# Materials Oceania 2019: Conference Report

International Conference on Materials Science and Engineering

September 16-18, 2019

# 

Event Venue

**Pullman Melbourne Albert Park** 65 Queens Road Melbourne Victoria 3004 Australia



# **Our Supporters**







Bus Charter







# Acknowledgements

The conference was headed by Prof. Manijeh Razeghi (Northwestern University, USA) and the sessions were governed by Prof. Osama O. Awadelkarim (Pennsylvania State University, USA), Prof. Yoshimine Kato (Kyushu University, Japan), Dr. Barbara Szpunar (University of Saskatchewan, Canada), Prof. Hiromitsu Takaba (Kogakuin University), Dr. Kun Qian (Shanghai Jiao Tong University, China), Dr. Katsumi Yoshida (Tokyo Institute of Technology, Japan), Dr. Shalini Bahel (Guru Nanak Dev University, India), Prof. Ivan Nemec (Charles University, Czech Republic), Dr. Frank Czerwinski (CanmetMATERIALS, Canada). The poster session was judged by Prof. Yusuke Yamauchi (The University of Queensland, Australia), Dr. Rajender Varma (U.S. Environmental Protection Agency, USA) and Prof. C. K. Jayasankar (Sri Venkateswara University, India).

Sincerest thanks to Lord Mayor Sally Capp (City of Melbourne) for her inspirational speech and inquisitive participation in the panel discussion on Women in Materials Science along with Prof. Jiazhao Wang (University of Wollongong, Australia), Prof. Manijeh Razeghi (Northwestern University, USA), Prof. Jing Li (Rutgers University, USA).

The congregation was generously supported by Across International Australia, Royal Society of Chemistry, Materials Today, Engineers without Borders Australia, Nanotechnology World Network, Innovation Leadership Forum, Medgate Today Magazine, Lanka Lion, Bio Based Press, EIN news and Bus Charter.

Revered members of organising committee were: Dr. Huijun Li (University of Wollongong, Australia), Dr. Almantas Pivrikas (Murdoch University, Australia), Dr. Tong Lin (Deakin University, Australia), Dr. Dusan Losic (The University of Adelaide, Australia), Dr. Chao Su (Curtin University, Australia), Dr. Yusuke Yamauchi (The University of Queensland, Australia), Dr. Wasim Saman (University of South Australia, Australia), Dr. Romila Devi Gopalan (University of South Pacific, Fiji), Dr. Manijeh Razeghi (Northwestern University, USA), Dr. Jian Liu (University of Surrey, UK), Dr. Gustaaf Schoukens (Ghent University, Belgium), Dr. Fabrice Charra (CEA, France), Dr. Felicia Iacomi (Alexandru Ioan Cuza University of Iasi, Romania), Dr. Vlad Stolojan (University of Surrey, UK), Dr. Anna Stoynova (Technical University of Sofia, Bulgaria) Dr. Jerome Tignon (Sorbonne University, France), Dr. Karolis Kazlauskas (Vilnius University, Lithuania), Dr. Charles Cornet (University of Rennes, France), Dr. Janis Grabis (Riga Technical University, Latvia), Dr. Milos Djukic (University of Belgrade, Serbia), Dr. Dragoslav Dobras (University of Banja Luka, Bosnia and Herzegovina), Dr. Tai-Shung Chung (National University of Singapore, Singapore), Dr. Abeer Abdullah Al Anazi (Australian College of Kuwait, Kuwait), Dr. Ivan Němec (Charles University, Czech Republic), Dr. Xiangang Wan (Nanjing University, China), Dr. Limin Wu (Fudan University, China), Dr. Roslina bt Ahmad (University of Malaya, Malaysia), Dr. Md. Abu Hashan Bhuiyan (Bangladesh University of Engineering and Technology, Bangladesh).

Staff support was provided by: Dr. Venkata Ravi Kumar Dasari, Mr. Raghav Gupta, Mr. Rakshith Kumar, Dr. Arindam Halder, Mrs. Bhavya Garg, Mr. Abhimanyu Sharma, Mr. Ankit Dahiya, Mr. Rakesh Kundra, Ms. Meg Blackie, Mr. Rishabh Sharma.

The organisers would like to thank all the participants for their unflinching and unparalleled contributions towards the Conference. Each and everyone of 160 plus participants from more than 25 countries played an indispensible role ranging from speakers, chairs and panelists to exhibitor and poster presenters, and participants of the breakout discussion sessions.





# of the

# Highlights of the Conference



# **Highlights of the Conference**

More than 160 ignited minds from over 25 countries met in Melbourne, Australia, from 16 to 18 September 2019 to exchange and explore ideas and best practices, foster debates, create and strengthen partnerships, and discuss the topic 'Core of innovations in materials science and engineering".

It was the first International Conference on Materials Science and Engineering (Materials Oceania), chiefly aiming towards providing a common platform to community of compatible professionals and academicians for new ideas to sprout, healthy discussions to bear fruit and academic/ business interests to propagate.

The call for conference proposals ran from 7 January - 15 July 2019. Materials Oceania 2019 received 224 proposals of abstracts for oral or poster presentation. The abstracts proposals were distributed to review committee for screening. The 3 days conference featured 12 Keynote presentations, 60 Oral presentations, 25 student presentations in 6 parallel sessions and 1 poster session with 30 poster presentations. "The conference is well organized and I get a lot of useful information. Thank you very much for your hard work".

**Yu Cong** Dalian Institute of Chemical Physics, CAS, China

Materials Oceania 2019 attracted over 160 attendees from over 25 countries, the largest percentage of overall conference attendance came from Asia. The attendees were from Australia, Belgium, Brazil, Canada, P. R. China, Czech Republic, France, Germany, Hong Kong, India, Israel, Japan, Malaysia, Philippines, Poland, Russia, Singapore, South Korea, Spain, Taiwan, Thailand, United States, United Kingdom and Vietnam. 38% of attendee's were women and 62% men; 48% represented academic/research communities, 21% were business delegates, 11% were consultants, 6% were technical staff, and 14% were categorised as others.

Pre-conference dinner was hosted before the first day of conference, for the keynote speakers and session chairs; Approximately 25 participants attended the dinner in Kitchen Workshop at Crown Towers, the largest casino complex in the Southern Hemisphere as well as in the world.

The conference kit was distributed among the attendees along with a mobile app providing information about the event was also available to download.

The Materials Oceania 2019 was a big leap towards connecting minds within the materials science community and beyond.

"I enjoyed the conference very much, the talks were of very high quality and the site and people were excellent. I find that the "customer service", i.e. the communication between you as organizer and me as attendee, has been always excellent, very fast and easy."

> **Pol Lloveras** olytechnic University of Catalonia Spain



"I enjoyed very much the conference – You and your co-organizers have done a terrific, impressive work! The Panel Discussion and Students Forum are all unique features of the conference, and the scientific quality of the program is high. There are plenty opportunities for discussions and communications".

> **Jing Li** Rutgers University USA



# Opening Ceremony





# **Opening Ceremony and Welcome Speech**

Prof. Manijeh Razeghi (Northwestern University, USA), officially opened the International Conference on Materials Science and Engineering on 16 September 2019. As the Honorary Chair of Materials Oceania 2019, she gave an overview of the event, noting that with over 160 people registered, the Materials Oceania Conference was a very well attended event with significantly more student participants than initially expected.

She commenced her address by appreciating the efforts put by the Prism Scientific Services team who made this conference a possibility. She then mentioned that the three day conference on 'Materials Science and Engineering' as a visionary leap ahead, in exposing the nascent minds of tomorrow to the literacy of modern science.

She noted the organising committee designed the Conference to stimulate interaction and dialogue through a variety of formats including Question and Answer sessions following presentations, breakout discussions, poster pitch presentations, exhibits and evening networking sessions.

Lord Mayor Sally Capp, City of Melbourne, began her speech by acknowledging the gathering on the traditional land of the Kulin Nation, and paid her respects to elders past and present. She welcomed all the participants, from Australia and beyond, to the City of Melbourne. She encouraged participants to take a walk around the city and explore historic arcades, colourful laneways, shops, galleries, fine dining, and beautiful gardens. She mentioned that for the best part of 10 years, Melbourne has been named one of the world's most liveable cities by The Economist.

She then congratulated Prism Scientific Services for organising this event and all the hard work the team had put into developing themselves and the fellow colleagues. She noted many in the community wouldn't automatically associate Melbourne as being an internationally recognised hub for Australia's materials science industry. She recognised that Melbourne is a global leader in areas including metals, polymers, photonics, composites biomaterials, electronics, coatings and emerging processes such as additive manufacturing. Melbourne has a proven track record in developing materials science and technology solutions with its advanced research and innovation capabilities in niche areas of advanced manufacturing. She added beyond Melbourne, Victoria is home to an innovative and dynamic cluster of minerals science companies, making the state a world leader in the delivery of products and service solutions for the Australian and international market.



"I'm often asked what's so special about our city – my answer is always – the people!"

Lord Mayor Sally Capp City of Melbourne



"We are scientists and our judgments have to be RIGHT!"

Manijeh Razeghi Northwestern University, USA





# Panel Discussion on Women in Materials Science



# Panel Discussion on Women in Materials Science

A panel discussion was planned during the materials science conference to pay tribute to the accomplishments of women in Materials Science field, inspire current early stage researchers to become innovators in the field, discuss issues facing by women in the materials science and engineering professions and provide girls and women with inspiring role models that could lead them to pursue careers in Materials Science.

The following speakers took the floor to start the panel discussion: Lord Mayor Sally Capp, City of Melbourne, Prof. Manijeh Razeghi, Northwestern University, USA, Prof. Jiazhao Wang, University of Wollongong, Australia, Prof. Jing Li, Rutgers University, USA.

The panel discussion was started with the inspirational and stimulating speech by Lord Mayor Sally Capp. Being an achiever herself, one of only three women to have been elected Lord Mayor of Melbourne in 176 years, she acknowledged the industry's leading women present in the conference and praised them for being pioneers in the materials field, and leaders in STEM subjects dominated by men for so long. She stated that the more voices we hear and stories we share about women making their mark across all spheres, the more leaders - and networks of leaders - we'll see emerge across the board. She encouraged women to stand up and take on these roles within the organisations and industries.



"The more voices we hear and stories we share about women making their mark across all spheres, the more leaders - and networks of leaders - we'll see emerge across the board"

Lord Mayor Sally Capp City of Melbourne

She appreciated the organizing committee for actively working to

support gender diversity through this conference program. She explained that recognising and celebrating the success of women in the industry is an important way to support change, promote materials science careers and encourage best practice approaches.

The women achievers of the field were facilitated by Lord Mayor with mementos and then each of them took stage to share their experiences and motivate the current early stage researchers to become innovators in the field. The conference participants were encouraged to share their thoughts and experiences and many of the comments were appreciated by Lord Mayor. The panel discussion was concluded by closing remarks from the Honorary Chair, Prof. Manijeh Razeghi.



# Conference Sessions Day 1 | 16 September 2019

### **Keynote Presentations**

Moderated by Prof. Manijeh Razeghi (Northwestern University, USA), the keynote session included the following speakers:

Dr. Amanda Barnard: Data61, CSIRO, Australia "Challenges and opportunities in data-driven materials design"

Prof. Dmitri Golberg: Queensland University of Technology, Australia "Nanomaterial properties as revealed via in situ transmission electron microscopy"

Prof. Jiazhao Wang: University of Wollongong, Australia "Efficient air cathodes for rechargeable lithium oxygen batteries"

Prof. Shizhang Qiao: The University of Adelaide, Australia "Nanostructured materials for energy-relevant electrocatalytic processes"

Prof. Manijeh Razeghi: Northwestern University, USA "The power of materials innovation; Breaking spectral and performance barriers for quantum devices"

Prof. Sean Smith: Australian National University, Australia "Cell membrane penetration without pore formation: Chameleonic properties of dendrimers in response to hydrophobic and hydrophilic environments"

Prof. Jing Li: Rutgers University, USA "Low-cost and high-performance hybrid phosphors for energy-efficient lighting technologies"

Dr. Rajender Varma: U.S. Environmental Protection Agency, USA "Magnetic nano-catalysts and carbonaceous waste for sustainable applications in chemical transformations"

Prof. Steven Denbaars: University of California, Santa Barbara, USA "Recent developments of advanced GaN materials for light emitting diodes (LEDs) and laser diodes for energy efficient lighting and displays"

Prof. Yusuke Yamauchi: The University of Queensland, Australia "Materials spacetectonics: New conceptual paradigm of functional porous system"

Dr. Hoydoo You: Argonne National Laboratory, USA "Advanced synchrotron x-ray diffraction and imaging techniques for catalysis and electrocatalysis"

Prof. Tierui Zhang: Technical Institute of Physics and Chemistry, CAS, China "Nano-structured layered double hydroxide based photocatalysts for solar fuels and value-added chemicals"





# **Networking cocktail**

One of the main reasons, professionals attend a conference, is to bridge a network. At the end of day 1 networking cocktail was organized to provide an opportunity for networking between delegates for exploring career options, expanding knowledge and broaden the business contacts. More than 60 participants attended the event which had a more casual and relaxed vibe but still maintained a professional decor.





# Conference Sessions Day 2 | 17 September 2019

#### **Invited Presentations**

Day 2 started with invited presentations with over 50 speakers presenting their work in 4 different sessions. Each session was chaired by 2 eminent personalities of their respective fields. The young researchers participated with great zeal and the best oral and poster presentations were motivated for their efforts, selected by different jury of leading experts.

#### Session 1: Electronic and Optical Materials

Chairs: Prof. Osama O. Awadelkarim, Pennsylvania State University, USA Prof. Yoshimine Kato, Kyushu University, Japan

Best Oral Presentation Award: Dr. Tam D. Nguyen- Nanyang Technological University, Singapore "Effective and stable heat modulation by smart window technology using advanced electrochromic and electrophoretic nanomaterials"

#### **Session 2: Energy and Environment Materials**

Chairs: Dr. Barbara Szpunar, University of Saskatchewan, Canada Prof. Hiromitsu Takaba, Kogakuin University, Japan

Best Oral Presentation Award: Dr. Piotr Cyganowski - Wroclaw University of Science and Technology, Poland "Nanocomposite catalysts for reduction of 4-nitrophenol"

#### Session 3: Biomaterials and Medical Devices

Chair: Dr. Kun Qian, Shanghai Jiao Tong University, China

Best Oral Presentation Award: Dr. Kun Qian - Shanghai Jiao Tong University, China "Design of new metabolic platforms for in vitro diagnostics"

# Session 4: Advanced Functional Materials

Chairs: Prof. Katsumi Yoshida, Tokyo Institute of Technology, Japan Dr. Shalini Bahel, Guru Nanak Dev University, India

Best Oral Presentation Award: Dr. Nattakan Soykeabkaew - Mae Fah Luang University, Thailand "Engineered woods based on rice straw: Structure, properties and uses"

#### **Poster Presentations**

Poster session was organized by the end of the day with more than 30 poster presentations on 6 major areas of interest in the studies of materials science, and related areas. The poster presentation awards were sponsored by Journal of Materials Chemistry A and Materials Horizons of Royal Society of Chemistry. 5 posters were selected as "Best Poster Presentations" and the certificates by Royal Society of Chemistry were awarded to the winners.

## **Best Poster Presentation Awardees:**

1. Ms. Gna Ahn: Chungbuk National University, Republic of Korea "Insulin receptor binding aptamer and milk exosome conjugates as promising therapeutic agents for Diabetes"

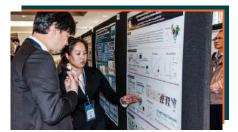
2. Ms. Natsuho Sugai: Chuo University, Japan "Synthesis of catalase microtube motors with controllable velocity and biodegradability"

3. Mr. Hiroshi Ikari: Tokyo University of Science, Japan "Development of selective hydrophilic/hydrophobic treatment towards future application to semiconductor substrate"

4. Mr. Shin Wook Kang: Korea Institute of Energy Research, Republic of Korea "A facile synthesis of supported metal nanoparticles with high dispersion by using the meltinfiltration method"

5. Mrs. Soohyun Kim: Korea Institute of Energy Research, Republic of Korea "The utilization of nanocellulose as catalyst support for methanol steam reforming" "I fully enjoyed my visit to the Conference, it was well organized".

**Dmitri Golberg** Queensland University of Technology, Australia







# Conference Sessions Day 3 | 18 September 2019

The final day of the conference started with invited presentations with 12 speakers presenting their work in 2 different sessions. Each session was chaired by a leading expert of the respective field. One young researcher was selected for Best Oral Presentation award.

Session 5: Materials Chemistry

Chair: Prof. Ivan Nemec, Charles University, Czech Republic

Session 6: Advance Structural Materials

Chair: Dr. Frank Czerwinski, CanmetMATERIALS, Canada

Best Oral Presentation: Dr. Heba Ahmed: RMIT University, Australia "Acousto-microfluidic one-step synthesis and activation of metal-organic frameworks (MOFs)"

#### **Students Session**

The most exciting part of the conference was the student oral presentations. The aim of the session was to provide an opportunity to the students from different races, genders, and nationalities to present their results and be patted for becoming great leaders and mentors for future generation. More than 25 students presented their work in the intensive session. 4 students were selected for "Best Student Presentation award".

Mr. Kamil Dydek: Warsaw University of Technology, Poland "The influence of thermoplastic nonwovens containing multi-walled carbon nanotubes on CFRPs properties"

Mr. Sanjit Gaikwad: Changwon National University, South Korea "Polyethyleneimine (PEI) impregnated bimetallic MIL-101 metal organic frameworks (MOF) for CO<sub>2</sub> capture study"

Ms. Olga Guselnikova: University of Chemistry and Technology, Czech Republic "Homochiral metal-organic frameworks functionalized SERS substrate for atto-molar enantioselective detection"

Ms. Anna Olszewska: AGH University of Science and Technology, Poland "GdBaCo2-xMnxO5+& layered perovskites as cathodes for solid oxide fuel cells"

# **Closing Ceremony**

Prof. Manijeh Razeghi closed the Materials Oceania 2019 conference by giving a vote of thanks to the delegates and the presenters for their agile participation. The excellent organisational work of the staff of the "Prism Scientific Services" was also admired. She extended her thanks to the organizing committee for their efforts, and expressed her contentment over the interactive nature of the discussions while congratulating participants on the extensive networking that had taken place, which she hoped would be carried miles ahead. She praised the young researchers for their excellent work and presentation skills and encouraged the participants to attend future Materials Oceania conferences. Dr. Rajender Verma presented the certificates for the Best Poster Award winners.

#### Social Tour Program

The Social Tour Program which included tours in and around Melbourne city was arranged after the scientific program to provide an extended networking opportunity among the conference attendees along with exploring the multi facets of Melbourne. The bus tour was thoroughly enjoyed by the participants and appreciation was received for the efforts.





"It was really nice to attend the conference Material Oceania 2019. Your team has done a wonderful work. Excellent planning, perfect execution and great hospitality".

> **Shalini Bahel** Guru Nanak Dev University India

# **Testimonials**

"I enjoyed the conference very much, the talks were of very high quality and the site and people were excellent. I find that the "customer service", i.e. the communication between you as organizer and me as attendee, has been always excellent, very fast and easy."

Pol Lloveras, Polytechnic University of Catalonia, Spain

"I fully enjoyed my visit to the Conference, it was well organized". Dmitri Golberg, Queensland University of Technology, Australia

"I enjoyed very much the conference – You and your co-organizers have done a terrific, impressive work! The Panel Discussion and Students Forum are all unique features of the conference, and the scientific quality of the program is high. There are plenty opportunities for discussions and communications". Jing Li, Rutgers University, USA

"It was really nice to attend the conference Material Oceania 2019. Your team has done a wonderful work. Excellent planning, perfect execution and great hospitality". Shalini Bahel, Guru Nanak Dev University, India

"Thank you for your great work on International Conference on Materials Science and Engineering. We had a very fruitful time". Yoshimine Kato, Kyushu University, Japan

"I and my students really enjoyed the Materials Oceania 2019! It was marvellous and friendly conference". Teru Komatsu, Chuo University, Japan

"Thanks a lot for successful organisation of the conference. Really, we enjoyed and benefited by participating and sharing of the knowledge". C.K. Jayasankar, Sri Venkateswara University , India

"The conference is well organized and I get a lot of useful information. Thank you very much for your hard work". Yu Cong, Dalian Institute of Chemical Physics, CAS, China

"I would like to congratulate the organizers, for doing great job by putting together an excellent program, bringing Outstanding Scientists from around the world. My favourite part was giving chance to the students from different race, gender, and nationality, to present their results and be encouraged for becoming great leaders". Manijeh Razeghi, Northwestern University, USA









VACUUM OVENS, VACUUM PUMPS, TUBE FURNACES, MUFFLE FURNACES, TUBE FURNACES, BALL MILLS, ROTARY EVAPORATORS, JACKETED REACTORS, CHILLERS AND HEATERS

Across International for over 25 years has been manufacturing lab equipment and ensuring each are tested for quality before shipment from our founding facility in New Jersey, and now Nevada and Melbourne, Australia.

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We have worked with industry leaders like Monash, Melbourne, NSW, Wollongong and Curtin universities, Toyota, NASA, the Australian government, DoD, Geoscience Australia, and Consolidated Tin Mines Ltd. to name a few like SGS, Boron Moleculars, Coogee Titanium and would like to assist you as we have them!

Thanks so much for your time, look forward to hearing from you and hope you have a great day!"

http://www.acrossinternational.com.au/



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# Monday, September 16, 2019

08:00-08:40	Conference Registrations	
	Arrival Tea & Coffee	@ Mercure Lounge
8:40-09:00	Opening Ceremony (State 3, Pullman Melbourne Albert Park)	
09:00-11:00	Keynote Presentations (State 3, Pullman Melbourne Albert Park)	
11:00-11:20	Coffee Break and Group Photograph	@ Mercure Lounge
11:20-11:40	Welcome Speech by Lord Mayor Sally Capp - City of Melbourne State 3, Pullman Melbourne Albert Park	
11:40-12:00	Panel Discussion	
12:00-13:00	Keynote Presentations (State 3, Pullman Melbourne Albert Park)	
13:00-13:40	Buffet Lunch	@ Mercure Lounge
13:40-15:40	Keynote Presentations (State 3, Pullman Melbourne Albert Park)	
15:40-16:00	Coffee Break	@ Mercure Lounge
16:00-17:00	Keynote Presentations (State 3, Pullman Melbourne Albert Park)	
17:00-18:00	Reception	@ Mercure Lounge

# Tuesday, September 17, 2019

08:00-10:00	Invited Session I: Electronic and Optical Materials (State 3, Pullman Melbourne Albert Park)	
	Invited Session 3: Biomaterials and Medical Devices (State 1, Pullman Melbourne Albert Park)	
10:00-10:20	Coffee Break @ Merc	ure Lounge
10:20-13:00	Invited Session 1: Electronic and Optical Materials (State 3, Pullman Melbourne Albert Park)	
	Invited Session 4: Advanced Functional Materials (State 1, Pullman Melbourne Albert Park)	
13:00-13:40	Buffet Lunch @ Mercure Loung	
13:40-16:00	Invited Session 2: Energy and Environment Materials (State 3, Pullman Melbourne Albert Park)	
	Invited Session 4: Advanced Functional Materials (State 1, Pullman Melbourne Albert Park)	
16:00-16:40	Coffee Break and Poster Presentations	@ Foyer
16:40-18:00	Invited Session 2: Energy and Environment Materials (State 3, Pullman Melbourne Albert Park)	
	Special Session: Computational Materials Science (State 1, Pullman Melbourne Albert Park)	

	Invited Session 6: Advance Structural Materials (State 1, Pullman Melbourne Alb	bert Park)
10:00-10:10	Coffee Break	@ Mercure Lounge
10:10-12:30	Oral Session 1: Students Forum (State 3, Pullman Melbourne Albert Park)	
	Oral Session 2: Students Forum (State 1, Pullman Melbourne Albert Park)	

# The city tour operated by Bus Charter starts at 13:30

# Monday 16 Sept

	Keynote Presentations	
09:00-09:30	Challenges and opportunities in data-driven materials design Amanda Barnard Data61, CSIRO, Australia	
09:30-10:00	Nanomaterial properties as revealed via in situ transmission electron microscopy Dmitri Golberg Queensland University of Technology, Australia	
10:00-10:30	<b>Efficient air cathodes for rechargeable lithium oxygen batteries</b> Jiazhao Wang University of Wollongong, Australia	
10:30-11:00	Nanostructured materials for energy-relevant electrocatalytic processes Shizhang Qiao The University of Adelaide, Australia	
11:00-11:20	Coffee Break and Group Photograph @ Mercure Lounge	
11:20-11:40	Welcome Speech by Lord Mayor Sally Capp - City of Melbourne	
11:40-12:00	Panel Discussion: Women in Materials Science	
12:00-12:30	The power of materials innovation; Breaking spectral and performance barriers for quantum devices Manijeh Razeghi Northwestern University, USA	
12:30-13:00	Cell membrane penetration without pore formation: Chameleonic properties of dendrimers in response to hydrophobic and hydrophilic environments Sean Smith Australian National University, Australia	
13:00-13:40	Buffet Lunch @ Mercure Lounge	
13:40-14:10	<b>Low-cost and high-performance hybrid phosphors for energy-efficient lighting technologies</b> Jing Li Rutgers University, USA	
14:10-14:40	Magnetic nano-catalysts and carbonaceous waste for sustainable applications in chemical transformations Rajender Varma Palacky University, Czech Republic	
14:40-15:10	Recent developments of advanced GaN materials for light emitting diodes (LEDs) and laser diodes for energy efficient lighting and displays Steven Denbaars University of California, Santa Barbara, USA	
15:10-15:40	Materials spacetectonics: New conceptual paradigm of functional porous system Yusuke Yamauchi The University of Queensland, Australia	

15:40-16:00	Coffee Break	@ Mercure Lounge
16:00-16:30	Advanced synchrotron x-ray diffract electrocatalysis Hoydoo You Argonne National Laboratory, USA	ion and imaging techniques for catalysis and
16:30-17:00	Nano-structured layered double hydroxide based photocatalysts for solar fuels an value-added chemicals Tierui Zhang Technical Institute of Physics and Chemistry, CAS, China	
17:00-18:00	Reception	@ Mercure Lounge

# Tuesday 17 Sept

State Room 3

Invited Session 1: Electronic and Optical Materials State 3, Pullman Melbourne Albert Park		
Chairs:	<b>Osama O. Awadelkarim,</b> Pennsylvania State University, USA <b>Yoshimine Kato,</b> Kyushu University, Japan	
08:00-08:20	<b>Superconductivity enhanced by a ferroelectric quantum critical point</b> Isao H. Inoue National Institute of Advanced Industrial Science and Technology, Japan	
08:20-08:40	<b>Exploring novel engineered materials for flexible electronic system</b> Osama O. Awadelkarim Pennsylvania State University, USA	
08:40-09:00	<mark>Si paste as a novel printing electronic material</mark> Yoshimine Kato Kyushu University, Japan	
09:00-09:20	<b>Gas bubbles, liquid droplets and sound: The new frontier for nonlinear optics</b> Ivan S. Maksymov Swinburne University of Technology, Australia	
09:20-09:40	<b>Vertically-aligned resonant tunnelling devices with organic molecules as quantum dots</b> Ryoma Hayakaw National Institute for Materials Science, Japan	
09:40-10:00	<b>A facile strategy to fabricate conductive fabrics-polyaniline based</b> Mohd Muzamir Mahat MARA University of Technology, Malaysia	
10:00-10:20	Coffee Break @ Mercure Lounge	
10:20-10:40	Femtosecond nonlinear four wave mixing for study of carrier dynamics in porous silicon Lap Van Dao Swinburne University of Technology, Australia	
10:40-11:00	Effective and stable heat modulation by smart window technology using advanced electrochromic and electrophoretic nanomaterials Tam D. Nguyen Nanyang Technological University, Singapore	
11:00-11:20	<b>RIKEN accelerator-driven compact neutron source as a material science investigation probe</b> Yoshie Otake RIKEN, Japan	
11:20-11:40	Size tuneable NiCr2O2 nanoparticles for high charge storage parallel plate supercapacitor Biplab Kumar Paul Jadavpur University, India	
11:40-12:00	<b>Wide band gap organic single crystal for thermal and third order nonlinear optical applications</b> Bincy I.P MES College, India	
12:00-12:20	Francisites as new geometrically frustrated quasi-two-dimensional magnets Alexander Vassiliev M.V. Lomonosov Moscow State University, Russia	

12:20-12:40	<b>Structure-property relationships in α-, β'-, γ and δ-modification</b> Olga Maximova M.V. Lomonosov Moscow State University, Russia	s of Mn₃(PO₄)₂
12:40-13:00	<b>Development of flexible carbon nanotube electrochemical sensor u</b> Soheli Farhana University in Kuala Lumpur, Malaysia	sing screen printed technique
13:00-13:40	Buffet Lunch	@ Mercure Lounge

# Invited Session 2: Energy and Environment Materials State 3, Pullman Melbourne Albert Park

Chairs:	<b>Barbara Szpunar</b> , University of Saskatchewan, Canada <b>Hiromitsu Takaba,</b> Kogakuin University, Japan
13:40-14:00	<b>Comparison of structural stability of β silcon carbide and thoria</b> Barbara Szpunar University of Saskatchewan, Canada
14:00-14:20	Molecular modeling of stability and emission properties of halide perovskites Hiromitsu Takaba Kogakuin University, Japan
14:20-14:40	<b>Enhancement of redox mediator effect at air electrode for rechargeable Li-O</b> <sub>2</sub> batteries Morihiro Saito Seikei University, Japan
14:40-15:00	Nanofabrication processes for catalysts on nano-silicon materials for energy conversion devices Ahmed Halima Monash University, Australia
15:00-15:20	Guest Li⁺ ion conductors based on Nal-NaBH₄ and their potential use for all-solid-state batteries Reona Miyazaki Nagoya Institute of Technology, Japan
15:20-15:40	Nanomaterials for energy conversion and storage Nasir Mahmood RMIT University, Australia
15:40-16:00	Hetero-structured titanium dioxide photocatalyst Chiaki Terashima Tokyo University of Science, Japan
16:00-16:40	Coffee Break and Poster Presentations @ Foyer
16:40-17:00	Nanocomposite catalysts for reduction of 4-nitrophenol Piotr Cyganowski Wroclaw University of Science and Technology, Poland
17:00-17:20	Efficient down/up-conversion rare earth pair doped luminescent materials for Si-solar cell applications C. K. Jayasankar Sri Venkateswara University, India
17:20-17:40	Two dimensional materials preparation and their properties of oxygen evolution reaction Chuanbao Cao Beijing Institute of Technology, China
17:40-18:00	Interaction of corrosion-induced hydrogen with nascent defects in steel under neutron irradiation Evgenii Krasikov Kurchatov Institute, Russia

# Parallel Session: II

State Room 1

Invited Session	on 3: Biomaterials and Medical Devices
State 1, Pullma	n Melbourne Albert Park
Chair:	<b>Kun Qian,</b> Shanghai Jiao Tong University, China
08:00-08:20	<b>Hemoglobin-albumin cluster as red blood cell substitute</b> Teruyuki Komatsu Chuo University, Japan
08:20-08:40	Use of multivalent-type compounds for enhancement of biological affinities Koji Matsuoka Saitama University, Japan
08:40-09:00	Tuning the size and composition of nanohydrogels using a "phantom monomer" for biological applications Gerardo Byk Bar Ilan University, Israel
09:00-09:20	Nanoparticle engineering towards highly efficient drug delivery systems and SERS-based bio-sensing Beatrice Fortuni Catholic University of Leuven, Belgium
09:20-09:40	Photocontrollable adhesion: A bioinspired microstructured transport device Emre Kizilkan Kiel University, Germany
09:40-10:00	<b>Design of new metabolic platforms for</b> in vitro <b>diagnostics</b> Kun Qian Shanghai Jiao Tong University, China
10:00-10:20	Coffee Break @ Mercure Lounge
	on 4: Advanced Functional Materials n Melbourne Albert Park
Chairs:	<b>Katsumi Yoshida,</b> Tokyo Institute of Technology, Japan <b>Shalini Bahel,</b> Guru Nanak Dev University, India
10:20-10:40	Development of highly microstructure-controlled boron carbide neutron absorbers for fast reactors Katsumi Yoshida Tokyo Institute of Technology, Japan
10:40-11:00	<b>Reflection studies of barium lanthanum titanates in 8.2 to 12.4 GHz frequency range</b> Shalini Bahel Guru Nanak Dev University, India
11:00-11:20	<b>Cold spray process for thick ceramic coatings</b> Motohiro Yamada Toyohashi University of Technology, Japan
11:20-11:40	Stimuli responsive and molecularly imprinted polymers for phthalates removal

- Joanna Wolska Wroclaw University of Science and Technology, Poland
- 11:40-12:00 Engineered woods based on rice straw: Structure, properties and uses Nattakan Soykeabkaew Mae Fah Luang University, Thailand

12:00-12:20	Improving molded pulp products from agro wastes via blending approach Nattaya Tawichai Mae Fah Luang University, Thailand
12:20-12:40	Theoretical assessment of wettability on silane coatings: From hydrophilic to hydrophobic Haiming Huang Guangzhou University, China
12:40-13:00	Nanofabrication technology for structure control of nano-materials and their applications Chi Won Ahn Korea Advanced Institute of Science and Technology, Korea
13:00-13:40	Buffet Lunch @ Mercure Lounge
13:40-14:00	Interfacing biomolecules with nanomaterials: Structure and function at the atomic-scale Tiff Walsh Deakin University, Australia
14:00-14:20	<b>Chemical engineering of nanostructured materials for varying applications</b> Xingmao Jiang Wuhan Institute of Technology, China
14:20-14:40	<b>Preparation of graphene based magnetic hybrids for dye removal application</b> Ing Kong La Trobe University, Australia
14:40-15:00	<b>The potential of using gold nanoparticle-based assay for target molecule detection</b> Dakrong Pissuwan Mahidol University, Thailand
15:00-15:20	Next-generation latent finger-mark detection using functionalised silicon oxide nano-particles Fehmida K Kanodarwala University of Technology Sydney, Australia
15:20-15:40	<b>Colossal reversible barocaloric effects in plastic crystals</b> Pol Lloveras Polytechnic University of Catalonia, Spain
15:40-16:00	Magnetic properties of LSMO, LSMKO and LSMPO superparamagnetic nanomaterials Sunita Keshri Birla Institute of Technology, India
16:00-16:40	Coffee Break and Poster Presentations @ Foyer

# Special Session: Computational Materials Science from Data61, CSIRO, Australia

State 1, Pullman Melbourne Albert Park

16:40-18:00	Active-learning directed simulation of small molecule surface binding Christopher A. Feigl Data61, CSIRO, Australia
	Feature selection for machine learning of surface catalysts Julia Melisande Fischer
	Data61, CSIRO, Australia Understanding and predicting defective graphene-oxide structures using machine Benyamin Motevalli Soumehsaraei

learning

Data61, CSIRO, Australia

# 16:00-16:40

# Location: Foyer

ICME001	<b>Synthesis and drug binding properties of recombinant canine serum albumin</b> Tomomi Hasegawa Chuo University, Japan
ICME002	Insulin receptor binding aptamer and milk exosome conjugates as promising therapeutic agents for Diabetes Gna Ahn Chungbuk National University, Republic of Korea
ICME003	Protection layer/semiconductor structure of photoelectrode for photoelectrochemical water splitting Jianyun Zheng Curtin University, Australia
ICME004	<b>Bacterial nanofibrial polymer (BNP) for wound-healing application</b> Seon Hyung Lee Chungbuk National University, Republic of Korea
ICME005	Super tough, thermally conductive composite hydrogel and its biomedical applications Yi Wang Sichuan University, China
ICME006	<b>Highly stretchable and self-healing "solid-liquid" elastomer with strain-rate sensing capability</b> Qi Wu Sichuan University, China
ICME007	Characterizing the multi-scale energy dissipation mechanism of natural rubber Cheng Huang Sichuan University, China
ICME008	Ultra-tough, defect-tolerant and humidity-responsive self-healing elastomers for intelligent actuators Yong Zhu Sichuan University, China
ICME009	Ionic modified halogenated elastomers with the capabilities of self-healing and water insensitivity Linjun Zhang Sichuan University, China
ICME010	<b>Synthesis of catalase microtube motors with controllable velocity and biodegradability</b> Natsuho Sugai Chuo University, Japan
ICMEOII	Structural and electrochemical properties of Li- and Mn-rich positive electrode materials exhibiting oxygen activity Katarzyna Redel AGH University of Science and Technology, Poland
ICME012	<b>Ecofriendly synthesis of gold nanoparticles using low-cost biosorbents from lower Silesia region</b> Dorota Jermakowicz-Bartkowiak Wroclaw University of Science and Technology, Poland

ICME013	Investigation on mechanical and frictional properties of barium titanate and PVDF using atomic force microscopy Yan Zhang Southeast University, China
ICME014	Overview of the composite nanoceramics prepared by sintering of in-situ made multiphase nanopowders in the bimetallic system aluminum nitride AlN/gallium nitride GaN Jerzy F. Janik AGH University of Science and Technology, Poland
ICME015	Comparison of two different metal sulfide systems used in the mechanochemical synthesis of kesterite Cu <sub>2</sub> ZnSnS <sub>4</sub> for photovoltaic applications Jerzy F. Janik AGH University of Science and Technology, Poland
ICME016	<b>Electrically colour tunable colloid in nonpolar solvents for the color reflective display film</b> Woo Jin Yim NSPECTRA Co., Ltd., Republic of Korea
ICME017	<b>Quantum-dot microcapsule film for an oxygen and moisture problems</b> Jinseok Song NSPECTRA Co., Ltd., Republic of Korea
ICME018	Effect of oleothermal synthesis parameters on TiO <sub>2</sub> quantum dots functionalized graphene Felipe Amorim Berutti Federal University of Rio Grande do Sul, Brazil
ICME019	NaLuGdF <sub>.</sub> :Yb³+/Er³+ up-conversion nanoparticles as an optical sensor Bui The Huy Changwon National University, Republic of Korea
ICME020	Paper-based sensors coupled with smartphone for fluorescence detection of phenolic pollutants based on amphiphilic quantum dots Salah M Tawfik Changwon National University, Republic of Korea
ICME021	Tuning the size and composition of nanohydrogels using a "phantom monomer" for biological applications Gerardo Byk Bar Ilan University, Israel
ICME022	Development of selective hydrophilic/hydrophobic treatment towards future application to semiconductor substrate Hiroshi Ikari Tokyo University of Science, Japan
ICME023	Effective and stable heat modulation by smart window technology using advanced electrochromic and electrophoretic nanomaterials Tam Duy Nguyen Nanyang Technological University, Singapore
ICME024	<b>Effect of W loading on TiO<sub>2</sub> electrochromic properties</b> Annelise Kopp Alves Federal University of Rio Grande do Sul, Brazil
ICME025	Effects of phase structure on up-conversion photoluminescence and dielectric performance in Er <sup>3+</sup> doped (Bi <sub>0.5</sub> Na <sub>0.5</sub> )TiO <sub>3</sub> -BaTiO <sub>3</sub> lead-free ceramics Chao Chen Jingdezhen Ceramic Institute, China

ICME026	A facile synthesis of supported metal nanoparticles with high dispersion by using the melt- infiltration method Shin Wook Kang Korea Institute of Energy Research, Republic of Korea
ICME027	<b>The utilization of nanocellulose as catalyst support for methanol steam reforming</b> Soohyun Kim Korea Institute of Energy Research, Republic of Korea
ICME028	Dipicolylamino quinoline derivative as novel dual fluorescent detecting system for Hg²+ and Fe³+ Waroton Paisuwan Chulalongkorn University, Thailand
ICME029	<b>Ultrasonic observation of H<sub>2</sub> gas replacement in a pipe</b> Takuya Kido Kyushu University, Japan
ICME030	Performance and durability of flat-tubular solid oxide 3-cell stack in the reversible electrolysis- fuelcell operation Sun-Dong Kim Korea Institute of Energy Research, Republic of Korea
ICME031	Effects of an inner coating of crystalline GDC nanosol in the porous metal support on the electrochemical properties of metal-supported SOFC cells Tae Woo Kim Korea Institute of Energy Research, Republic of Korea

**Invited Session 5: Materials Chemistry** State 3, Pullman Melbourne Albert Park Chair: Ivan Nemec, Charles University, Czech Republic 08:00-08:20 Advanced phase characterization of novel prospective materials for NLO hydrogen-bonded salts and cocrystals of heteroaromatic bases Ivan Nemec Charles University, Czech Republic 08:20-08:40 Material design of porous coordination polymer for high performance adsorbent of NH, and NH<sup>4+</sup> Tohru Kawamoto National Institute of Advanced Industrial Science and Technology, Japan 08:40-09:00 Temperature dependent crystal structure of LaSr, Fe, O10 with intercalated H, O and OH Isao Kagomiya Nagoya Institute of Technology, Japan Insights into the activation of molecular oxygen for alcohol oxidation over Pd single-atom 09:00-09:20 catalyst Yu Cong Dalian Institute of Chemical Physics, CAS, China 09:20-09:40 Ceramic composites with zero-thermal-expansion property Ikuo Yanase Saitama University, Japan 09:40-10:00 Gelcasted solid-state-sintered SiC ceramic foams with excellent permeability Haibo Wu Shanahai Institute of Ceramics, China **Coffee Break** 10:00-10:10 @ Mercure Lounge

Oral Sessi	on 1: Students Forum	@ State 3, Pullman Melbourne Albert Park
10:10-10:20	Development of a 3D printed sca metastasis in breast cancers Habib Belaid European Institute Des Membra	iffold allowing multiple drug delivery for the treatment of bone nes, France
10:20-10:30	<b>Uptake, permeability and diffus</b> <b>cell assemblies</b> Indra Van Zundert Catholic University of Leuven, B	s <mark>ion of multifunctional mesoporous silica nanoparticles in 3D</mark> elgium
10:30-10:40	Development of antimicrobial nanocomposite films for biomed Somtirtha Kool Banerjee Jadavpur University, India	l and biocompatible fluorescent Hydroxyapatite-chitosar ical applications

10:40-10:50	Polybutylene succinate porous scaffold prepared by fused deposition modeling and salt leaching techniques for drug delivery application Kasidis Teerasuchai Silpakorn University, Thailand
10:50-11:00	<b>Characterization of calceined waste shells</b> Wiranchana Srichanachaichok Mahidol University, Thailand
11:00-11:10	The influence of thermoplastic nonwovens containing multi-walled carbon nanotubes on CFRPs properties Kamil Dydek Warsaw University of Technology, Poland
11:10-11:20	<b>3D printed PLA/BN scaffolds for bone tissue engineering application</b> Habib Belaid European Institute Des Membranes, France
11:20-11:30	Effect of co-solvent on the properties of non-woven porous neomycin-loaded poly(lactic acid)/ polycaprolactone fibers Thiphathai Hongthipwaree Silpakorn University, Thailand
11:30-11:40	Properties of nonwoven polylactic acid fibers from prepared by simple rotational jet spinning method Worapon Rodchanasuripron Silpakorn University, Thailand
11:40-11:50	Magnetic nanoparticles for monocyte separation Porntida Wattanakull Mahidol University, Thailand
11:50-12:00	<b>Doped ZnO in hybrid nanostructure for lighting and solar cell applications</b> Yu Zhang Lyon Institute of Nanotechnology, France
12:00-12:10	Polyethyleneimine (PEI) impregnated bimetallic MIL-101 metal organic frameworks (MOF) for CO <sub>2</sub> capture study Sanjit Gaikwad Changwon National University, South Korea
12:10-12:20	Generation of charged Ti nanoparticles and their deposition behaviour under the applied bias during RF magnetron sputtering Ji Hye Kwon Seoul National University, South Korea
12:20-12:30	Development of a self-charged photo-power cell based on <i>in situ</i> synthesized electroactive and large dielectric SrF <sub>2</sub> /PVDF nanocomposite film Farha Khatun Jadavpur University, India

# Parallel Session: II

State Room 1

Invited Session 6: Advance Structural Materials State 1, Pullman Melbourne Albert Park		
Chair:	<b>Frank Czerwinski</b> , CanmetMATERIALS, Canada	
08:00-08:20	Recycled AA6111 Al alloys manufactured by me thermomechanical forming processes Isaac Chang Brunel University London, UK	It conditioned direct chill casting and
08:20-08:40	Improving thermal stability of aluminum alloys throu Frank Czerwinski CanmetMATERIALS, Canada	ugh additions of rare earths
08:40-09:00	<b>PM production of tungsten and its alloy: A multi-sca</b> Xizhong An Northeastern University, China	le numerical study
09:00-09:20	<b>Refractories; An essential evil?</b> Michael Walton RefMet, Australia	
09:20-09:40	Acousto-microfluidic one-step synthesis and activation Heba Ahmed RMIT University, Australia	on of metal-organic frameworks (MOFs)
09:40-10:00	Effect of chicken feather and its carbon derivative mortar Bryan Pajarito University of the Philippines, Philippines	s on the compressive strength of cement
10:00-10:10	Coffee Break	@ Mercure Lounge

# Oral Session 2: Students Forum @ State 1, Pullman Melbourne Albert Park

10:10-10:20	Role of colossal dielectric Cu impregnated α-MnO <sub>2</sub> nanoparticles in highly durable asymmetric solid state supercapacitor Dheeraj Mondal
	Jadavpur University, India
10:20-10:30	Homochiral metal-organic frameworks functionalized SERS substrate for atto-molar enantio- selective detection Olga Guselnikova
	University of Chemistry and Technology, Czech Republic
10:30-10:40	A route to reach the absorption limit of perovskite solar cells by using metal-oxide front contacts Mohammad Ismail Hossain
	The Hong Kong Polytechnic University, Hong Kong
10:40-10:50	Capacitive organic anode based on fluorinated-contorted hexabenzocoronene: Applicable to lithium-ion and sodium-ion storage cell Jaehyun Park
	Ulsan National Institute of Science and Technology, Republic of Korea

10:50-11:00	Deterministic growth of a sodium metal anode on a pre-patterned current collector for highly rechargeable seawater batteries Jaeho Jung Ulsan National Institute of Science and Technology, Republic of Korea
11:00-11:10	<b>GdBaCo<sub>2.x</sub>Mn<sub>x</sub>O<sub>5+6</sub> layered perovskites as cathodes for solid oxide fuel cells</b> Anna Olszewska AGH University of Science and Technology, Poland
11:10-11:20	A statistical and systemic study of the interaction between lubricin (LUB) on different substrate surfaces Mingyu Han Deakin University, Australia
11:20-11:30	Bulk deformation and toughness behavior of titanium alloys comprising the C15-type laves and beta phase Chirag Dhirajlal Rabadia Edith Cowan University, Australia
11:30-11:40	<b>Cyclic deformation behaviors of a nickel based superalloy: Potential competing failure mechanism</b> Wei-Wen Kong Institute of Metal Research, CAS, China
11:40-11:50	Influence of relative contents of materials in coating mortars with natural river sand andlimestone binder filer with similar granulometric distribution Ieda Maria Fagundes Zanolla Private University in São Leopoldo, Brazil
11:50-12:00	Preparation of inorganic porous adsorbent by gasification fly ash and adsorption behavior for Cr(VI) removal Yang Guo China University of Mining and Technology, China
12:00-12:10	Enhanced electrochemical properties of ultrathin Ni(OH) <sub>2</sub> -MnO <sub>2</sub> hybrid nanosheets by plasmaInduced grafted MWCNTs as binder-free electrode for high performance supercapacitor Ai-Wen Chai National Cheng Kung University, Taiwan
12:10-12:20	<b>Thermolysis behavior of microcrystalline cellulose at low heating rates</b> Mohamed Rashid Ahmed-Haras RMIT University, Australia

# **City Tour**

## Schedule

13:30	Depart from the Conference Venue
13:30-16:00	Explore the City by Bus Charter 16:00-16:15 Refreshment
16:15-19:00	Continue the Exploration
19:00	Back to the Conference Venue

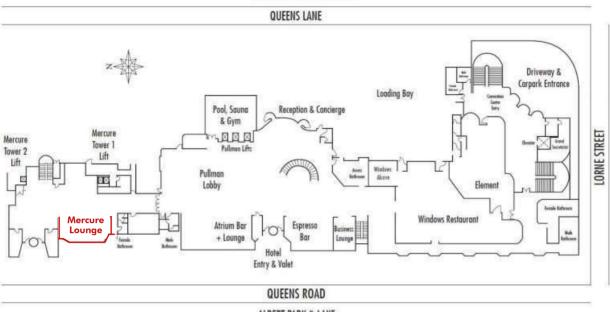
**Spotlight on Melbourne** Melbourne's charm is characterised by its enchanting laneways, stunning waterfront precincts and trendy neighbourhoods, and provides an endless choice of shopping hot spots and culturallydiverse, award-winning restaurants, cafés and bars in weird and wonderful locations. There are plenty of things to do in Melbourne. Easily navigated on foot, the city's confidence and success are infectious; whether closing a deal or relaxing with colleagues and new friends, Melbourne is the perfect destination.

# The following are places covered during city tour.

- St Kilda Pier
- Brighton Huts
- Melbourne Star (Docklands)
- Melbourne Cricket Ground
- Royal Exhibition Building

# **Venue Floor**

GROUND FLOOR



ALBERT PARK & LAKE

# **CONFERENCE AND EVENT CENTRE**



QUEENS ROAD

**ALBERT PARK & LAKE** 

# **Keynote Presentations**

# Challenges and opportunities in data-driven materials design

# Amanda S. Barnard\*

CSIRO Data61: Door 34 Village Street, Docklands, VIC, 3008

## Abstract

A fundamental aim of nanomaterials research is to identify features of materials that can be tuned to control how the nanomaterial performs under specific application conditions. The combination of computational chemistry, computational materials science with machine learning provides a powerful way of relating structural features with functional properties, but combining these fundamentally different scientific approaches is not as straightforward as it seems. Machine learning methods were developed for large data sets with small numbers of consistent features. Typically materials data sets are small, with high dimensionality and high variance in the feature space, and suffer from numerous destructive biases. None of the established data science or machine learning methods in widespread use today were devised with materials data sets in mind, but there are ways to overcome these issues and use them reliably. In this presentation we will discuss the impact of domain-specific constraints on data-driven materials design, and explore the differences between materials simulation and materials informatics that can be leveraged for greater impact.

# Biography

Dr. Amanda Barnard is Chief Research Scientist at the Commonwealth Scientific and Industrial Research Organisation (CSIRO) in Data61. She received her Ph.D. (Physics) in 2003, followed by a Distinguished Postdoctoral Fellow in the Center for Nanoscale Materials at ANL, and a Violette & Samuel Glasstone Fellow at the University of Oxford. She joined CSIRO as an ARC Queen Elizabeth II Fellow in 2009, and now leads research developing structure/property relationships using computational physics and chemistry, machine learning, deep learning and artificial intelligence (AI). For her work she has won the 2009 Young Scientist Prize in Computational Physics from the IUPAP, the 2009 Malcolm McIntosh Award from the Prime Minister of Australia for the Physical Scientist of the Year, the 2014 ACS Nano Lectureship (Asia/Pacific), and the 2014 Feynman Prize in Nanotechnology (Theory) from the Foresight Institute.



# Nanomaterial properties as revealed via in situ transmission electron microscopy

# **Dmitri Golberg**

School of Chemistry, Physics and Mechanical Engineering, Science and Engineering Faculty, Queensland University of Technology (QUT), 2<sup>nd</sup> George st., Brisbane, QLD 4000, Australia

## Abstract

Uncovering structural, electromechanical, thermoelectric and optoelectronic properties of a material, in particular down to the nanoscale range of dimensions, is the key with respect to its smart integration into modern nanotechnologies. However, in many cases such properties have been measured by means of scientific instruments with no direct access to the nanomaterials' atomic structure, its crystallography, spatially-resolved chemistry and defects. This fact largely limits the relevance of the collected data because all particular structural features of a nano-object prior, during and after its testing have typically been hidden. Therefore, the acquired results can hardly be linked to a particular material morphology, its atomic structure and defect network. Thus, a wide scatter of the reported data has been observed while studying various samples within different research groups. Such drawback has often confused practical engineers and led to many uncertainties with respect to real nanomaterials' potentials. I will demonstrate the striking usefulness of diverse state-of-the-art in situ transmission electron microscopy methods for the precise property analyses of numerous advanced nanomaterials, e.g. individual inorganic nanotubes, graphene-like nanosheets, nanowires, nanoparticles, nanocomposites and heterostructures. The Young's modulus, tensile strength and strains, electrical conductance, thermal gradients, photocurrents, and spatially-resolved cathodoluminescence of prospective nanomaterials have be unambiguously determined under atomic resolution inside a high-resolution transmission electron microscope, while employing piezo-driven electrical probes, mechanical sensors, nanomanipulators and optical fibers adjusted within the microscope column.

Acknowledgement: This work was financially supported by the Australian Research Council (ARC) in the frame of the Australian Laureate Fellowship FL160100089 and QUT Projects No. 322170-0355/51 and 322170- 0348/07.

# Biography

Dmitri Golberg has a wide background and strong command in the synthesis, electron microscopy, and physical property measurements of BN and other inorganic nanotubes and related nanomaterials. In 1995 he became one of first world scientists to launch a full scale research on BN nanotubes. Over the last few years he became fully engaged in the electrical, mechanical, thermal, optical and optoelectronic property measurements of individual nanotubes, nanowires and graphene-like nanostructures in a high-resolution transmission electron microscope. Golberg is author or co-author of more than 580 original papers in peer-reviewed International journals and over 100 patents. In 2005 Golberg was awarded the 16th Tsukuba Prize for his studies of inorganic nanotubes and nanothermometers. In 2012, he became a recipient of the Thomson Reuters Research Front Award for his



outstanding contributions to emerging global research fronts. In 2014 he obtained the "Seto Award" from the Microscopy Society of Japan for his pioneering development of in situ TEM techniques for inorganic nanomaterial property analysis. In consecutive 2014 and 2015 years Golberg was elected as a highly-cited researcher by "Thomson Reuters". In 2016 he won the NIMS President Award. At present, Golberg is listed among top-150 most- cited world materials scientists on the Web of Science. His works have been cited more than 25000 times and H-factor of his publications is 84.

# Efficient air cathodes for rechargeable lithium oxygen batteries

# Jiazhao Wang<sup>a\*</sup>, Wenbin Luo<sup>a</sup>, Chaozhu Shu<sup>a,b</sup>

<sup>a</sup>Institute for Superconducting and Electronic Materials, University of Wollongong, Wollongong, NSW 2500, Australia <sup>b</sup>College of Materials and Chemistry&Chemical Engineering, Chengdu University of Technology, P. R. China

# Abstract

A Li–air battery could reach an energy density 3–4 times higher than state-of-the-art Li-ion cells at the cell level. Research on the Liair battery, however, is currently still in the early stages of understanding the basic scientific principles and mechanisms, and there are significant technical challenges confronting the development of advanced materials for Li-air batteries [1]. Transition metal-doped perovskite oxide, ruthenium-carbon composite and Pd-based compotes have been invested in our group and will be reported in this presentation!

Transition metal-doped perovskite oxide  $LaNi_{0.9}M_{0.1}O_3$  (M=Cu, Co, Zn) has been grown on nickel foam with different morphology as carbon and binder free 3D air electrod. Excellent cycling performace under 1000 mAh g<sup>-1</sup> capacity limited mode is demonstrated, the discharge terminal voltage of stays above 2.36 V for 100 cycles under a current density of 0.1 mA g<sup>-1</sup>[2]. Ru decorated hierarchically porous carbon (Ru@HPC) cathodes were synthesized using a facile and rapid puffing process followed by decoration of Ru nanoparticles. Ru@HPC cathode demonstrates a reduced overpotential, enhanced specific capacity and superior cyclability. Density functional theory calculations indicated that the interfacial interaction between Ru nanoparticles and carbon substrate, which triggers electron transfer from ruthenium to carbon and thus optimizes the surface adsorption energy of the reactants and intermediate, facilitates the performance improvement of Li-O<sub>2</sub> battery [3].

Carbon-free porous AgPd–Pd composite NTs were synthesized via a galvanic replacement reaction. The composite was used as a bifunctional electrocatalyst, showing favorable rechargeability and good electrocatalyst performance with a high round-trip efficiency, owing to the high catalytic activity of the electrocatalyst and the abundant catalytic active sites provided by the porous NT structure [4]

# References

- [1] C. Z. Shu, J.Z Wang et al, Adv. Mater., 2019, 1804587.
- [2] T. V. Pham, J.Z. Wang et al, J Mater. Chem A 5 (2017) 5289.
- [3] C. Z. Shu, J.Z Wang et al, Nano Energy, 57 (2019) 166-175.
- [4] W. B. Luo, J.Z. Wang et al, H.K. Liu, Adv. Mater 27 (2015) 6862.

# Biography

Jiazhao Wang is a Professor at the Institute for Superconducting and Electronic Materials, University of Wollongong, Australia. Her research activities focus on electrochemical energy storage in batteries, including Li-ion batteries, Na-ion batteries, metal-air batteries (Li, Na & Zn), and Li-S batteries. She has won 30 research grants including 20 Australian Research Council (ARC) grants as a chief investigator (CI). She is current a team leader of an ARC DP on Na-air batteries, and a team leader of an ARC LP on Li/S batteries. She has published



more than 200 papers in international journals (Citations>16000, H index = 70, Google Scholar, April. 2019). She is 2018 Highly Cited Researcher (Clarivate Analytics). She has supervised 29 PhD students.

# Nanostructured materials for energy-relevant electrocatalytic processes

# **Shizhang Qiao**

School of Chemical Engineering and Advanced Materials, The University of Adelaide, SA5005, Australia

# Abstract

Replacement of precious metal catalysts by commercially available alternatives is of great importance among both fundamental and practical catalysis research. Nanostructured carbon-based and transition metal materials have demonstrated promising catalytic properties in a wide range of energy generation/storage applications. Specifically engineering carbon with guest metals/metal-free atoms can improve its catalytic activity for electrochemical oxygen evolution reaction (OER) and hydrogen evolution reaction (HER), thus can be considered as potential substitutes for the expensive Pt/C or IrO<sub>2</sub> catalysts in metal-air batteries and water splitting process. In this presentation, I will talk about the synthesis of nonprecious metal and metal free elements-doped graphene, and their application on electrocatalysis [1-4]. The excellent OER and HER performance (high catalytic activity and efficiency) and reliable stability indicate that new materials are promising highly efficient electrocatalysts for clean energy conversion. I will also present some research results of CO2 electrocatalytic reduction conducted in my research group [5, 6].

# References

(1) Jin H., Qiao S.Z., et al., Chem. Rev. 2018, 118, 6337-6408.

- (2) Zhao Y., Qiao S.Z., et al., Angew. Chem. Int. Ed., 2019, 58, 12252-12257.
- (3) Shan J., Qiao S.Z., et al., Advanced Materials 2019, 31, 1900510.
- (4) Ling T., Qiao S.Z., et al., Nature Communications 2017, 8, 1509.
- (5) Zheng Y., Qiao S.Z., et al., J. Am. Chem. Soc. 2019, 141, 7646-7659.
- (6) Jiao Y, Qiao S.Z., et al., J. Am. Chem. Soc. 2017, 139, 18093.

# Biography

Dr. Shi-Zhang Qiao is a Chair Professor at School of Chemical Engineering and Advanced Materials of the University of Adelaide. His research expertise is in nanostructured materials for new energy technologies. He has co-authored more than 385 papers in refereed journals (over 52,000 citations withh- index 119).



Prof. Qiao was honoured with a prestigious ARC Australian Laureate Fellow (2017), ExxonMobil Award (2016), ARC Discovery Outstanding Researcher Award (DORA, 2013) and an Emerging Researcher Award (2013, ENFL Division of the American Chemical Society). He is a Clarivate Analytics Highly Cited Researcher (Chemistry, Materials Science).

# Cell membrane penetration without pore formation: chameleonic properties of dendrimers in response to hydrophobic and hydrophilic environments

# Sergio de Luca<sup>1</sup>, Prasenjit Seal<sup>2</sup>, Harendra S. Parekh<sup>3</sup>, Karnaker R Tupally<sup>3</sup> & Sean C. Smith<sup>1</sup>

<sup>1</sup>Research School of Physics and Engineering, Australian National University. <sup>2</sup>Department of Chemistry, University of Helsinki, P.O. Box 55 (A.I. Virtasen aukio 1), Helsinki 00014, Finland. <sup>3</sup>School of Pharmacy, The University of Queensland, Brisbane, Australia.

# Abstract

The mechanism by which cell-penetrating peptides and antimicrobial peptides cross plasma membranes is unknown, as is how cellpenetrating peptides facilitate drug delivery, mediating the transport of small molecules. Pore formation, including toroidal, barrelstave, or carpet models, have nearly reached the status of a dominant paradigm. Spontaneous pores have been observed in coarsegrained simulations and less often in molecular dynamics simulations. While pores are widely assumed and inferred, there is no unambiguous experimental evidence of the existence of pores. Some recent experimental studies actually contradict the mechanistic picture of pore formation. We propose a model for peptide (linear and dendritic) translocation which does not require the presence of pores and which potentially accords with such experiments. We suggest that a charged peptide, as it experiences an increasingly hydrophobic environment within the membrane surface, can shed its protons to membrane phosphate groups, thereby becoming compatible with the hydrophobic interior of the membrane. This increases the likelihood to move into the highly hydrophobic core of the membrane and ultimately reach the opposite leaflet to re-acquire protons again, suggesting a potential "chameleon" mechanism for non-disruptive and non- endocytotic membrane translocation. Our molecular dynamics simulations also reveal stability of peptide bridges joining two membrane leaflets and demonstrate that this can facilitate cross-membrane transport of small drug molecules.

# Biography

Sean Smith commenced as Director of the NCI in January 2018 and is conjointly Professor of computational nanomaterials science and technology at the ANU. He has extensive theoretical and computational research experience in chemistry, nanomaterials and nano-bio science and technology. He returned to Australia in 2014 at UNSW Sydney, founding and directing the Integrated Materials Design Centre to drive an integrated program of materials design, discovery and characterization. Prior to this, he directed the US Department of Energy funded Center for Nanophase Materials Sciences (CNMS) at Oak Ridge National Laboratory, one of five major DOE nanoscience research and user facilities in the US, through its 2011-2013 triennial phase. During his earlier career, he joined The University of Queensland as junior faculty in 1993 after post-doctoral research



at UC Berkeley (1991- 1993) and Universität Göttingen (Humboldt Fellow 1989-1991); became Professor and Director of the Centre for Computational Molecular Science 2002-2011; and built up the computational nanobio science and technology laboratory the Australian Institute for Bioengineering and Nanotechnology (AIBN) at UQ 2006-2011.Sean has published over 260 refereed journal papers with more than 15000 citations. In 1998 he was elected Fellow of the RACI. In 2006 he was recipient of a Bessel Research Award of the Alexander von Humboldt Foundation in Germany. In 2012 he was elected Fellow of the American Association for the Advancement of Science (AAAS) and in 2015 he was elected Fellow of the Institution of Chemical Engineers (IChemE). He received his PhD in theoretical chemistry from the University of Canterbury, New Zealand, in 1989.

# Low-cost and high-performance hybrid phosphors for energy-efficient lighting technologies

# Jing Li

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# Abstract

Current energy-efficient general lighting technologies (e.g. CFLs, LEDs) rely heavily on rare earth element (REE) based phosphors. Developing alternative phosphor materials that have little or no dependence on REEs is much needed due to the potential cost and supply risks of REEs, as well as their negative impact on the environment. In the recent years, we have developed several crystalline inorganic-organic hybrid material families, all of which are free of REEs. This talk will focus on our recent effort in systematic tuning and optimizing optical properties of copper iodide based hybrid materials by rational design and engineering of their crystal structure and chemical bonding at the

inorganic-organic interface. A powerful combination of experimental and theoretical methods has enabled us to investigate the correlation between their crystal structures and electronic/optical properties and to understand the relationship between chemical bonding and emission behavior as well as framework stability. These studies also provide helpful insight into the origin and mechanisms of luminescence observed in these systems. With high luminescence quantum efficiency (comparable to that of benchmark commercial phosphors), low synthesis cost, excellent thermal- and photo-stability, good solution processability and strong scalability, these hybrid materials exhibit substantial potential for possible use in energy-efficient general lighting technologies.

# Biography

Jing Li is a Distinguished Professor in the Department of Chemistry and Chemical Biology at Rutgers University, USA. She received her Ph.D. degree from Cornell University in 1990 under the guidance of Professor Roald Hoffmann. She joined the chemistry faculty at Rutgers University in 1991 as Assistant Professor. She was promoted to Associate Professor in 1996, to Full Professor in 1999, and to Distinguished Professor in 2006. She has published +330 research articles, invited book chapters and reviews, and holds 14 issued and pending patents. She currently serves as Associate Editor for Crystal Growth & Design.



## Magnetic nano-catalysts and carbonaceous waste for sustainable applications in chemical transformations

#### Rajender S. Varma<sup>\*a,b</sup>

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#### Abstract

Sustainable efforts for the greener syntheses of assorted nanoparticles, nanocomposites and their applications as retrievable nano-catalysts are important in synthesis and remediation.<sup>1-5</sup> Pd, Ni, Ru, Ce, Cu etc. immobilized on biodegradable and earth-abundant supports namely cellulose, chitosan, tree gums or their conjugates on magnetic ferrites via ligands such as dopamine or glutathione will be presented.<sup>1-4</sup> The solubility problems in water have been addressed via polymer conjugates of chitosan with poly(3– hydroxybutyrate).<sup>4</sup> The unprecedented fabrication of bioplastic fibers from Gum Arabic, a natural tree gum exudate, blended with PVA via 'green' electrospinning process will be featured for greener food wrapping applications<sup>5</sup> including sustainable routes to nanoparticles using waste from winery,<sup>6a</sup> or biodiesel byproduct, glycerol<sup>6b,c</sup> and their applications as magnetic nano-catalysts or organocatalysis.<sup>7</sup> The value of heterogenized bimetallic Ag-Pd nanoparticles on graphitic carbon nitride (AgPd@g-C<sub>3</sub>N<sub>4</sub>) will be underscored in upgrading of biofuel via hydrodeoxygenation of vanillin under visible light conditions using formic acid as a hydrogen source<sup>8a</sup> and conversion of lignin-derived guaiacol to cyclohexanol.<sup>8b</sup> Photocatalytic C-H activation<sup>10a</sup> using VO@g-C<sub>3</sub>N<sub>4</sub> catalyst for direct oxidative esterification of alcohols, <sup>10D</sup> oxygen insertion reaction in hydrocarbons<sup>10c</sup> and selective oxidation of alcohols<sup>10d</sup> and hydrogenation of alkenes and alkynes<sup>10e</sup> using visible light as the source of energy will be described; these strategies capitalize on the use of waste that can sustainably generate N-enriched carbonaceous catalytic materials valuable in performing greener transformations and environmental remediation with minimal impact.<sup>11</sup>

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#### Biography

Prof. Varma (H-Index 106; Highly Cited Researchers 2016-18; Publons Awardee 2018) was born in India (Ph.D., Delhi University 1976). After postdoctoral research at Robert Robinson Laboratories, Liverpool, U.K., he was faculty member at Baylor College of Medicine and Sam Houston State University prior to joining the Sustainable Technology Division at the US Environmental Protection Agency in 1999 with appointment at Regional Centre of Advanced Technologies and Materials, Palacky University at Olomouc, Czech Republic. He has over 45 years of research experience in management of multidisciplinary technical programs ranging from natural products chemistry to development of more environmentally friendly synthetic methods using microwaves, ultrasound, etc. Lately, he is focused on greener approaches to assembly of nanomaterials and sustainable applications of magnetically retrievable nanocatalysts in benign media. He is a member of the editorial advisory board of



several international journals, has published over 540 papers, and has been awarded 16 US Patents, 6 books, 26 book chapters and 3 encyclopedia contributions with 38,000 citations.

# Recent developments of advanced GaN materials for light emitting diodes (LEDs) and laser diodes for energy efficient lighting and displays

#### Steven P. DenBaars<sup>\*</sup>, Shuji Nakamura, James Speck

Solid State Lighting and Energy Electronics Center, University of California, Santa Barbara, CA 93106USA

#### Abstract

LEDs fabricated from gallium nitride have led to the realization of high-efficiency white solid-state lighting. Currently, commercial GaN white LEDs exhibit luminous efficacy greater than 120 lm/Watt, and external quantum efficiency higher than 50%. This has enabled LEDs to compete with traditional lighting technologies such as incandescent and CFL. Further improvements in materials quality and cost reduction are necessary for wide-spread adoption of LEDs for lighting. In particular, solving both current "droop" and thermal "droop" has been identified by the USA Department of Energy as key roadblocks to cost reduction and further improvements in LED Lighting. Using advanced light extraction structures we have fabricated advanced GaN white LEDs structures which exhibit luminous efficacy greater than 198 lm/Watt, and external quantum efficiencies higher than 76% at low current densities. Looking even further into the future we see Laser Diode based solid state lighting as impacting high brightness specialty lighting. Recently, we have demonstrated laser based white lighting with luminous efficacies of 87 lm/watt, and over 1000 lumens from a single emitter. The US DOE estimates LED lighting is now posed to save the world tens of billions of USD in energy costs and a large reduction of greenhouse gases. This work was supported by the Solid State Lighting and Energy Electronics Center.

#### **Biography**

Dr. Steven P. DenBaars is a Professor of Materials and Co-Director of the Solid-State Lighting and Energy Electronics Center (SSLEEC) at the University of California Santa Barbara. In 2005 he was appointed the Mitsubishi Chemical Chair in Solid State Lighting and Displays. Specific research interests include growth of wide-bandgap semiconductors (GaN based), and their application to Blue LEDs and lasers and high power electronic devices. Prof. DenBaars has been an active in entrepreneurship, having helped co-found 3 start-up companies in the field of optoelectronics and electronics. He received the IEEE Fellow award in 2005, Aron Kressel Award – IEEE Photonics Society, elected member of the National Academy if Engineers 2012, and National Academy of Inventors in 2014. He has authored or co-authored over 980 technical publications, 350 conference presentations, and over 185patents.



## Materials spacetectonics: New conceptual paradigm of functional porous system

#### Yusuke Yamauchi<sup>a,b\*</sup>, Tang Jing,<sup>b</sup> and Md. Shahriar A. Hossain<sup>b,c</sup>

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#### Abstract

Porous materials have unique features such as high surface areas and large pore volumes, and they have been actively applied as catalyst materials, adsorption materials, etc. Mesoporous materials have been actively studied worldwide since the 1990s and have been synthesized using amphiphilic molecules. Thousands of papers on mesoporous materials are published every year, and it can be said that that field has become mature. On the other hand, unique coordination polymers (PCPs/MOFs) has been extensively studied worldwide. These examples, however, are formed based on 'coordination bonds' using organic ligands and metal ions, and their applications are limited to gas adsorption, separation, molecular recognition, etc. Considering applications to (electro)catalysts, supercapacitors, secondary batteries, fuel cells, etc. to solve serious global energy issues, the discovery other types of novel porous materials composed of stable inorganic solids in which atoms are linked by covalent bonds or metal bonds is essential. Our group has focused on new "self-organization" phenomenon involving interactions between molecules to introduce many conductive inorganic frameworks in porous systems. This has been an important breakthrough representing a substantial advance for the porous material community. In this presentation, we will introduce our recent advance on functional porous materials towards energy-related applications.

#### Biography

After receiving his Ph.D. (Waseda Univ.), he joined the National Institute of Materials Science (NIMS), Japan to start his own research group. Currently, he is a full-time professor at the School of Chemical Engineering and a senior group leader at AIBN at the University of Queensland. He serves concurrently as an honorary group leader of NIMS, a visiting/honorary professor at many universities over the world, and an associate editor of Journal of Materials Chemistry A published by the Royal Society of Chemistry (RSC). He has published more than 650 papers in international refereed journals with > 35,000 citations (h-index > 90). He is selected as one of the Highly-Cited Researchers in Chemistry in 2016, 2017, and 2018.



# Advanced synchrotron x-ray diffraction and imaging techniques for catalysis and electrocatalysis

#### Hoydoo You

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#### Abstract

We will review advanced synchrotron x-ray diffraction and imaging techniques and their applications for catalytic and electrocatalytic systems relevant to energy storage and conversion technologies. An important characteristics of synchrotron x-rays is the high sensitivity to the interfaces and nanoparticles through the power penetrating electrolytes or high-pressure gas environments. For the reason, the x-ray techniques are powerful for operando or in-situ studies on structure determination of surfaces, dynamics study of interfaces, and imaging nanoparticles. In each category, we will present a short description of the technique followed by the important results obtained by the techniques. (i) Application of crystal truncation rods (CTR) for light elements in electrified interfaces will cover the water life cycle on oxide surfaces, nascent oxidation on metal surfaces, and electrified Stern layers. (ii) Use of coherent x-ray reflectivity will be discussed in measuring the dynamics and transitions of electrode surfaces and interfaces such as step dynamics and dissolution reactions. (iii) A new x-ray imaging technique, Bragg coherent diffraction imaging, is used to study nanoparticles under insitu conditions such as silver nanoparticle dissolution reactions, showing highly nonlinear behavior of dissolution, and visualizations of dealloying processes of Ag-Au alloy nanoparticles, showing that the dealloying characteristics are critically dependent on particle environments. In more recent studies, we examined gas-induced core-shell segregation behavior of alloy nanoparticles under gas environments.

#### Biography

Dr. Hoydoo You graduated from University of Washington, Seattle, WA USA with Ph.D. in Physics from Seoul National University, Seoul, Korea, with BS in Physics Education. Later on he worked in the area of Synchrotron x-ray studies at Physics Department of Brookhaven National Laboratory as a postdoc initially and then as an Assistant Physicist later. Presently he is working at Argonne National Laboratory, Materials Science Division, Argonne, IL USA



# Anostructured layered double hydroxide based photocatalysts for solar fuels and value-added chemicals

#### **Tierui Zhang**

*Key Laboratory of Photochemical Conversion and Optoelectronic Materials, Technical Institute of Physics and Chemistry, CAS, Beijing, 10190, China* 

#### Abstract

Layered double hydroxide (LDH) based nanostructured materials have been considered as very promising photocatalysts for chemical fuels and products. Herein, some very recent research progress in my group has been summarized on the rational design of Layered double hydroxide (LDH)-based photocatalysts for improved water splitting into hydrogen,  $CO_2$  photoreduction into fuels and photofixation of N<sub>2</sub> into NH<sub>3</sub> by introducing defects in their surfaces and/or constructing heterointerface structure. For instance, I) By creating more oxygen defects in ultrathin ZnAl-LDH nanosheets, the photocatalytic reduction of  $CO_2$  with water over ZnAl-LDH exhibited stable activity of  $\approx 7.6 \,\mu\text{mol g}^{-1} \,\text{h}^{-1}$ ; in ultrathin ZnAl-LDH nanosheets N<sub>2</sub> can be efficiently reduced into NH<sub>3</sub> under visible-light irradiation; II) By constructing heterointerface structure, NiO/Ni nanocatalysts exhibited an unexpectedly high selectivity of 60% for  $C_2$ -  $C_7$  hydrocarbons in the CO hydrogenation reaction under visible-light irradiation.<sup>[1-8]</sup>

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## Biography

Dr. Tierui Zhang is a full Professor in Technical Institute of Physics and Chemistry, Chinese Academy of Sciences. He received Ph.D. in Organic Chemistry in 2003 from Jilin University in China. His research activity focuses on catalyst nanomaterials for energy conversion. He has published more than 180 peer reviewed SCI journal articles. These publications have earned him to date over 10000 citations with H- index 54. He was named in the annual Highly Cited Researchers 2018 List by Clarivate Analytics. Dr. Zhang is the associate editor of Science Bulletin and also serves as an editorial board member for peer- reviewed journals including Advanced Energy Materials. He is the recipient of a number of awards including Alexander von Humboldt Fellowship, Royal Society-Newton Advanced Fellowship. He was named a fellow of the Royal Society of Chemistry in 2017.



# **Invited Presentations**

## Session 1: Electronic and Optical Materials

# Superconductivity enhanced by a ferroelectric quantum critical point

## Yasuhide Tomioka, Naoki Shirakawa, Keisuke Shibuya, Isao H. Inoue\*

National Institute of Advanced Industrial Science and Technology (AIST): Tsukuba 305-8565, Japan

## Abstract

SrTiO<sub>3</sub> is a well-known insulator with a band gap of ~3.3 eV and shows many interesting properties. Notably, due to the substantial dielectric constant  $\varepsilon \sim 24,000$  at low temperatures, the effective Bohr radius becomes extremely large (~0.5 µm), driving the insulator to metal transition even at a very low carrier density of  $2 \times 10^{16}$  cm<sup>-3</sup>. Although  $\varepsilon$  is huge, SrTiO<sub>3</sub> does not show ferroelectricity; this is called a quantum paraelectric because the low- temperature phase is close to a quantum critical point (QCP). Studies on QCPs so far have revealed remarkable phenomena such as superconductivity, but only around magnetic QCPs. In this talk, I will focus on the non-magnetic counterpart: ferroelectric QCP of SrTiO<sub>3</sub>. We explore the relationship between the superconductivity and the ferroelectric QCP of SrTiO3. We have prepared high-quality Sr<sub>1-x</sub>La<sub>x</sub>Ti(<sup>16</sup>O<sub>1-z</sub><sup>18</sup>O<sub>2</sub>)<sub>3</sub> single crystal and systematically investigated the La substitution of Sr as an alternative of introducing oxygen vacancies. The superconducting transition temperature T<sub>c</sub> shows a dome-like behaviour against the carrier density n. Analysis of the data based on a theoretical model predicts an appearance of the ferroelectric QCP for Sr<sub>1-x</sub>La<sub>x</sub>TiO<sub>3</sub> around  $3 \times 10^{18}$  cm<sup>-3</sup>. The QCP raises the superconducting dome of Sr<sub>1-x</sub>La<sub>x</sub>TiO<sub>3</sub> upwards. Further enhancement of T<sub>c</sub> (~0.6 K) is achieved by <sup>18</sup>O exchange on the Sr<sub>1-x</sub>La<sub>x</sub>TiO<sub>3</sub> crystals. These findings provide a new knob for observing intriguing physics around the ferroelectric QCP. Details are given in the talk.

## Biography

Dr Isao H. Inoue received BSc, MSc, and DSc degrees in Physics from the University of Tokyo in 1990, 1992 and 1998, respectively. He became a researcher with tenure of the Electrotechnical Laboratory (ETL) in 1992 and a senior researcher in 1999. From 1999 to 2001, he was a visiting scholar at Cavendish Laboratory, University of Cambridge. In 2001, ETL was reorganised to AIST; since then, he has been a senior researcher of the National Institute of Advanced Industrial Science and Technology (AIST). He has been investigating on a wide range of research field: from the strongly correlated oxides to the neuromorphic electronic devices.



# Exploring novel engineered materials for fl'exible electronic system

## Ibrahim H. Khawaji<sup>a</sup>, Osama O. Awadelkarim<sup>b,c</sup>, and Akhlesh Lakhtakia<sup>b</sup>

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#### Abstract

Silicon-based CMOS material set is rather restrictive for the realization of the full potential of flexible electronics and, hence, new material compositions are currently being explored. Because of its extensive applications in medical devices as well as its chemical inertness and thermal stability Parylene C can play different roles in flexible systems. Columnar microfibrous thin films ( $\mu$ FTFs) of Parylene C are grown using an oblique-angle variant of standard physicochemical vapor deposition, whereby a collimated flux of Parylene C monomers is directed at an angle on to a substrate. Columnar  $\mu$ FTFs for different as well as bulk Parylene-C are grown and characterized as blanket layers or as dielectrics in metal– Parylene C  $\mu$ FTF–metal and metal-bulk Parylene C –semiconducting pentacene device structures. With decreasing  $\mu$ FTF deposition, it is observed that: the porosity of the  $\mu$ FTF is increased; its Young's modulus is decreased; its flexibility is significantly enhanced; and up to 30% decrease in its dielectric constant is attained. The d.c. leakage current in the  $\mu$ FTF is found to be dominated by the Poole–Frenkel conduction mechanism, whereas the a.c. conduction is temperature-activated and follows a power law in frequency. Also, constant-voltage stress (CVS) reliability testing of bulk Parylene-C reveals trapped charge build up induced by CVS in the bulk of Parylene-C and at its interface with pentacene. Overall, both the mechanical and dielectric properties of the Parylene-C columnar  $\mu$ FTFs can be engineered by selecting  $\chi_V$  therefore rendering Parylene-C, in columnar  $\mu$ FTF or bulk forms, a promising candidate for deployment as a multifunctional dielectric in integrated flexible electronics.

#### Biography

Dr. Awadelkarim received his Ph. D. from Reading University, UK, and prior to joining Pennsylvania State University, he worked as a Research Scientist at Linkoping University, Sweden, and the Swedish Defense Research Establishment. His research interests are in electronic materials and devices. He was selected by the US National Academy of Sciences as a Jefferson Science Fellow and is currently a Science Advisor at the US Department of State, and Emeritus Member of the Board of Directors for the Arab Science and Technology Foundation.



## Si paste as a novel printing electronic material

#### **Yoshimine Kato**

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#### Abstract

The Si microcrystalline pastes were prepared by a planetary ball miller to pulverize Si source material. p- and n-type Si pastes were prepared individually and pn homo-junction was formed by coating the Si pastes onto Al/Fe or Mo substrates, followed by annealing under Ar or Ar+H2 atmosphere. Influences of annealing temperatures ranging from 400 °C to 1100 °C to crystal quality and oxidation have been investigated and discussed. The optimal annealing temperature was found to be around 1050 °C that exhibits the lowest resistivity. A pn junction was successfully formed with a rectifying ratio of around 440 at  $\pm$ 1V. A slight photovoltaic was also was observed. Raman spectra was also observed and relaxation phenomena of the tensile stress after the PBM process and improvement in crystalline quality of the Si paste were confirmed after annealing at higher temperature. Oxidation of Si paste was recognized at higher annealing temperature according to FT-IR spectra. It is important to reduce the Si oxide during the annealing process. It is anticipated that Si microcrystalline pastes have potential for low cost device fabrication such as printing solar cells. All CZ Si ingot growth and slicing procedures could be skipped, consequently it is expected that the manufacturing cost for the Si solar cell can be greatly reduced.

## Biography

Dr. Yoshimine Kato has been graduated from Keio University, Japan in 1991 with a Ph.D. in engineering. He received Bachelor's and Master's from Keio University in 1988 and 1985, respectively. He also received Master's degree in engineering from Colorado State University, USA in 1984. Since 1988 he was a research staff member of IBM Tokyo Research Center. In 2004 he became an Associate Professor in Kyushu University, Japan. His wide research interests include ultrasonic gas sensors and its application, paste electronic materials, wide bandgap semiconductors and their applications to electronics.



# Gas bubbles, liquid droplets and sound: The new frontier for nonlinear optics

#### Ivan S. Maksymov

Centre for Micro-Photonics, Swinburne University of Technology, Hawthorn, VIC 3122, Australia and Australian Research Council Centre of Excellence for Nanoscale BioPhotonics

#### Abstract

Nonlinear optical processes are vital for telecommunications, signal processing, data storage, spectroscopy, sensing, and imaging. As an independent research area, nonlinear optics began with the invention of the laser, because practical sources of intense light needed to generate optical nonlinearities were not previously available. One of the current research directions in

nonlinear optics focuses on new materials and resonant structures capable of producing nonlinear optical phenomena with lowpower light emitted by inexpensive and compact sources. Acoustic nonlinearities, especially giant acoustic nonlinear phenomena in gas bubbles in liquids and liquid droplets, are much stronger than their optical counterparts [1]. Here, we suggest to employ acoustic nonlinearities of gas bubbles and plasmonic liquid-metal nanoparticles [2] to generate new optical frequencies, thereby effectively reproducing nonlinear optical processes without the need for laser light. We show that the conversion of acoustic nonlinearities into optical signals is possible with incoherent light sources such as light-emitting diodes that cost less than one dollar, which would usher new classes of low-power photonic devices that are more affordable for

remote communities and developing nations

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#### Biography

Dr Ivan Maksymov is an Australian Research Council Future Fellow in the Centre for Micro- Photonics at Swinburne University. He is also an Associate Investigator for the ARC Centre of Excellence for Nanoscale BioPhotonics. He received a joint-badged PhD degree in Theoretical Physics and Electronic Engineering from the University Rovira i Virgili (Spain) and NURE University (Ukraine). He has over 50 peer-reviewed journal publications with an h-index of 23.



#### Ryoma Hayakawa\*

International Center for Materials Nanoarchitectonics (WPI-MANA), National Institute for Materials Science (NIMS), 1-1 Namiki, Tsukuba 305-0044, Japan

#### Abstract

Quantum molecular devices hold promise for evolution of new data processing architectures that would not be realized by current Si technology. In this regard, we have proposed a vertically-aligned resonant tunneling devices with organic molecules as quantum dots. A striking point of our devices is that the molecules are embedded in an insulating layer of a metal-oxidesemiconductor structure, which works as a double tunnel junction. Moreover, the molecules are fully isolated from each other. The feature enables us to evaluate quantum transport via single molecules in the devices with the same analogy of scanning tunneling spectroscopy, although many molecules (1012-1013 cm-2) are present in the insulating layer. So far, we have achieved stepwise currents in the devices, which originate from resonant tunneling through discrete energy levels of the embedded molecules. Specially, the employment of C60 molecules as quantum dots attained the room-temperature observation of the tunneling current. In addition, the adoption of diarylethene photochromic molecules allowed for optical manipulation of the tunneling. Consequently, we demonstrated a vertical resonant tunneling transistor, given above achievements. The transistor permitted a multilevel operation, which is controlled by molecular orbitals. Our proposed transistor thus has the potential to realize unique device operations unobtainable with inorganic quantum dots.



#### Biography

Dr. Ryoma Hayakawa is a senior researcher at International Center for Materials Nanoarchitechtonics (MANA) of National Institute for Materials Science (NIMS). In 2006, he received his Ph.D. in Engineering from Osaka Prefecture University. He then earned a postdoctoral fellowship from Japan Society for the Promotion of Science (JSPS) in 2006. Thereafter, he held positions as a fellow at International Center for Young Scientist (ICYS) in 2010 and an independent researcher at MANA in 2012. Currently, he works in the field of molecular electronics, with his special interests in the development of unique devices with attractive molecular functions.



## A facile strategy to fabricate conductive fabrics-polyaniline based

#### Mohd Muzamir Mahat<sup>\*</sup>, Nazreen Che Roslan

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#### Abstract

The advancement of bioelectronics requires devices to be flexible and wearable. Fabric, is one of the interests due to the unique properties it can offer. Important considerations include the simplicity and ease in their fabrication. Here, we report a facile strategy to fabricate a conductive fabric by incorporating a conducting polymer-Polyaniline (PANI). PANI was used as a conductive agent embedded into the fabric and this was achieved by immersing the bare fabric into several concentrations of PANI solution, followed by a drying process. Prior to this, PANI was synthesized by chemical oxidation method, using phosphoric acid as a dopant. The fabrics were then characterised using Impedance Spectroscopy, Scanning Electron Microscope (SEM) and Fourier Transform Infra-Red Spectroscopy (FTIR) to reveal their conductivity, morphology, and functional group, respectively. The highest conductivity of the fabrics was obtained at 30 v/v % of dopant concentration which was found to be  $1.62 \times 10-4 \pm 2.30 \times 10-4 \text{ s/m}$ . The increase in the concentration of dopant had significantly improved the conductivity of the fabrics although according to SEM images, their morphology showed no significant differences. We found that PANI was uniformly distributed and had embedded well into the fabrics, suggesting a good incorporation of PANI into the fabrics, bridged by the phosphoric acid. The interaction of the dopant within the PANI structure was confirmed by the presence of phosphate peak in the FTIR spectra. Further investigation into the elemental composition using X-ray florescence (XRF) spectroscopy suggested that more phosphate groups were present on the fabrics with a higher concentration of dopant, justifying the increase of conductivity values.

#### Biography

Dr. Mohd Muzamir Mahat obtained his PhD from the Department of Materials, Imperial College London, specialised in surface chemistry and bio-stability of conducting polymers for biomedical applications. During his PhD in Imperial College, he worked with Professor Molly Stevens, Dr. David Payne and Dr Damia Mawad (now in University New South Wales, Australia). Presently, he is working as a senior lecturer at the Faculty of Applied Sciences, Universiti Teknologi MARA (UiTM), Malaysia. He continued his research in UiTM focusing on the fabrication of conductive fabrics, using polyaniline as the conductive agents. In the meantime, he hold a position as corporate communication coordinator of the faculty, facilitating the formal and scientific events.



## Femtosecond nonlinear four wave mixing for study of carrier dynamics in porous silicon

#### Lap Van Dao<sup>1</sup> and Nguyen Dai Hung<sup>2</sup>

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#### Abstract

Macro- and meso- porous silicon (PS) have also received much attention as good candidates for making microcavities and photonic crystals or mirrors with porous multilayers. However, since meso-PS consists of Si wires with diameters 6-10 nm, the quantum confinement does not strongly modify their electronic states and quantum efficiency for light emission is rather low, making studies of the optical properties of meso-PS more difficult. We report the use of spectrally resolved femtosecond 2 colour 3 pulse wave-mixing for studying the optical properties and carrier dynamics of meso-porous silicon, which is an example of an indirect band gap system. Control of two independent time delays, between the first and second pulses and between the second and third pulses, reveals the dynamics of the coherence and population ensembles, respectively. Furthermore, the wavelengths of the pump and probe pulses can be independently selected to drive particular quantum pathways and to study the dynamics of the electron or hole systems. With this

technique more than three degrees of freedom can be independently controlled to provide detailed information about the energy structures and dynamics of the charge systems. We study the hopping of the electrons among the localised states. Short timescales for electron localisation (~500 fs) and electron hopping (~3 ps) are observed which are dependent on the porosity of the samples.

#### Biography

Lap Van Dao is a Professor and Leader of Ultrafast Laser Science group at Centre for Quantum and Optical Science, Swinburne University of Technology. His research activities are the development and application of ultrafast and high power laser for imaging and ultrafast time-resolved laser spectroscopy in semiconductor quantum structures and biological systems

# Effective and stable heat modulation by smart window technology using advanced electrochromic and electrophoretic nanomaterials

#### Tam Duy Nguyen,<sup>a,b,\*</sup> Loo Pin Yeo,<sup>a,b</sup> Daniel Mandler,<sup>b,c</sup> Shlomo Magdassi,<sup>b,c</sup> Alfred Iing Yoong Tok <sup>a,b</sup>

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#### Abstract

Along with the development of renewable energy technologies, effective management of energy consumption is another key factor to address the increasing global energy demand coupled with the depletion of fossil fuel resources. In 2010, it is reported that more than 32% of global energy was spent in building industry, mainly for lighting as well as to conduct the room heating/cooling for indoor comfort [1, 2]. Recently, this energy consumption has been quickly growing as many modern buildings are commonly assembled with large scale glass window panels, where the effect of heat and light transfer through the windows is significantly enhanced. In this case, smart window technologies possess a huge potential for indoor energy savings due to the ability to modulate the transmittance of heat and light. However, the practical application of smart windows is restricted by the poor effectivity of heat modulation, low visible transparency, or short device lifespan. Our research recently has achieved two novel solutions to improve the performance of smart windows technology. Firstly, the electrochromic technology based on hybrid multilayered  $SnO_2$ -TiO<sub>2</sub>-WO<sub>3</sub> inverse opal nanostructure allows a highly transparent, effective and stable modulation of heat radiation through glass window. During colored state, this material can block approximately 90% of near infrared radiation while allows nearly 70% of visible transmittance. Secondly, the electrophoretic technology using graphene quantum dots thin film is able to control the heat conduction through glass window, with the minimal influence on the transparency. These advanced nanomaterials can significantly promote the application of smart window technology.

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#### Biography

Dr. Tam Nguyen obtained his bachelor degree in engineering physics and nanotechnology from Vietnam National University, Hanoi (VNUH) in 2012. He was also received the Temasek Foundation Leadership Enrichment and Regional Networking (TF-LEaRN) award from National University of Singapore (NUS) in 2012. Later on, he obtained his Ph.D. degree in materials science from Nanyang Technological University (NTU) in 2017. He is currently working as a Research Fellow at School of Materials Science and Engineering (MSE), NTU. His research interests include electro-catalysis and electrochemistry; materials for energy storage and conversion; semiconductor and electrochromic nanomaterials, carbon and graphene-based materials; membranes and polymer thin films.



## RIKEN accelerator-driven compact neutron source as a material science investigation probe

#### Yoshie Otake\*

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#### Abstract

RIKEN Accelerator-driven compact neutron source, RANS, has been operated since 2013. There are two major goals of RANS research and development. One is to establish a new compact low energy neutron system of floor-standing type for industrial use. Another goal is to invent a novel transportable compact neutron system for the preventive maintenance of large scale construction such as a bridge. The low energy transmission imaging, neutron diffractometer, small angle scattering instruments, fast neutron transmission imaging, fast neutron reflected (back scattered) imaging, neutron induced prompt gamma-ray analysis for elemental analysis and neutron activation analysis are available with RANS. Based on the success of RANS, we have developed more compact neutron system for popular use of neutron beam at any institutes, or universities, or industries with the name of RANS-II. It is now ready to generate neutrons in the RANS experimental hall with individual shielding system. The novel proton accelerator tube and 500 MHz solid state high-frequency amplifier for RANS-III, of a transportable neutron system as a non-destructive test for the infrastructures on-site, is started be developed in RIKEN. Such compact neutron systems enable material science

#### Biography

Dr. Yoshie OTAKE has been graduated from Institute of Science and Engineering, Waseda University: Doctor of Science in Elementary Particle Theoretical Physics. Later on she obtained her associate professor position at Ibaraki National College of Technology, and Research Fellow at Elementary particle experimental group in Kyoto University, became Visiting Scientist at Institute of Laue-Langevin, Grenoble France (Search for neutron EDM with crystal technology) in 1995, became research scientist of RIKEN in 1996. Presently she has been working at RIKEN for compact neutron systems development as a team leader of Neutron beam technology team in RIKEN center for advanced Photonics.



## Size tuneable NiCr2O4 nanoparticles for high charge storage parallel plate supercapacitor

#### Biplab Kumar Paul, Ananda Lal Gayen and Sukhen Das

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#### Abstract

Size tunable nickel chromite (Ni<sub>1+x</sub>Cr<sub>2-x</sub>O<sub>4</sub> where x=0.01, 0.05 and 0.1) nanoparticles have been successfully synthesized by simple coprecipitation method. Sintering temperature and molar concentration variation of Ni and Cr [NC<sub>1</sub> (Ni<sub>1.01</sub>Cr<sub>1.99</sub>O<sub>4</sub>), NC<sub>2</sub> (Ni<sub>1.05</sub>Cr<sub>1.95</sub>O<sub>4</sub>) and NC<sub>3</sub>(Ni<sub>1.1</sub>Cr<sub>1.9</sub> O<sub>4</sub>)] make the composite sample very imperative for capacitative application. XRD and FTIR patterns confirm the single phase FCC lattice of NiCr<sub>2</sub>O<sub>4</sub> as well as nano-dimensional distribution of the synthesized particles. The Field Emission Scanning Electron Microscopy (FESEM) illustrates that the particles are very small in size (<10 nm) and homogeneously distributed in the whole matrix without making any agglomeration. The obtained average size of the particles from the Transmission Electron Micrograph (TEM) is 4.5 nm for NC<sub>3</sub>, which agree well with the calculated size from Debye-Scherer equation. The presence of intrinsic defects/ oxygen vacancies has been confirmed by photoluminescence spectroscopy (PL) analysis. Enormous dielectric constant ( $_r=6.8x10^4$ ) and little tangent loss (tan=0.5) for the sample NC<sub>3</sub> at 50 Hz ensure the superiority of the material as a high dielectric separator compared to previously reported NiCr<sub>2</sub>O<sub>4</sub> based literature. Utilizing the synthesized material as high dielectric separator, a highly charge storage parallel plate supercapacitor (1cm×1cm) has been fabricated. The handmade device can able to enlighten 73 no of LEDs for 5 min. Therefore, we can conclude the synthesized NiCr<sub>2</sub>O<sub>4</sub> can be used as a promising candidate for cheap, unconventional and environment friendly energy storage device which can fulfill the exponentially increasing requirements of power supply for the civilization to a greater extent.

#### Biography

Dr. Biplab Kumar Paul has acquired his Ph.D. degree in 2016 from Department of Physics, Jadavpur University, India. Previously, he completed the M.Sc. and B.Sc. degree in Electronic Science in 2012 and 2010 respectively from West Bengal State University and Calcutta University respectively. Further, he acquired his extended knowledge and expertise in NOCCD at CSIR-CGCRI, India, as Research Associate from Jan-2017 to Apr-2019. Currently he is continuing his research work in Jadavpur University as a Post-Doctoral Fellow. His research focuses on the development of advanced multifunctional materials and fabrication of cheap, unconventional and environment friendly energy storing smart devices for civilization.

# Wide band gap organic single crystal for thermal and third order nonlinear optical applications I.P.

#### Bincy<sup>a\*</sup> and V. Ramkumar<sup>b</sup>

<sup>a</sup>Department of Physics, MES College, Nedumkandam, Idukki- 685553, Kerala, India. <sup>b</sup>Department of Polymer Science and Technology, Council of Scientific and Industrial Research (CSIR)-Central Leather Research Institute (CLRI), Adyar, Chennai, 600020, Tamil Nadu, India.

#### Abstract

Good quality single crystals of an organic third order nonlinear optical (NLO), 3-Hydyoxyanilinium p-toluenesulfonate (3HAPTS) were grown by slow evaporation solution technique (SEST) using constant temperature bath (CBT). Single crystal XRD reveals that grown 3HAPTS crystal belongs to triclinic system with centrosymmetric space group Pī. The lattice parameters obtained from single crystal X-ray diffraction are a = 9.578 (3) Å, b = 10.822 (3) Å, c = 14.145 (4) Å,  $\alpha$  = 96.787 (2)°,  $\beta$  = 109.701 (1)°,  $\gamma$  = 91.324 (2)°. Functional groups present in 3HAPTS were identified by FT-IR studies. FT-NMR spectral study confirms the number of protons and carbon present in 3HAPTS. Thermal behavior and stability of 3HAPTS were assessed by thermogravimetric and differential thermal analyses. A sharp endothermic peak at 181.44 °C in the DTA curve is assigned to the melting point of the title compound. Transparency of 3HAPTS in UV–vis–NIR region was analyzed and the optical band gap energy was found to be 4.01 eV. There is no significant absorption in the range of 310 – 1100 nm with a lower cut off wavelength at 310 nm. The mechanical behavior of the grown crystal in the (101) plane was analyzed with Vicker's microhardness tester. The negative third order nonlinear optical parameters were estimated by Z-scan studies, which affirm 3-Hydyoxyanilinium p-toluenesulfonate is a promising material for nonlinear optical application.

#### Biography

Dr.BINCY.I.P have been graduated and Post graduated in Physics from Providence Women's College, Kerala, India (under University of Calicut). I did my Ph.D in Physics from Anna University, Chennai under the guidance of Dr.R.Gopalakrishnan with thesis entitled 'Single crystal growth of new organic compounds and their characterization for third order nonlinear optical applications'. Presently I am working as Assistant Professor and Head of the Department of Physics in MES College Nedumkandam, Kerala, India. So far twelve post graduate students completed their project under my guidance in the field of nonlinear optical properties of Organic Crystals.



## Francisites as new geometrically frustrated quasi-two-dimensional magnets

#### Alexander N. Vasiliev<sup>a,b</sup>

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#### Abstract

New geometrically frustrated quasi-two-dimensional magnets represent exclusive scientific and practical interest due to the presence of multitude of quantum ground states of very similar energy which prevents the formation of "simple" long-range order. In case of strong ferromagnetic interaction within the layer and weak interlayer antiferromagnetic coupling the ground state of quasi-two-dimensional antiferromagnet can be easily destroyed by external magnetic field. This opens the possibility of reversible switching between states with "zero" and maximal magnetization. The phenomena of metamagnetism as sharp change of the volume magnetization is the effect of demand in spintronic and magnetic memory devices. Besides, the nearest antiferromagnetically ordered magnetic moments in frustrated systems can't simultaneously minimize their exchange energies which results in their canting. It is accompanied by formation of non-collinear long-range order i.e. spiral or cycloidal structures which in turn leads to multiferroelectricity and magneto-electric effect. The synthesis of new geometrically frustrated layered systems stimulate the experiment and a progress in theoretical research of quasi-two-dimensional magnetism on the background of three-dimensional crystal lattice. We present magnetic and electric properties of the whole family of compounds Cu3RE(SeO3)2O2X, where RE = Bi, Pr, Nd, Gd, Dy, Tb, Ho, Er, a X = Cl, Br. Assumingly, these objects form non-collinear magnetic structures and demonstrate the metamagnetic behavior in weak magnetic field similar to properties of mineral francisite Cu3Bi(SeO3)2O2CL. Recently found broadband absorption of electromagnetic waves at metamagnetic transitions in francisites seems to be

important to construct new devices (filters, delay lines) for information and communication technologies.

#### Biography

Dr. Alexander N. Vasiliev has been graduated from Lomonosov Moscow State University as physicist with the specialties including Materials Science and Nanotechnology. Later on he obtained Ph.D. and D.Sc. degrees on superconductivity and magnetism in the same university. He authored about 400 papers in peer-reviewed journals on these topics.



## Structure-property relationships in $\alpha$ -, $\beta'$ -, $\gamma$ and $\delta$ -modifications of Mn3(PO4)2

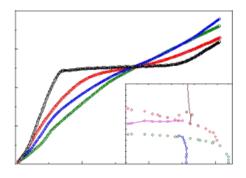
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#### Abstract

The manganese orthophosphate, Mn3(PO4)2, is characterized by the rich variety of polymorphous modifications, alpha-, beta'-, gamma- and delta-phases, crystallized in monoclinic P2(1)/c (P2(1)/n) space group type with unit cell volume ratios of 2:6:1:2 [1,2].

The crystal structures of these phases are constituted by three-dimensional framework of corner- and edge-sharing [MnO5] and [MnO6] polyhedra strengthened by [PO4] tetrahedra. All compounds experience long-range antiferromagnetic order at Neel temperature TN = 21.9 K (alpha-phase), 12.3 K (beta'-phase), 13.3 K (gamma-phase) and 13.6 (delta-phase). Additionally, second magnetic phase transition takes place at T\* = 10.3 K in beta'-phase and at 7.7 K in delta-phase. The magnetization curves of alpha-, beta'- and delta-modifications evidence spin-flop-like features at B = 1.9, 3.7 and 2.5 T, while the gamma-Mn3(PO4)2 stands out for an extended one-third magnetization plateau stabilized in the range of magnetic field B = 7.5-23.5 T, as shown in the Figure. Complex B-T phase diagram for delta-Mn3(PO4)2 is shown in the inset to the Figure. The first-principles calculations define the main paths of superexchange interaction between Mn spins in these polymorphs. The spin model for alpha-phase is found to



be characterized by collection of uniform and alternating chains, which are coupled in all three directions. The strongest magnetic exchange interaction in gamma-phase emphasizes the trimer units, which make chains that are in turn weakly coupled to each other. The spin model of beta'-phase turns out to be more complex compared to alpha- or gamma-phase. It shows complex chain

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#### Biography

Olga Maximova received PhD in physics from Moscow State University in 2015. At the moment she is working as a researcher at Low temperature physics and superconductivity department of Moscow State University. Her research interests are focused on the field of low dimensional magnetic system.



## Session 2: Energy and Environment Materials

## Comparison of structural stability of $\beta$ silcon carbide and thoria

#### B. Szpunar<sup>\*</sup>, J.A. Szpunarb

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#### Abstract

The good mechanical, thermal, and chemical properties of SiC such as high stiffness, high hardness, high mechanical strength at high temperature, high thermal conductivity and melting point make SiC a candidate for various applications in nuclear industries. On the other hand thoria based fuel has been considered as an alternative fuel, since it does not oxidises and has high melting point

and higher thermal conductivity than traditionally used urania. Many factors need to be investigated before alternative nuclear fuel can be adapted to the service in the harsh environment in the nuclear reactor. In this work we evaluated the effect of temperature on the structural stability of SiC and ThO2. We use first-principles molecular dynamics as implemented in CASTEP Density Functional code, since for example, as reviewed previously, each of the available potentials of SiC for classical molecular dynamics has some deficiencies. Therefore although our calculations, are limited to 64 atoms for  $\beta$  SiC and 96 atoms for ThO2, with periodic boundary conditions they provide important information about the structural stability over a wide range of temperatures up to 3000 K. We evaluated mean square displacement of atoms and found that SiC covalent structure is very stable up to 3000 K temperature and in contrast to urania or thoria, no sub-lattice premelting was observed.

#### Biography

Dr Barbara Szpunar's current research interests are: First principles, predictive simulations of properties of accident tolerant and recycled nuclear fuels; Multidisciplinary studies of reactor safety and accidents in nuclear reactors and artificial transmutation. She has ~200 publications and over 60 AECL technical documents. She has been visiting many international universities and laboratories, and after working for over seven years at Atomic Energy Canada Limited, where she pursued her interest in the simulations of nuclear accidents she moved to the University of Saskatchewan in Canada. She introduced there an innovative course, based on simulations and became interested in experiential learning.



# Molecular modeling of stability and emission properties of halide perovskites

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#### Abstract

Recently, organic-inorganic lead halide perovskites nanocrystals become one of key materials of solar cell application and emission diode. The electronic structure and structural stability of these materials significantly depends on its chemical composition. Therefore, the optimal emission properties and desirable durability of the halide perovskites can be controlled by varying the chemical composition. In this study, using density functional theory (DFT) and molecular dynamics, theoretically investigation of a crystal structure and electronic structure of the partially substituted cubic  $MA_{0.5} X_{0.5} PbI_3 (MA = CH_3NH_3^+, X = NH_4^+ \text{ or } (NH_2)_2CH^+ \text{ or } Cs^+)$  will be presented. Our calculation results indicate that a partial substitution of A position ions of MA by other ions induces a lattice distortion, resulting in changing the electronic structures. Their bandgaps slightly decrease compared to that of MAPbI\_3. Our results mean that partial substitution in halide perovskite is effective to induce the structural distortion of arrangement of octahedral structure, which resulting in the changing ion diffusion rate as well as emission properties. The detailed ionic diffusion properties, which is related to the stability of materials, and emission properties of various kind of chemical composition of halide perovskites will be reported.

#### Biography

Dr. Hiromitsu Takaba was completed his Ph.D. from Tohoku University in Japan at 1998. After working in The University of Tokyo as Research Associate, and Tohoku University as Associate Professor, he becomes Professor at the current university from 2014. He has published more than 170 papers and was awarded from Japanese membrane society in 2006.



# Enhancement of redox mediator effect at air electrode for rechargeable Li-O2 batteries

#### Morihiro Saito\*

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#### Abstract

As increasing electric vehicles, next-generation battery systems instead of the conventional Li-ion batteries (LIB) has been much expected in recent years. Li-air batteries (LABs) is one of the candidates because of the high energy density over 5 times larger than LIBs. However, before the commercialization, there still remain some serious problems to be solved, i.e. Li dendrite growth at Li metal anode, large overpotentail due to Li2O2 decomposition at air electrode during charge process in glyme-based electrolytes, etc. Especially, the latter was reported to be able to solved by using redox mediators (RMs) such as both inorganic (LiI, LiBr, LiNO3)

and organic (2,2,6,6-tetramethyl-piperidinyloxyl (TEMPO)) ones. While many researchers focused on the kinds of RMs, and investigation on the RM effect mechanism was not sufficient for clear understanding the RM function. Recently, we have investigated the environment to enhance the RM effect by controlling the electrolyte viscosity and dissociation of RM, i.e. Li salts, in the electrolyte using mixed solvent systems and operating temperature of LABs, and suggested the importance of diffusivity for free RM species in electrolytes. Namely, the RM effect can be efficiently enhanced by providing the comfortable conditions for RMs. In this study, we will demonstrate the importance of diffusivity control for RMs parallelly using a pulsed gradient spin-echo (PGSE)-NMR method, and point out the problem related to shuttle effect. Also, an excellent way to both more enhance the RM effect and suppress the shuttle effect will be introduced in the conference.

#### Biography

Dr. Morihiro Saito (Ph.D.-engineering) is an Associate Professor of Department of Materials and Life Science in Seikei Univ. He received Ph.D. in 2003 from Graduate School of Science and Engineering, Tokyo Institute of Technology. He has worked on electrochemical energy storage and coversion systems at National Institute of Advanced Industrial Science and Technology (AIST) (2003-2005), Tokyo Univ. of Science (2005-2009), Doshisha Univ. (2009-2012), Tokyo Univ. of Agriculture & Technology (2013-2019) and Seikei Univ. (2019-present). His research interests are materials science for Li-ion batteries, fuel cells and LAB system. He has authored 80 peerreviewed papers, 5 book chapters and 7 patents.



## Nanofabrication processes for catalysts on nano-silicon materials for energy conversion devices

#### Ahmed Farid Halima\*, Douglas Robert MacFarlane<sup>a</sup>

<sup>a</sup>ARC Centre of Excellence for Electromaterials Science, School of Chemistry, Monash University, Victoria 3800, Australia

#### Abstract

Realizing a green economy envisages solar-to-fuel (STF) conversion as the promising pathway for reliable energy storage and utilization. To facilitate this, efficient catalysts are optimized for nanostructured semiconductors towards highly performing devices. Silicon is regarded an advantageous photoelectrode support for a range of fuel reactions, provided enhancement to its chemical stability. One challenge prevails for nanostructured Silicon-based devices; to identify scalable and reliable chemical fabrication methods, especially for noble or earth-abundant metal catalysts (such as Pt, Pd, Au, Ag, Cu) for respective/simultaneous photocatalysis of Hydrogen or Carbon Dioxide. The work presented herein demonstrates detailed investigations for cost-effective, reliable and scalable nanofabrication processes, and display device functionality/efficiency characterization in STF conversion.

#### **Biography**

Dr Ahmed Farid Halima is a passionate materials scientist with expertise in advanced functional nanomaterials for energy, quantum and biomedical technologies. He was awarded his PhD in Physical Chemistry from Monash University for innovation in energy photocatalysis, and MSc in Quantum and Materials Physics from the University of Melbourne while benchmarking diamond nanomaterials for neural interfaces. He contributed to cutting-edge science with the ARC Centre of Excellence for Electromaterials Science and Bionic Vision Australia. He is interested in innovative research to solve grand challenges such as energy and quantum topological materials through prospective postdoctoral opportunities.



## Guest Li+ ion conductors based on NaI-NaBH4 and their potential use for all-solid-state batteries

#### Reona Miyazaki<sup>a</sup>, Yasuto Noda<sup>b</sup>, Isao Sakaguchi<sup>c</sup>, and Takehiko Hihara<sup>a</sup>

<sup>a</sup>Department of Physical Science and Engineering, Graduate School of Engineering, Nagoya Institute of Technology, Gokiso-cho, Showa, Nagoya 466-8555, Japan

<sup>b</sup>Division of Chemistry, Graduate School of Science, Kyoto University, Kitashirakawa-Oiwakecho, Sakyo, Kyoto 606-8502, Japan <sup>c</sup>National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

#### Abstract

The conduction ions in the solid electrolytes can be divided into two types; the host ions and the guest ions. Solid electrolytes for the all-solid-state lithium ion batteries have been mainly developed based on the host Li<sup>+</sup> ion conductors where Li compounds have been the material candidates. On the other hand, our group has been focused on the guest Li<sup>+</sup> ion conduction in the "Li-free" compounds

in which the small doped guest Li<sup>+</sup> ions play a major role for the total ionic conduction. We have reported that NaI, NaBr and KI form the solid solution with  $\text{LiBH}_4$  (6 mol%) and become the guest Li<sup>+</sup> ion conductors [For example Miyazaki et al., 2016]. Furthermore, the contribution of the host Na<sup>+</sup> ions in NaI-LiBH<sub>4</sub> systems was proven to be quite small [Miyazaki et al., 2018]. One thing should be emphasized here is that the mobility of the guest Li<sup>+</sup> ions in NaI is higher than that of host Li<sup>+</sup> ions in LiI. This result strongly suggests that solid electrolytes are not restricted to the Li compounds but other Li-free compounds have the potential to become a novel solid electrolyte.

In this presentation, we will show the fabrication process of the solid solution of NaI-NaBH<sub>4</sub>-LiI systems. Subsequently, the guest Li<sup>+</sup> conduction properties in NaI-NaBH<sub>4</sub> systems are presented. Finally, we will demonstrate that the guest Li<sup>+</sup> conductors well work as the solid electrolytes for all-solid-state batteries.

#### Biography

Dr. Reona Miyazaki has been graduated from Graduate School of Engineering (Tohoku University, Japan) as a Doctor of engineering with the specialties including solid state ionics and battery materials at 2013. He obtained his post-graduation from Tohoku University with subject titled "Fabrication of Li fluoride and hydride compounds and their ion conduction properties" and then started the research of high capacity anode materials for all-solid-state lithium batteries at National Institute for Materials Science (NIMS, Japan) from 2013 to 2015. Presently he has been working at Nagoya Institute of Technology, Nagoya City. His hobbies are playing Violin and Sumo watching.



## Nanomaterials for energy conversion and storage

#### Nasir Mahmood

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#### Abstract

The renewable energy systems are playing major roles in transforming our lifestyle with almost zero  $CO_2$  emissions, where their efficiencies are mainly controlled by the electrodes used. Such electrodes use rationally tuned nanomaterials with rich surface chemistries and unique electronic structures which are technologically intriguing and are potential candidates for renewable energy. The nanostructuring and tuning of chemistry at a molecular level of electrode/catalyst materials may introduce a new concept of energy storage and conversion and give birth to advanced technologies in next generation devices that have the ability to touch the theoretical prediction of electrochemical energy conversion and storage and deliver electrical energy rapidly and efficiently.

Here, we have developed several nanostructured materials like carbonaceous and transition meta oxides, sulphides, phosphides as well as their hybrids through wet chemistry and physical methods to explain the structural fundamentals at the atomic level thickness with rationally tuned surface chemistry introduced through defective structures and/or unsatisfied surface atoms. We further studied how the catalytic activities/electrode capacities of various materials can be enhanced by tuning their aforementioned-features. We have found very exciting results by achieving highly stable performances for batteries up to 5000 cycles and current densities up to 350 mA/cm<sup>2</sup> required for the commercialization of water electrolysis at extremely low overpotentials. Recently, we also found that by developing 2D heterostructures with the genuine features of unilamellar sheets of two different materials will be very exciting, which can revolutionize various technological fields, especially the energy sector.

#### Biography

Dr Nasir Mahmood, is a Vice-Chancellor Fellow at School of Engineering, RMIT University, obtained his PhD (with distinction) in Materials Science and Engineering from Peking University, China in 2015. His early career began at the University of Wollongong, Australia (2015-16) followed by a research fellow position at Tianjin University, China (2016-17). He co-founded a Center of Micro-Nano Functional Materials and Devices, University of Electronic Science and Technology of China in Sichuan. Nasir's research interests include the chemical design of nanomaterials for electronics, catalysis, energy conversion and storage, sensors, microwave absorption, wastewater treatment and biomedical applications. Nasir's team has also begun work on developing 2D heterostructures to harvest both nanoscale and microscale features in one structure, boosting surface reactions for catalytic water-splitting, supercapacitors and batteries.



## Heterostructued titanium dioxide photocatalyst

#### Chiaki Terashima<sup>a,b,c,\*</sup>, Mao Sasaki<sup>a,b</sup>, Shoki Suzuki<sup>a,b</sup> and Akira Fujishima<sup>a</sup>

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#### Abstract

Titanium dioxide  $(TiO_2)$  has been widely investigated as photocatalyst because of its environmentally and economically advantages with high chemical stability, earth abundant and bio compatible properties. However, its large band-gap for the activity to only UV light region, and the high recombination rate of photogenerated electron and hole pairs have to be overcome to utilize effectively sunlight, and to enhance the photocatalytic performance. Recent enormous efforts to overcome the above-mentioned drawbacks have resulted in the one-dimensional  $TiO_2$  nanotubes, nanofibers and nanorods to suppress the carrier recombination, and/or the heterojunction structure of  $TiO_2$  with another semiconductor to achieve larger separation of the photogenerated electron and hole, as well as the modification of  $TiO_2$  nanoparticles with gold clusters to expand the light conversion from UV to visible and nearinfrared region. Another interesting approach on black  $TiO_2$  nanoparticles succeeded in narrowing the band gap of pure white  $TiO_2$ nanoparticles (X. Chen, et al., Science, 11 (2011) 746). The present study focused to treat pristine  $TiO_2$  nanoparticles by the discharge in water-based solution, which is named as solution plasma, follow to make heterostructured  $TiO_2$ , and to investigate the material properties as well as the photocatalytic activities for decomposing organics.

#### **Biography**

Dr. Chiaki Terashima received his Ph.D. degree (2003) in Electrochemical Analysis from the University of Tokyo under the supervision of Profs. Akira Fujishima and Kazuhito Hashimoto. His academic career started at Nagoya University as an Associate Professor (2010–2011) in Prof. O. Takai's group, and then moved to Tokyo University of Science in 2012. He is currently a Professor at the Photocatalysis International Research Center, Tokyo University of Science. His research interests focus on photoelectrochemistry, diamond electrochemistry, and plasma processing in liquids.



## Nanocomposite catalysts for reduction of 4-nitrophenol

#### Piotr Cyganowski\*

Department of Polymer and Carbonaceous Materials, Faculty of Chemistry, Wroclaw University of Science and Technologu, Wybrzeze S. Wyspianskiego 27, 50-370 Wroclaw, Poland

#### Abstract

Among a number of organic pollutants, 4-nitrophenol (4-NP) is accounted as a major one. 4-NP has drawn much attention in recent years because it is not only characterized by increased discharge in water but also can originate from verous waste sources [1, 2]. Hence, finding an effective and stable catalysts allowing to reduce 4-NP under mild conditions is of greatest concern. Polymeric nanocomposite catalysts can address this issue. Within the present studies a new in-situ method for synthesis of polymeric nanocomposites (NCs) with nanoparticles (NPs) of Au, Pt and Pd is proposed. The approach involves synthesis of amino functionalized anion exchange resins followed by reduction-coupled adsorption of Au(III), Pt(VI), and Pd(II). The so-obtained nanomaterials were the employed in catalytic decomposition of 4-NP.

Based on the results, it may be concluded that the application of polymeric matrices characterized by less developed internal surface area allowed the amino functionalities to efficiently reduce and precipitate NPs within the polymeric network. Changes of pH of a solution combined with the analyzed FT-IR spectra allowed to link the redox reaction with amino functionalities, which character (as well as a number of nitrogen atoms they contain) influences characteristics of the obtained NPs. A nanocomposite catalyst with AuNPs and PdNPs stabilized on a functionality derived from 1-(2-aminoethyl)piperazine effectively reduced 4-NP to 4-aminophenol (4-AP).

[1] electronic document: https://www.epa.gov/sites/production/files/2016-09/documents/4-nitrophenol.pdf, access date: Jan 21st 2019.

[2] B, in: P.G. Urben (Ed.), Bretherick's Handbook of Reactive Chemical Hazards (Seventh Edition), Academic Press, Oxford, 2007, pp. 65-133.

#### Biography

Scientific interests of Dr Piotr Cyganowski focus on the design and synthesis of polymer adsorbents, as well as ion exchange and chelating resins, able to concentrate, recover and reduce valuable metals such as Au, Pt and Pd. Dr Piotr Cyganowski began his doctoral studies in the field of Chemical Technology working on the development of new polymeric materials for separation and recovery of noble metals from wasted electric and electronic equipment (WEEE). He obtained PhD degree in September 2017. Currently, he is an Assistant Professor at the Faculty of Chemistry of Wroclaw University of Science and Technology (Poland).



## Efficient down/up-conversion rare earth pair doped luminescent materials for Si-solar cell applications

#### C.K.Jayasankar

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#### Abstract

Ultraviolet/visible to near-infrared quantum cutting and photon conversion through up/down conversion mechanisms have been proven as promising tools to enhance the efficiency of many optical devices. Currently, the photon conversion by selection and combination of rare earth ( $RE^{3+}$ )/ytterbium ( $Yb^{3+}$ ) ion pairs doped materials are attracting the attention of researchers. Hence, our group has prepared a variety of glasses/glass-ceramics/nano-crysals doped with  $RE^{3+}/Yb^{3+}$  ions and characterized their excited state dynamics systematically and uniformly by using well known theoretical models. For example, in the case of  $Sm^{3+}/Yb^{3+}$  codoped tellurite glasses, the energy transfer efficiency is found to be 41% which confirms that these glasses can be used as spectral convertors for the silicon solar cells. Similar results have also been obtained in  $Ho^{3+}/Yb^{3+}$  and  $Er^{3+}/Tm^{3+}$  co-doped tellurite glasses. On the other hand, different concentrations of  $RE^{3+}$ -doped calcium orthosilicate ( $Ca_2SiO_4$ ) phosphors have also been synthesized by the conventional high temperature solid-state reaction method from agricultural waste (egg shell and rice husk). It is observed that the luminescence phenomena involved in  $Ca_2SiO_4$  phosphors is due to cooperative energy transfer from  $Ce^{3+}$  to  $Yb^{3+}$  with an efficiency of 25 %. These results confirm that the  $RE^{3+}$  ion pairs doped materials can be a best choice as spectral converters for multi functional applications, in particular for Si-solar cells, which will be reviewed along with latest advances besides future scope in this challenging field.

#### Biography

Prof. Jayasankar has been graduated from Department of Physics, Sri Venkateswara University, Trupati-517502, India where he continues and at present works as a UGC-BSR Faculty Fellow. He has four decades of rich experience in lanthanide-doped optical quality glasses/nano-glass ceramics, phosphors and nanocrystalline materials for various applications like the development of lasers, optical fiber amplifiers, sensors, biolabels, W-LEDs and buried waveguides (Google-Citations:7950, h-index:52 and i10-index:178). A recent scientometrics analysis of rare earths research in India published in Current Science (110, 1184-7(2016)) lists Prof.Jayasankar as one of the most prolific Indian authors in the field of rare earths research in the order of z-index



# Two dimensional materials preparation and their properties of oxygen evolution reaction

#### Chuanbao Cao\*

Research Center of Materials Science, Beijing Institute of Technology : Beijing 100081, China

#### Abstract

Water splitting provides an appealing pathway for clean and sustainable energy conversion and storage. Therefore, development of a noble metal-free, efficient and robust electrocatalyst oxygen evolution reaction (OER) is still a great challenge. Herein, we introduced

to synthesize two dimensional nanostructure especially freestanding nanosheets materials such as  $Co(OH)_2$ ,  $Co_2O_3$ , CoS, CoP, FeNi et.al. We find that the planar sheet area was up to several micrometres and exhibited an ultrathin thickness (< 1 nm) with a mesoporousfeature. Hence, the highly exposed surface atoms afforded high electrochemical activity, whereas the ultrathin and mesoporous features facilitated charge and mass transfer along the 2D nanostructure to efficiently perform the surface dependent electrochemical reactions: HER, OER, and the overall water splitting. We demonstrate in situ surface substitution of the hydroxyl functional groups on the surface of  $Co(OH)_2$ . FeNi LDH et.al, and found that the in situ surface modification maintains the initial structure and morphology while increasing the areal density of active sites and reducing the energy barrier of



the OER. These results are embodied by the increase of the electrochemically active surface area (ECSA) and the lowering of the OER onset overpotential. We have found that several substitutes can enhance the properties. The mechanisms are also discussed. The findings provide a new way to improve the OER properties and extend their applications.

#### Biography

Dr. Chuanbao Cao is currently the Chair Professor of School of Materials Science and Engineering, Director of Research Center of Materials Science of Beijing Institute of Technology. He received B.S (1983) degree in Chemistry from Nanjing University, M.S(1989) and PhD (1992) degrees in Materials Science from University of Science and Technology of China. He was a postdoctoral fellow in Fudan University (1992-1994). In 1994, he joined Beijing Institute of Technology. His current research focuses on the low dimensional materials synthesis and their energy application, . Until now, he was granted more than 40 patents, authored more than 320 peer-reviewed papers, cited by more than 8100 times, H index 47.

## Session 3: Biomaterials and Medical Devices

## Hemoglobin-albumin cluster as red blood cell substitute

#### Teruyuki Komatsu\*

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#### Abstract

Hemoglobin (Hb)-based  $O_2$ -carriers of several kinds have been developed and evaluated as red blood cell (RBC) substitutes. Nevertheless, because of several concerns, none has been assigned yet for practical use. Recently, we have synthesized covalent coreshell structured protein cluster comprising Hb in the center and human serum albumins (HSA) at the periphery, Hb-HSA<sub>3</sub> cluster, as a novel  $O_2$ -carrier designed for RBC substitute (the product name: HemoAct<sup>™</sup>). The protein cluster was prepared by covalent linkage between surface Lys amino groups of Hb and Cys-34 residue of HSA using heterobifunctional cross-linker, N-succinimidyl 3-maleimido-propionate. The major product was isolated using anion exchange chromatography. The 3D reconstruction of Hb-HSA<sub>3</sub> based on cryo-TEM images revealed a complete triangular structure. The HemoAct<sup>™</sup> showed higher  $O_2$ -affinity ( $P_{50} = 9$  Torr) than the native Hb. Intravenous administration of HemoAct<sup>™</sup> into anesthetized rats did not elicit an unfavorable increase in systemic blood pressure by vasoconstriction. The half-life of <sup>125</sup>I-labeled HemoAct<sup>™</sup> in the blood circulation was markedly longer than that of HSA. These results suggest that the HemoAct<sup>™</sup> solution can be of great medical importance not only for alternative material of RBC transfusion, but also for  $O_2$ -providing therapeutic reagent in various clinical situations. Moreover, we have recently prepared recombinant canine serum albumin (rCSA) and feline serum albumin (rFSA) by yeast expression technique, and synthesized HbrCSA<sub>3</sub> and Hb-rFSA<sub>3</sub> clusters as RBC substitutes for dogs and cats.

#### Biography

Dr. Teruyuki Komatsu is Professor of Biomolecular Chemistry at Chuo University, Tokyo, Japan. He studied polymer chemistry at Waseda University, Tokyo, Japan, where he received his Ph.D. After post-doctoral work at Freie Universität Berlin, Germany, as a JSPS fellow for research abroad, he returned to Waseda University, where he was appointed as an Associate Professor until 2009. From 2006–2010, he held additional post of a PRESTO researcher of JST. His current research interest is synthesis of biofucntional micro/nanomaterials and their practical applications.



# Use of multivalent-type compounds for enhancement of biological affinities

#### Koji Matsuoka\*

Division of Material Science, Graduate School of Science and Engineering & Medical Innovation Research Unit (MiU), Advanced Institute of Innovative Technology (AIIT), Saitama University, Sakura, Saitama 338-8570, Japan

#### Abstract

Glycoproteins, glycolipids, and proteoglycans are known as glycoconjugates and these are generally existing on cell surfaces. In biological events, the glycoconjugates play roles not only as carriers of information in cell-cell interactions but as markers of cellular

differentiation, aging, malignant alteration, and so on. The oligosaccharide chains of glycoconjugates are, therefore, the third chains of biomacromolecules next to nucleic acids and proteins. Since the saccharide chains have highly complex structures, functions of the glycoconjugates were not completely investigated. Affinity of a monomeric saccharide chain against the appropriate protein, such as a carbohydrate-binding protein, a lectin and an enzyme, is not so high, usually in the mM range. In the 70's, Lee reported remarkable enhancement of the binding affinity by means of multivalent-type sugar substrates, so-called "sugar clustering effect".<sup>11</sup> The clustering effect has been expanded to other bioactive substances.<sup>21</sup> In this presentation, our recent progress on design, synthesis, and biological evaluation of our multivalent-type substances will be discussed.

Y.C. Lee, et al., J. Biol. Chem. 1983, 258, 199.
R. Hayama, et al., Molecules 2018, 23, 2875.

#### Biography

Dr. Koji Matsuoka is a Professor of Material Science, Graduate School of Science & Engineering, Saitama University (SU), Saitama, Japan. He received a Bachelor degree from Seikei University in 1990 and a Ph.D. from Hokkaido University (with Prof. S.-I. Nishimura) in 1995. He did his postdoctoral research at RIKEN, Saitama, Japan. He joined Department of Functional Materials Science, Faculty of Engineering, Saitama University in 1995 as an assistant professor, and was promoted an associate professor in 2001 and professor in 2011. He has published more than 100 research articles and book chapters in organic chemistry and polymer chemistry field.



## Tuning the size and composition of nanohydrogels using a "phantom monomer" for biological applications

#### Gerardo Byk and Sarin Palakkal

Bar Ilan University, dept. of Chemistry, 52900-Ramat Gan, Israel

#### Abstract

We have designed series of monodispersed nanohydrogels (NHG's) size raging from 20 nm to 400 nm, generated from mixtures of N-isopropylacrylamide, di-block (hydrophilic-hydrophobic) and tri-block (hydrophobic-hydrophilic-hydrophobic) copolymer acrylamide macro-monomer. When the monomers are mixed at high temperature they collapse into well-defined self-assemblies, which can be further polymerized leading to particles with sizes matching the intermediate self-assemblies. The size of the self-assemblies can be tuned/calibrated by combining different ratios of the starting monomers mixtures at high temperature<sup>1</sup>.

Herein, we defined the concept of "phantom monomers" which are the closest structure that mimic a selected monomer but lacks the active function for polymerization. The phantom monomer co formulated with the other monomers will be present in the intermediate self-assemblies due to their similarity with one of the active monomers, however, upon polymerization, different materials will be generated since the phantom will be excluded due to lack of reactivity. The comparative analyses of the classical systems (first generation) with those obtained with the phantom monomers (second generation) not only put in evidence the self-assembly mediated mechanism, but also prove the generation of new monodispersed NHG's. The second generation NHG's were found to be nontoxic based on the XTT assay. We have observed different loading and different phenotypes of the cells treated with the same amounts of DOX loaded into different NHG's or free as seen by confocal microscopy.

#### References

Khandadash, R.; Machtey, V.; Sheiner, I.; Gotilied, H.; Gothilf, A.; Ebenstein Y.; Weiss A. and Byk G. Journal of Nanoparticle Research (2014) 16(12), 1-18.

#### Biography

Gerardo Byk received his PhD (summa cum laude) at the Hebrew University of Jerusalem. In his PhD work, he developed a new generation of peptidomimetic molecules by the introduction of the new concept of backbone cyclization. Since August 1992, he has been in AVENTIS, where he was involved in the development of novel non-viral gene delivery complexes for gene therapy. He joined Bar Ilan University/Israel in 1999, was promoted to Associate Professor in 2002, where he is currently associated with the Marcus Center of Pharmaceutical Chemistry. His main scientific interests: peptide, peptidomimetics, combinatorial chemistry and gene therapy. Lastly, his group entered the field of nanotechnology with the design and development of biocompatible nanoparticles suited both for peptide synthesis, and for in vivo applications.

## Nanoparticle engineering towards highly efficient drug delivery systems and SERS-based bio-sensing

## Beatrice Fortuni<sup>\*a</sup>, Monica Ricci<sup>a</sup>, Tomoko Inose<sup>b</sup>, Indra Van Zundert<sup>a</sup>, Susana Rocha<sup>a</sup> and Hiroshi Uji-i<sup>a,b</sup>

<sup>a</sup>KU Leuven: Celestijnenlaal 200F/2404, Leuven, Belgium, 3001 <sup>b</sup>RIES Hokkaido University, N20W10 Kita-Ward Sapporo, Japan, 0010020

#### Abstract

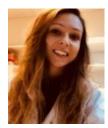
Most targeting strategies of anticancer drug delivery systems (DDSs) rely on the surface functionalization of nanocarriers with specific ligands for receptors, which are overexpressed in cancer cells. In such a way, DDSs are internalized via endocytosis, which implies their accumulation inside the acidic compartments (endosomes and lysosomes) and their eventual ejection by exocytosis. This endocytic process reduces the bioavailability of the drug in the intracellular environment, hindering the therapeutic efficiency at low drug dose. Here, we propose a simple method to functionalize DDSs with a polymeric bilayer of hyaluronic acid and polyethylenimine (PEI) which, besides providing targeting capability and controlled drug release, can induce the escape of the system from the undesirable endo-lysosomal cycle.

To advance the scientific knowledge on the controversial concept of PEI-induced endosomal escape and to boost the field of drug delivery, along with demonstrating a high therapeutic efficiency, we report a full in cellulo study of the intracellular route followed by our multifunctional DDS, from the cellular uptake to the drug release (Sci. Rep. 2019, 9, 2666, doi:10.1038/s41598-019-39107-3).

The in cellulo drug release experiments via fluorescence microscopy turned out to be extremely problematic due to the fluorescence quenching of the compound upon the intercalation between the DNA base-pairs in the nucleus. In order to investigate the drug cellular distribution and to further understand the action mechanism, we developed an alternative technique to fluorescence based on our previously reported work entitled "Live-Cell SERS Endoscopy Using Plasmonic Nanowire" (Adv. Mater. 2014, 26, 5124–5128).

#### Biography

Dr Fortuni completed her doctorate in chemistry at the KU Leuven in 2017, under the supervision of Prof. Uji-i. Her PhD was focused on nanoparticles engineering towards drug delivery and bio-sensing. After her graduation she got a postdoctoral fellowship of 3 years from the Research Foundation - Flanders (FWO), starting from October 2018. Her postdoctoral research is performed in the same group (KU Leuven) in collaboration with Prof. Kasai in Tohoku University (Japan).



# Photocontrollable adhesion: A bioinspired microstructured transport device

## Emre Kizilkan<sup>1</sup>, Jan Strueben<sup>2</sup>, Anne Staubitz<sup>2</sup>, Stanislav N. Gorb<sup>1</sup>

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<sup>2</sup>Otto-Diels-Institute for Organic Chemistry, Kiel University, Otto-Hahn-Platz 4, 24118 Kiel, Germany <sup>2</sup>Institute for Organic and Analytical Chemistry, University of Bremen, LeobenerStraße NW 2 C, 28359 Bremen, Germany <sup>2</sup>MAPEX Center for Materials and Processes, University of Bremen Bibliothekstraße 1, 28359 Bremen, Germany

#### Abstract

Highly dynamic attachment and detachment movements are crucial for the legged locomotion of numerous animal species in nature. It is well established that in this process a hierarchical surface topography plays the main role. For example, geckos have fibrillar setae which branch out into spatula-shaped nano-structures. This fibrillar hierarchical structure has a non-sticky default state which can be switched to the adhesive state through the action of the shear force using leg movements. Inspired by such stimuli-responsive adhesive systems in nature, we developed a bio-inspired photocontrollable microstructured material as a transport device. The material consists of three layers; i) mushroom-shaped adhesive microstructured surface made of polydimethylsiloxane (PDMS), ii) porous light responsive liquid crystal elastomer film and iii) a PDMS layer to seal the whole structure. Through ultraviolet (UV) light

illumination, the material experiences a switch from the adhesive state to the non-adhesive state. By varying the UV light intensity, the adhesive forces were able to accordingly be varied. Moreover, the three layered design allowed the material to recover its initial shape without any other illumination of light or thermal-stimulus. Finally, the material was demonstrated as a pick-up and drop-down device for transporting planar and 3D solid objects.



#### Biography

Dr. Emre Kizilkan's research involves photoresponsive polymers, bioinspired adhesives, and surface microstructuring. He is pursuing his research activities as PostDoc in Kiel University, Germany. Thanks to 2019 Micromachines Travel Award, he is able to present his work in this conference.

## Design of new metabolic platforms for in vitro diagnostics

#### Kun Qian

School of Biomedical Engineering, Shanghai Jiao Tong University

#### Abstract

Profiling and quantitation of small metabolites are essential for monitoring the physiological and pathological process in bio-systems and can lead to the set-up of new biomarkers benchmark. Despite that mass spectrometry (MS) enjoys huge application benefits over traditional methods, present MS approaches, particularly laser desorption/ionization (LDI) MS techniques, urgently need designed materials as efficient matrices and their LDI mechanism is still to be explored, in order to overcome the major limitations in terms of sensitivity, selectivity, throughput, accuracy, and practicability for metabolic diagnostics in clinical laboratory. In this talk, we show our recent progress on the design of inorganic particles as novel matrices for LDI MS analysis and their practical application in detection of small metabolites in bio-fluids for advanced metabolic diagnostics toward large-scale clinical use.

#### Reference

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- [3] Huang, L. et al. and Qian, K.\* Nature Communications 2017, 8, 220.
- [4] Wu, J. et al. and Qian, K.\* Advanced Functional Materials 2016, 26, 4016.

#### Biography

BS/MS at Fudan University, PhD at University of Queensland, Research Fellow at Stanford University. He is now a principle investigator (PI) at School of Biomedical Engineering, Shanghai Jiao Tong University. His research is focused on development and commercialization of ultra-sensitive and high-throughput bio-analytical methods and mass spectrometry techniques towards large-scale clinical use through design, synthesis, and engineering of materials and devices. He has co-authored over 50 peer-reviewed articles in top international journals. Dr. Qian has attracted grants from top research programs and received prestigious awards for research excellence. He held key patents and had strong connections with domestic/international industry partners.



## **Session 4: Advanced Functional Materials**

## Development of highly microstructure-controlled boron carbide neutron absorbers for fast reactors

#### Katsumi Yoshida<sup>a\*</sup>, Tohru S. Suzuki<sup>b</sup>, Koji Maeda<sup>c</sup>

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#### Abstract

Boron carbide ( $B_4C$ ) pellets have been used as neutron absorber materials in fast reactor system because they have low radioactivity after irradiation, excellent thermal stability and high neutron absorbability. During fast reactor operation, neutron irradiation causes cracking of  $B_4C$  pellets and fractured into pieces due to swelling, helium gas produced by (n, a) reaction and thermal stress. Finally cracks are caused in the cladding tube by the mechanical interaction induced by the swelling of  $B_4C$  pellets and relocation of  $B_4C$ fragments (absorber-cladding mechanical interaction (ACMI)). The ACMI limits the use period of control rods in fast reactors. Therefore high performance  $B_4C$  pellets for fast reactor system have been urgently required to extend the duration of the use of control rods and to enhance the safety for fast reactor operation. In our attempt to develop high performance  $B_4C$  ceramics with excellent mechanical and thermal properties, the authors have paid attention to controlling microstructure of  $B_4C$  ceramics with the addition of carbon nanotubes (CNTs). In addition highly-oriented pores were introduced in  $B_4C$  ceramics to release helium gas produced by (n, a) reaction.

In this study, the authors focused on two fabrication processes; normal slip casting and slip casting under strong magnetic field (12T), and microstructure-controlled  $B_4C$  ceramics with CNTs and highly-oriented pores was fabricated by these processes, and its mechanical and thermal properties were evaluated.

#### Biography

Dr. Katsumi Yoshida is an Associate Professor at Laboratory for Advanced Nuclear Energy, Institute of Innovative Research, Tokyo Institute of Technology (Tokyo Tech), Japan. He received Ph.D. in Engineering from Tokyo Tech in 2001. He was a research fellow of the Japan Society for the Promotion of Science (JSPS) from 2000 to 2001. He worked at Chiba Institute of Technology as a research associate from 2001 to 2004, and at National Institute of Advanced Industrial Science and Technology (AIST) as a researcher form 2004 to 2007. He moved to Tokyo Tech in 2007 and worked as an assistant professor. He has been in the current position from 2015.

## Reflection studies of barium lanthanum titanates in 8.2 to 12.4 GHz frequency range

#### Shalini Bahel\*, Ranjeet Singh, Mandeep Kaur, S. Bindra Narang

Department of Electronics Technology, Guru Nanak Dev University, Amritsar, India, 143005

#### Abstract

Pollution from electromagnetic (EM) radiation has increased many-folds due to recent development in wireless communication, microwave, and millimeter-wave electronic systems. This problem could be tackled by using effective EM wave shields with strong reflection or absorption from thin samples over a wide band of frequencies. In the present work, efficient microwave reflectors were synthesized and studied for their structural, dielectric and reflection properties in 8.2 to 12.4 GHz frequency range at room temperature. Barium Lanthanum Titanates with general formula  $Ba_{3-x}La_{4+1.5x}Ti_9O_{27}$ , x = 0.6 and 0.7 were synthesized using solid-state reaction technique by calcining at 1100°C and sintering at 1350°C for 2h in air. Both the studied solid solutions possess orthorhombic crystal structure with closely packed elongated grains and a high relative density (> 90%). Relative permittivity changed between 16.5 to 18.3 for composition x = 0.6 and between 15.5 to 17.6 for composition x = 0.7 in the studied frequency range. Similarly, loss tangent varied between 0.1744 to 0.8672 for composition x = 0.6 and between 0.2369 to 0.6242 for composition x = 0.7. A high reflection of around 98% was observed for composition x = 0.6 with a sample thickness of 3.6 mm from 8.6 GHz to 9.5 GHz. Composition x = 0.7 with thickness = 3.4 mm showed more than 95% reflection in almost entire studied frequency range (i.e. 8.6 GHz to 12.3 GHz). These ceramics are promising candidate for microwave reflectors in 8.2 GHz to 12.4 GHz frequency range.

#### Biography

Dr. Shalini Bahel Graduated from R.G.P.V., Bhopal (M.P.) with specialization in Electronics. Later on, she obtained her post-graduation from Maulana Azad National Institute of Technology, Bhopal (M.P.) in Digital Communication and then started working as Assistant Professor in the Department of Electronics Technology at Guru Nanak Dev University, Amritsar, where she has continued her research. Presently, she has been working on synthesis and characterization of low loss dielectric ceramic and their applications.



# Cold spray process for thick ceramic coatings

#### Motohiro Yamada<sup>\*</sup>a Noor irinah binti Omar<sup>a,b</sup>, Toibah Abd Rahim<sup>b</sup>, Kosei Fukudome<sup>a</sup>, Kodai Ogasawara<sup>a</sup>, Masahiro Fukumoto<sup>a</sup>

<sup>a</sup>Toyohashi University of Technology: 1-1, Tempaku, Toyohashi, Aichi, 441-8150, Japan <sup>b</sup>Universiti Teknikal Malaysia Melaka: 76100, Durian Tunggal, Melaka, Malaysia

#### Abstract

Cold spray has been developed as a high-quality coating process. In this process, feedstock particles are accelerated by a supersonic gas stream at a temperature that is lower than the melting point of the material, resulting in a coating formation from particles in a solid state. Therefore, this process can form pure metallic coatings without oxidation under an atmospheric ambient. On the other hand, it has been difficult to fabricate ceramic coatings through this process due to the lack of ductility. In this study, titanium dioxide

a wide range of photocatalytic applications. In order to understand the bonding mechanism of solid ceramic particles, the structure of feedstock particles was carefully observed and the effect of substrate materials was examined. The observation result revealed the importance of the unique applemented structure of the feedstock particles. The applemented particle enabled

(TiO<sub>2</sub>) ceramic particles are deposited on several substrate materials and fabricated thick coatings, making this approach suitable for

importance of the unique agglomerated structure of the feedstock particles. The agglomerated particle enabled to deposit on the substrate as the deformation like behavior. The substrate materials also had an important role for the adhesion strength of the coatings. The hardness, surface oxide, and temperature affected the adhesion strength. Concludingly, the formation mechanisms of cold sprayed  $TiO_2$  coatings were investigated and the importance of feedstock powder structure and the substrate properties were described.

## Biography

Dr. Yamada received his PhD degree in Engineering, in 2006 from Toyohashi University of Technology, Japan. He worked as Research Associate in same university just after his graduation. He is currently Assistant Professor at the Department of Mechanical Engineering in Toyohashi University of Technology. His principal interests are ceramic coating processes using thermal spray and cold spray.

# Stimuli responsive and molecularly imprinted polymers for phthalates removal

## Joanna Wolska<sup>\*</sup>, Katarzyna Smolińska-Kempisty, Marek Bryjak

<sup>a</sup>Wroclaw University of Science and Technology: Poland, Wybrzeze Wyspianskiego 27, Wroclaw 50-370

## Abstract

There is a great number of chemicals that are used in industry, agriculture and by customers every day and that can be released to water. For over 20 years, many reports have shown the presence of new compounds, called "emerging pollutants", in aquatic environments. They are new chemicals without regulatory status and whose effects on environment and human heath are still unknown. To this group are included chemicals called "endocrine disruptors" (EDs) that perturb the endocrine system either by acting as agonists or antagonists to sex hormone receptors, thus mimicking or preventing the action of endogenous estrogens and androgens. Many classes of chemicals including phthalates, dioxins, reveal the ability to interfere with hormonal system. The presented studies were focused on preparation of molecularly imprinted polymers (MIPs) for selective recognizing ED, such as phthalates. They were focused on the application of pH-responsive molecularly imprinted polymers in the adsorption–membrane filtration process (AMF) for DEP removal from aqueous solutions. The goal of this study was to determine the optimum parameters that govern the efficiency of AMF process. During the research the sorption and desorption properties of the synthesized pH-responsive polymers were also evaluated. The investigated MIPs revealed pH-sensitivity, as the greatest affinity towards phthalates was observed at pH 5, while the greatest pHdriven desorption was noted at pH 8.

## Biography

Dr. Joanna Wolska is the working at Wroclaw University of Science and Technology. She has published 29 papers on the subject of polymeric resins, sorbents for boron removal, MIPs, smart structures, biomimmetic polymers, hybrid processes. After graduating from Wroclaw University of Science and Technology in 2003 she has begun Ph.D. studies at this University. During this time she was working with synthesis of sorbents for boron removal from wastewaters obtaining Ph.D. in 2008. She continue her work at Wroclaw University of Science and Technology, she is working with MIPs and smart polymers and try to obtained sensors for "Endocrine disruptors".



# Engineered woods based on rice straw: Structure, properties and uses

Nattakan Soykeabkaew\*, Manunchaya Kerdporn, Sakaowduen Preampree, Kadsaraporn Wonghankul, Uraiwan Intatha, Nattaya Tawichai, Kitiphong Khongphinitbunjong

Center of Innovative Materials for Sustainability (iMatS), School of Science, Mae Fah Luang University, Chiang Rai, Thailand 57100

## Abstract

Agricultural residues including rice straw are constantly a matter of attention due to their availability, abundance, and most important problem in waste management. In this research, rice straw was utilized to produce biocomposite materials with two thermosetting polymer matrices (unsaturated polyester and epoxy). The rice straw based biocomposites were prepared by using a compression molding technique. The effects of rice straw pretreatment, fiber size, fiber and pore volume fraction on the biocomposites were



studied. The biocomposites' structure, physical and mechanical properties, water resistance, and flammability were then characterized and tested.

For the specific uses (bee nucs and furniture), the structure of these biocomposite materials were designed, then shaped and fabricated into the prototypes. With high density structure (1.3 g/cm<sup>3</sup>) and water resistant surface after molded, the biocomposite panels were assembled into bee nucs and tested. It was found that this rice straw based bee nuc was more durable and could better control an inside humidity and temperature as compared to a typical wooden one. However, for larger and thicker products such as tables and chairs, the biocomposite panel was engineered into a light-weight sandwich structure with density lowered to 0.6-0.7 g/cm<sup>3</sup> which was in the same range with real woods. It was found that the skin and core thickness ratio significantly influenced the mode of failure and mechanical properties of this biocomposite sandwich panels. According to the American

National Standards Institute (ANSI), the current sandwich structures exceeded the requirement for wood particleboards exhibiting high strength and high water resistance



#### Biography

Dr. Nattakan Soykeabkaew is an Assistant Professor of Materials Science at Mae Fah Luang University, Chiang Rai, Thailand. Her research of interest is in the fields of Eco-Materials, Wastes Utilization and Nanocomposites, which focus mainly on the extraction, treatment, and modification of applicable raw materials from biomass as well as processing, structure, properties, and applications of its potential products. The materials of interest include: 1) agricultural wastes, 2) bio-based materials, 3) cellulose nanocomposites. Assist. Prof. Soykeabkaew received her D.Phil. (Materials Science and Engineering) from Queen Mary, University of London, UK in 2007.

## Improving molded pulp products from agro wastes via blending approach

#### Nattaya Tawichai\*, Phattharasaya Rattanawongkun, Uraiwan Intatha, Nattakan Soykeabkaew

Center of Innovative Materials for Sustainability (iMatS), School of Science, Mae Fah Luang University, Chiang Rai, Thailand 57100

#### Abstract

Due to the shortage of raw materials and cost increment in molded pulp industry, agro residues such as rice straw (RS), pineapple leaf (PL), and banana stem (BS) have been considered as an alternative sustainable resource for pulp. In this work, the molded sheets from RS, PL and BS pulps were prepared by compression molding and their physical and mechanical properties were then evaluated. The results showed that the paper sheet made from BS pulp had the lowest strength (19 MPa); while the samples made from PL and RS pulps exhibited the higher strength (52 and 57 MPa, respectively). To reach a good quality or improve performance a weak product, the concept of blending with stronger fibers was applied here to provide more fiber bonding and enhance strength of a final product. Thus, the molded sheets of BS pulp blended with 10 - 50% of PL or RS pulp were prepared. It was found that the blended paper qualities could significantly improve when increasing PL and RS contents. The tensile strength of the blended BS/PL and BS/ RS paper sheets were increased more than 60% compared to the unblended paper. From these results, the blending pulp concept was next conducted in the manufacturing line of the molded pulp factory (Chainart, Thailand). The PL and RS pulps (10-20%) were added into bagasse (BG) pulp and then formed into molded pulp containers. The mechanical properties, surface morphology, oil, and water resistance of the products were then investigated. The results revealed that the agro blended pulps offered much better strength and smoother surface than the BG pulp alone. This has confirmed the promising of blending pulp approach and thus, agro pulps can be utilized and possibly reduce the production cost in molded pulp manufacturing.



#### Biography

Dr. Nattaya Tawichai earned her Ph.D. in Materials Science from Chiang Mai University, Thailand (2012). She is now an Assistant Professor of Materials Science and Assistant director of Northern Science Park at Mae Fah Luang University, Chiang Rai, Thailand. She has long been engaged in teaching and researching on materials science. Her research of interests lie in Eco-Materials, Wastes Utilization and Biomass pellet, which focus mainly on the extraction, treatment, and modification of applicable raw materials from biomass as well as processing, structure, properties, and applications of its potential products.



## Theoretical assessment of wettability on silane coatings: From hydrophilic to hydrophobic

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<sup>1</sup>School of Physics and Electronic Engineering, Guangzhou University, Guangzhou, 510006, P. R. China <sup>2</sup>Advanced Institute of Engineering Science for Intelligent Manufacturing, Guangzhou University, Guangzhou, 510006, P. R. China <sup>3</sup>State Key Laboratory of Optoelectronic Materials and Technologies, School of Physics, Guangdong Province Key Laboratory of Display Material and Technology, Sun Yat-sen University, Guangzhou, 510275, P. R. China <sup>4</sup>School of Chemistry and Chemical Engineering, Guangzhou University, Guangzhou, 510006, P. R. China

#### Abstract

The potential distribution and work function of a graphene surface modified by various types of silanes are investigated by first principles quantum mechanical calculations to establish its surface hydrophobicity hierarchy. It is found that the work function relies on the electronegativity of atoms on silane. The localization feature of interaction between silane and the graphene surface is demonstrated by the electron density difference. The work function is demonstrated to be a critical quantity in understanding the surface polarizability and thereby the surface wetting properties. By performing contact angle measurements experimentally using water as the probe fluid, surfaces grafted with different silanes show hydrophobicity variation that is found to follow the reverse trend to that of the proposed surface polarizability obtained through the work function calculation. The work function-dependent contact angle can be fitted with a linear equation.

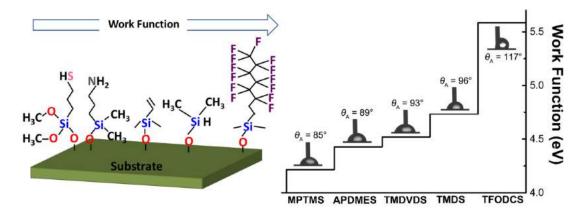


Figure. 1. Relationship between wettability and work function on silane coatings.

#### Reference

1 .H. Huang, W. Wang, and L. Wang, Phys. Chem. Chem. Phys. 21, 8257 (2019).

#### Biography

Haiming Huang received hisPh.D. degree onTheoretical Physics from Sun Yat-senUniversity in 2014. After 3 years working at National Supercomputer Center in Guangzhou, he joined Guangzhou University in May 2017. His current research interests includemodeling and simulation onelectronics and optoelectronicsoflow-dimensional carbon nano-materials, and surface wettability and adhesion from the micro-to nanometre scale, etc.



#### Chi Won Ahn<sup>1,2\*</sup>

<sup>1</sup>NNFC-Drexel-SMU FIRST Nano Co-op Center, National Nanofab Center, KAIST, Korea <sup>2</sup>Dept. Chemical and Biomolecular Eng., Korea Advanced Institute of Science and Technology, Korea

#### Abstract

Nano-fabrication and in-situ observation technologies of nano-structured materials are very important to control on the nano-scale phenomena associated with atomic movement, phase change, electrical or optical properties, and even reactions which take place in gas or liquid phases.

We have applied the in-situ observation technologies on 0D, 1D, and 2D nanomaterials, such as nano-pore, nano-cluster, nanowire, nanotube, graphene, and MXene et al. We have controlled various nanoscale interactions; formation of solid state nano-pores in the ultrathin graphene [1] or nano-gap thin  $Au/SiO_2$  substrate [2], phase changes in nanowire devices [3], direct observations of metal nano-droplets [4] and fusion of CNT [5], and new 2D materials on a freestanding graphene [6], and nano-structured electrode for energy and sensor applications [7] et al.

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## Biography

Dr. Chi Won Ahn is presently a director of FIRST Nano Co-op Global Research Center and group leader of Nano-Materials division, National Nanofab Center at KAIST and adjunct professor of KAIST.

He received his PhD.and M.S. in Materials Science and Engineering from Korea Advanced Institute of Science and Engineering (KAIST). He was with Advanced Materials Research Institute at KUN, Nijmegen, Netherlands, where he worked on nano-pattern induced self-assembly, scanning force microscope, and opto-magnetics. He was with Kavli Institute of Nanoscience, TU Delft in the Netherlands, where he worked on in-situ and cryo-observation by TEM, nano-fluidics, and nano-reactor for synthesis, assembly, and analysis of the nano-scale reactions of macromolecules and nano-materials.



His research interests include synthesis and analysis of nano-materials (graphene, Mxene, nano-pore, nano-fiber, nanowire, and nano-cluster et al.), and nano-structuring, applications to nano-patterning and nano-devices (for sensor, energy, environment) et al. He has published over 70 technical papers and is the holder of over 25 patents.

# Preparation of graphene based magnetic hybrids for dye removal application

## Ing Kong<sup>a\*</sup>, Zheng Yu Ng<sup>b</sup>

<sup>a</sup>School of Engineering and Mathematical Sciences, La Trobe University, Bendigo, Victoria 3552, Australia <sup>b</sup>Department of Mechanical, Materials and Manufacturing Engineering, The University of Nottingham Malaysia, Jalan Broga 43500

#### Semenyih, Selangor, Malaysia

#### Abstract

Graphene-based magnetic hybrids were synthesized through an in-situ co-precipitation method using expandable graphite and metal ions as raw materials. The hybrids were then characterized by using X-ray powder diffraction (XRD), field emission scanning electron microscopy (FESEM), vibrating sample magnetometer (VSM) and thermal gravimetric analysis (TGA) to study the microstructure, morphology, magnetic and thermal properties. The SEM micrograph showed that the magnetic nanoparticles were dispersed across the graphene sheets and the hybrids displayed magnetic properties (30.84 emu/g) which made them able to be retrieved out easily by an external magnetic field during the dye removal process. Malachite green (MG) and crystal violet (CV) were the two chosen dyes due to their widely-used applications in the modern industries (pen ink, leather treatment etc.). The dyes adsorption mechanism on the hybrid was justified by the adsorption kinetics. It was found that over 94% of MG and CV with 5 ppm concentration can be removed by a dosage of 30 mg hybrids within 3 h of experimental duration. Magnetite hybrid appeared to perform better than nickel-zinc ferrite hybrid across several experimental parameters (pH, dosage and time). Moreover, these hybrids can be regenerated after dye removal application completed just to restore back to its primary absorption capabilities again to be reused. Once the optimal operating conditions have been determined, this hybrid could turn out to have an easier separating ability and a cost effective along with promising regeneration method in removing the toxic dye particles present in waste water nowadays.

#### Biography

Dr Ing Kong is an Associate Professor in the Department of Engineering at La Trobe University. She received both her first degree and PhD in Materials Science from the National University of Malaysia in 2005 and 2009, respectively. She completed her Postgraduate Certificate in Higher Education (PGCHE) at University of Nottingham in 2015. Prior to joining La Trobe, she worked as a Postdoctoral Research Fellow for two years at National University of Malaysia (2009-2010) and RMIT University (2010-2011) and as an Associate Professor in the Department of Mechanical, Materials and Manufacturing Engineering at University of Nottingham from 2012 to 2017. Her research interests are in the development of advanced materials, particularly functional polymer composites, magnetic nanoparticles, carbon nanomaterials and superconductors.



# The potential of using gold nanoparticle-based assay for target molecule detection

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#### <sup>a</sup>Materials Science and Engineering Program

<sup>b</sup>Nanobiotechnology and Nanobiomaterials Research Laboratory (N-BMR), School of Materials Science and Innovation <sup>c</sup>Toxicology Graduate Program, Faculty of Science, Mahidol University, 272 Rama VI Road, Ratchathewi, Bangkok 10400, Thailand

#### Abstract

Due to an increase of dangerous molecules that can cause adverse health impacts, a rapid, precise, sensitive, and low cost assays are needed. Gold nanoparticles have shown a high potential to be used as a key part of diagnostic tool because of their unique optical property and friendly surface chemistry. Here, we have developed gold nanoparticle-based assay for detection of interest/ target molecules. We evaluated the possibility of using a mixed size of gold nanoparticles to see whether it can help increase detection sensitivity or provide any different colorimetric characteristics. The demonstration of using gold nanoparticles as a tool to detect foodborne pathogenic bacteria is also included. Lastly, the use of gold-based nanoshell for detection arsenic (III, V) will be demonstrated. We have found that gold nanoparticle-based assay could provide a high potential to be a diagnostic tool especially in point of care testing.

#### Biography

Assistant Professor Dakrong Pissuwan completed her PhD in Nanobiotechnology from University of Technology Sydney under supervision of Prof. Michael Cortie. Currently, she is a Principal Investigator of Nanobiotechnology and Nanobiomaterials Research Laboratory at Faculty of Science, Mahidol University. She was recently awarded for Australia-APEC Women in Research Fellowship in 2018 and received the latest competitive funding from Thailand Toray Science Foundation.



## Next-generation latent finger-mark detection using functionalised silicon oxide nanoparicles

## Lee P L T<sup>a</sup>, Kanodarwala F K<sup>b+</sup>, Moret S<sup>b</sup>, Spindler X<sup>b</sup>, Spikmans V<sup>a</sup>, Lennard C<sup>a</sup>, Roux C<sup>b</sup>

<sup>a</sup>Western Sydney University, School of Science and Health, Richmond, NSW 2753, Australia <sup>b</sup>University of Technology Sydney, Centre for Forensic Science, Broadway, NSW 2007, Australia

#### Abstract

Despite the reliability of routine latent fingermark development techniques in use by law enforcement agencies worldwide, a recent study indicated that conventional development methods struggle to detect some fingermarks that are present [1]. This is a major drawback with respect to latent fingermark detection using current techniques. Therefore, new and advanced methods are needed to assist law enforcement agencies.

There has been increased interest in using nanoparticles (NPs) for latent fingermark development. First, the small size of NPs permits high-resolution enhancement of fingermarks without the risk of over-development. Second, through surface functionalisation, various molecules can be grafted onto the surface of NPs to selectively strengthen interactions with fingermark residues. Finally, some NPs possess luminescence properties that are beneficial for substrates where background interference is problematic.

Silicon oxide nanoparticles (SiO<sub>2</sub> NPs) are one of a few NPs that possess all three of the aforementioned characteristics. Our recent publication thoroughly evaluated the application of functionalised SiO<sub>2</sub> NPs for latent fingermark detection; modification and optimisation of a set of previously published detection parameters were performed [2]. The improved performance of the technique indicates that SiO<sub>2</sub>-based NPs have the potential to become a breakthrough for latent fingermark detection.

This presentation aims to depict the most up-to-date application protocols and characterisations of functionalised  $SiO_2$  NPs for latent fingermark detection, together with potential new  $SiO_2$  NPs with altered surface functionalisation and optical properties. This research is part of an Australian Research Council funded project in collaboration with the Australian Federal Police, Victoria Police and Rofin Australia.

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#### Biography

Fehmida Kanodarwala is currently working as Postdoctoral Research Fellow at Centre for Forensic Science on the Australian Research Council (ARC) linkage project "Next-generation latent Fingermark detection using functional nanomaterials".

## Colossal reversible barocaloric effects in plastic crystals

Pol Lloveras<sup>a,\*</sup>, A. Aznar<sup>a</sup>, M. Barrio<sup>a</sup>, Ph. Negrier<sup>b</sup>, C. Popescu<sup>c</sup>, A. Planes<sup>d</sup>, L. Mañosa<sup>d</sup>, E. Stern-Taulats<sup>e</sup>, A. Avramenko<sup>e</sup>, N. D. Mathur<sup>e</sup>, X. Moya<sup>e</sup>, and J.-Ll. Tamarit<sup>a</sup>

<sup>a</sup>Grup de Caracterització de Materials, Departament de Física, EBE and Barcelona Research Center in Multiscale Science and Engineering, Universitat Politècnica de Catalunya, Eduard Maristany, 10-14, 08019 Barcelona, Catalonia, Spain <sup>b</sup>Université de Bordeaux, LOMA, UMR 5798, F-33400 Talence, France <sup>c</sup>CELLS-ALBA Synchrotron, E-08290 Cerdanyola del Vallès, Catalonia, Spain <sup>d</sup>Departament de Física de la Matèria Condensada, Facultat de Física, Universitat de Barcelona, Martí i Franquès 1, 08028 Barcelona, Catalonia, Spain <sup>e</sup>Department of Materials Science, University of Cambridge, Cambridge, CB3 0FS, UK

#### Abstract

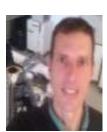
Pressure-driven liquid-vapor transition permits the exchange of latent heat using external work and is the basis for current refrigerators. However, these devices use massively hydrofluorocarbons with huge greenhouse potential, which poses a serious environmental problem. Alternatives based on solid-state first-order phase transitions that are sensitive to an external field such as



magnetic, electric or mechanic, have been explored but the magnitude of the latent heat associated with such transitions is usually much smaller compared to evaporation. We show that the pressure-driven caloric response (i.e. barocaloric effect) at phase transitions in plastic crystals is comparable to that in hydrofluorocarbons due to the emergence of molecular orientational disorder. We also identify the reversible range where barocaloric effects can be obtained upon cyclic application and removal of pressure as this is key for technological implementation. Our demonstration of colossal reversible barocaloric effects in plastic crystals should inspire the future development of environmentally-friendly solid-state barocaloric cooling devices.

#### Biography

Dr. Pol Lloveras obtained his Ph.D. in Condensed Matter Physics from the University of Barcelona (Spain) modeling studies on ferroelastic and magnetoestructural systems. After a first postdoc in the École Polytechnique he joined the Grup de Caracterització de Materials at the Universitat Politècnica de Catalunya (Spain) where he pressure-driven solid-state caloric effects for future eco-friendly cooling methods. He has also been Research University of Cambridge. Recently, he has analyzed the barocaloric response of a wide range of materials including ferroelectrics, superionic conductors and plastic crystals.



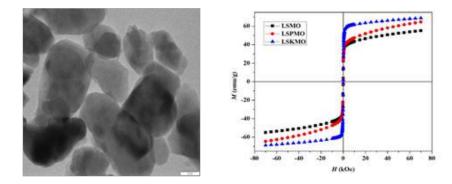
## Magnetic properties of LSMO, LSMKO and LSMPO superparamagnetic nanomaterials

#### Sunita Keshri\* and Sonali Biswas

Department of Physics, Birla Institute of Technology, Mesra, Ranchi-835215, Jharkhand, India

#### Abstract

Perovskite manganites with chemical formula (R: trivalent rare earth element and = alkaline earth) have been the subject of intense research in the last two decades because of their inherent potential to exhibit a wide variety of interesting physical properties which include colossal magnetoresistance (MR), magnetoimpedance (MI), half-metallicity, superparamagnetism and magnetocaloric properties. These properties open up several applications in the field of magnetic transducers, magnetic refrigerants and magnetic sensors. Superparamagnetic nanoparticles with large saturation magnetization and a Curie temperature above room temperature have potential for use in hyperthermia, MRI contrast enhancement and drug delivery applications. In the present paper, we have studied the magnetization, MR and MI of the optimally doped manganites, (LSMO),(LSKMO) and(LSPMO), synthesized by solgel method. The Rietveld refinement of the Xray diffraction data of these samples confirm their rhombohedral structure with space group whereas the grain size has been found to lie in the range of 3550 nm as estimated using high resolution transmission electron microscope (HRTEM). The HRTEM image of LSMO sample is shown in Figure 1(a). The room temperature magnetization as a function of the applied magnetic field is shown in Figure 1(b). The results indicate that the nanoparticles have superparamagnetic behavior with almost zero remanence and coercivity at room temperature and are of interest for biomedical applications. The theoretical study shows a good fit of these data with Langevin function.



#### Biography

Dr. Sunita Keshri is currently working as Professor and Head of the Department of Physics, Birla Institute of Technology, Mesra, Jharkhand, India. Her field of interest includes different types of functional materials, including colossal magnetoresistive materials, dielectric materials, semiconducting thin films, etc. Till now she has handled eight research projects including an Indo-Russian (DST-RFBR) bilateral project. So far, she has guided four PhD students; two more will submit their theses shortly. She has also guided several PG projects. Till the date she has published around fifty research papers in SCI indexed journals and forty eight communications in national or international conferences.



## Feature selection for machine learning of surface catalysts

#### Julia Melisande Fischer<sup>1</sup>, Michelle Hunter<sup>2</sup>, Marlies Hankel<sup>2</sup>, Debra Searles<sup>2,3</sup>, Amanda Parker<sup>1</sup>, Amanda Barnard<sup>1</sup>

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<sup>2</sup>Centre for Theoretical and Computational Molecular Science, Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, Brisbane, Queensland 4072, Australia

<sup>3</sup>School of Chemistry and Molecular Biosciences, The University of Queensland, Brisbane, Queensland 4072, Australia

#### Abstract

Most machine learning research on chemical systems study either materials, with periodic structures, or molecules. Often for surface catalysis, the relevant information is in-between both systems. For this study, our dataset contains molecules on different surface defects, namely catalytic active centres. These are N-doped graphene pores supporting one or two single metal atoms.

The binding energies (BE) is an indicator for the strength of the interaction of the molecule with the surface and is used as the label. The data includes around 1600 structures of molecules on various different active centres and their BE. The geometric data comprises of the 3-dimensional coordinates of all atoms in a periodic cell. The main problem is describing features which are meaningful for a wide number of structures, as different structures have different atom types, adsorbed species and number of atoms. Through different descriptions of the geometrical structure in the systems, we try to link the BE to essential geometric features.

## Understanding and predicting defective graphene-oxide structures using machine learning

#### Benyamin Motevalli, Amanda Barnard

#### Data61, Docklands, Australia

#### Abstract

Graphene is a two-dimensional sheet of carbon atoms discovered in 2004 by Nobel Prize winners Andre Geim and Konstantin Novoselov [1], which is the lightest, strongest, most electrically conductive substance on earth; exhibiting a range of unique and exceptional properties that will revolutionise everyday products [2]. Since its discovery more than 12,000 graphene related patents have been filed, with research continuing to grow rapidly across the public and private sectors [3]. Proposed graphene applications include real-time sensing of changes in stress, temperature, moisture and the concentration of gases (including toxins). However, after well over a decade of intense research and development graphene products are still almost non-existent, because the level of control exercised in laboratories cannot be delivered at scale [4]. To better understand the challenges, computational material science and machine learning are ideal for characterising atomic-scale structure-property relationships of graphene oxides (GOs) [5]. To date, most available studies are limited to few cases of specific topologies, sizes, and oxygen concentrations.

Here, we use 20,396 virtual experiments developed using electronic structure simulations. To characterize the virtual samples, 829 features were extracted via a range of post-processing techniques, from which 223 were identified to effectively describe GO. These include details descriptions of defects, which are known to impact performance. Using defects as labels for machine-learning we were able to determine which structural features are important in defining defective GO, as well as predicting how the level of defects is related to the oxygen concentration.

A classification model was selected to separate defective structures from non-defective structures, using a grid-search to optimize the hyper-parameters and improve precision and recall. This model isolated the parameters responsible for defects formation. Thereafter, a regression model was fitted to predict defect concentration from the feature set, following a similar grid-search. The regression model was able to predict the defect concentration of the GO samples with an accuracy of higher than 94%, and identify what gives rise to defects, and how they can be enhanced or suppressed.

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#### **Biography:**

Dr. Benyamin Motevalli is a Postdoctoral Fellow at Data61. He has years of experience in developing/employing computational and numerical analysis techniques to establish fundamental understanding of novel intelligent nanomaterials. His current research focuses on rational design of materials through innovative data-driven models that offer the advantage of fusing complex experimental and computational data for a higher-level understanding of structure-processing-property relationships. He is also highly interested in developing professional software packages capable of providing analytics for decision support in industry.



# Session 5: Materials Chemistry

# Advanced phase characterization of novel prospective materials for NLO hydrogen-bonded salts and cocrystals of heteroaromatic bases

#### Ivan Němec<sup>a,\*</sup>, Irena Matulková<sup>a</sup>, Róbert Gyepes<sup>a</sup>, Matouš Kloda<sup>a</sup>, Ivana Císařová<sup>a</sup>

<sup>a</sup>Charles University, Faculty of Science, Department of Inorganic Chemistry, Hlavova 8, Prague 2, CZ 128 40, Czech Republic

#### Abstract

The hydrogen-bonded salts and cocrystal of nitrogen-containing heteroaromatic bases are forming a very promising family of novel materials for nonlinear optics (NLO). Their NLO properties can be utilized in several technical applications ranging from harmonic generations and optical limiting processes to stimulated light scattering. A very actual utilization of these molecular crystals is based on stimulated Raman scattering (SRS). This third-order NLO phenomenon was recently used for the development of compact and efficient frequency converters of the one-micron laser emission based on neodymium or ytterbium lasants.<sup>1</sup>

The title materials are based on properly arranged organic molecules (carriers of NLO properties) interacting with selected inorganic or organic anions/molecules via the system of hydrogen bonds, which positively influences not only packing of the crystals but also their chemical and physical properties.

This contribution deals with phase characterization of selected representative examples of molecular crystals containing aminopyrimidines by the combination of experimental (i.e. IR and Raman spectroscopy, X-ray diffraction and calorimetric methods) and theoretical (solid state quantum-chemical calculations) approaches. Particular attention will be focused on combination of temperature-dependent vibrational spectroscopic and X-ray diffraction methods for phase characterization and monitoring of phase transformation. The mechanism of the observed solid state transformations will be discussed in detail.

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1. A.A. Kaminskii, Laser and Photonics Reviews 1 (2007) 93.

Acknowledgements: Financial support from the CUCAM project (project No. CZ.02.1.01/0.0/0.0/15\_003/ 0000417) is gratefully acknowledged.

#### Biography

Prof. Ivan Němec has been graduated from Faculty of Science, Charles University, Prague as M.Sc., with the Inorganic Chemistry specialty. Later on he obtained his post-graduation from Faculty of Science, Charles University with subject Inorganic Chemistry and then started working at the Department of Inorganic Chemistry, Faculty of Science, Charles University where he has continued his research. Presently he has been working at the same department as professor and leading the Solid-State and Material Chemistry Group.



# Material design of porous coordination polymer for high performance adsorbent of NH3 and NH4+

## Tohru Kawamoto<sup>\*</sup>, Akira Takahashi, Durga Parajuli, Kimitaka Minami, Tohru Nakamura, and Hisashi Tanaka

National Institute of Advanced Industrial Science and Technology (AIST), 1-1-1 Umezono, Tsukuba 305-8565, Japan

#### Abstract

Ammonia is one of the chemical materials that are the most highly produced in the world, produced about the 180 million tons in a year. The major use of ammonia is for fertilizer, implying the release of the tremendous amount of chemicals into the environment. As the result, various prolusion issues occur such as eutrophication and PM2.5. To solve the issues, the recovery of the ammonia from the environment, both atmosphere and water, is quite important.

We developed a new adsorbent of ammonia in atmosphere and ammonium in water. Its adsorption capacity of ammonia is the highest among the porous materials. In addition, the adsorbent can be recycled only by washing with water, acid, or salty solutions. The adsorbent was developed with the optimization crystal structure of Prussian blue, a porous coordination polymer used as a blue pigment invented in 18th century. Prussian blue has a sub-nm scale porous network in its crystal, suitable for small molecules. In addition, we can implement the vacancies of hexacyanoferrate ions in wide range to control the amount of the of alkali cations used for the ion-exchange reaction, and that of the open-metal sites for the coordinating adsorption. In this talk, the concept of the materials design, typical performance as the adsorbent, and the examples for application are discussed.

#### Biography

Dr. Tohru Kawamoto has been graduated from Osaka university as PhD. He worked in AIST from 1997, and became a research group leader on 2010. The main research theme is the material chemistry for porous coordination polymers and the development of their application such as adsorbent for toxic materials, and electrochromic devices. Presently he is working at the Tsukuba City in Japan.



## Temperature dependent crystal structure of LaSr3Fe3O10 with intercalated H2O and OH-

#### Isao Kagomiya\*, Yudai Wakita, Ikuya Matsue, Yutaro Yagi, Ken-ichi Kakimoto, Daijyu Matsumura<sup>b,</sup> Yasuhiro Yoneda<sup>b</sup>

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<sup>b</sup>Materials Sciences Research Center, Japan Atomic Energy Agency: Kouto 1-1-1, Sayo-cho, Sayo-gun, Hyougo, 679-5148, Japan

#### Abstract

Layered perovskite  $LaSr_{3}Fe_{3}O_{10}$  (LSF) shows an intercalation reaction that water and hydroxide are incorporated into the interlayers of the perovskite. Crystal structure of the intercalated LSF is different from that of LSF. The recent study reported that ion conductivity of the intercalated LSF was as large as that of Nafion, suggesting fast diffusion of OH<sup>-</sup> or H<sup>+</sup> in LSF. [1] However, the detailed diffusion behavior is still unclear. This study tries to investigate the crystal structure and the structure change resulting from H<sub>2</sub>O and OH<sup>-</sup> desorption. It is a key to clarify the diffusion behavior.

 $LaSr_{3}Fe_{3}O_{10}$  (LSF) was prepared by a solid state reaction. The obtained LSF was annealed at 600°C under reduced atmosphere. After annealing, the samples were leaved under ambient air for approximately two weeks. The crystal structure was investigated by x-ray powder diffraction (XRPD) and x-ray absorption fine structure (XAFS).

The XRPD pattern at 25°C for the LSF leaved under air after annealing showed that  $H_2O$  and  $OH^-$  were intercalated into LSF. The XRPD pattern at 150°C was different from that at 298 K, suggesting that the intercalated  $H_2O$  was removed during heating. From the XAFS for the intercalated LSF at 25°C, we found that Sr-O length was larger than that of La-O. With increasing temperature, Sr-O length decreases, whereas the La-O remains constant. The result suggest that the intercalated  $OH^-$  and  $H_2O$  is located near Sr. The  $H_2O$  and  $OH^-$  desorption short Sr-O length.

[1] T. Takeguchi et al., J. Am. Chem. Soc., 135 (2013) 11125-11130.

#### Biography

Dr. Isao Kagomiya has been graduated and then received Dr. of. Sci. degree (2002) from Waseda University, Tokyo, Japan, with the specialties including Condensed Matter Physics and Materials Science. After working as a post-doctoral researcher, he joined Nagoya Institute of Technology (NITech), Nagoya, Japan, as a research



associate in 2005. He is now an associate professor in the Department of Life Science and Applied Chemistry, NITech, where he has studies electro-ceramics and solid state ionics used for advanced energy materials.

## Insights into the activation of molecular oxygen for alcohol oxidation over Pd single-atom catalyst

#### Qinghao Shang, Nanfang Tang, Guoliang Xu, Chuntian Wu, Yu Cong\*

CAS Key Laboratory of Science and Technology on Applied Catalysis, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, China

#### Abstract

To efficiently activate molecular oxygen under mild reaction conditions is a critical challenge in aerobic oxidation of alcohols. Homogeneous organometallic catalysts are normally used owing to their defined coordination geometry, uniform metal active centers and ligands, but a major drawback exists in their separation from the products and recycling. Heterogeneous catalysts are easy to recycle and separate, but usually with low reactivity. Single-atom catalysts (SACs) have attracted great attention due to their theoretically 100% metal utilization, unique electronic properties, and excellent catalytic performances, since the concept was proposed by Zhang et al. in our laboratory in 2011. These special catalysts are considered as connecting bridges between homogeneous and heterogeneous catalysis. In this work, single-atom  $Pd/Al_2O_3$  catalysts were prepared by anchoring Pd on  $Al_2O_3$  rich in coordinatively unsaturated  $Al^{3+}$  sites. High conversions (>90%, 8 h) were obtained for the selectively aerobic oxidation of cinnamyl alcohol under mild conditions (80 °C, 1 atm). With the aid of XPS, XAS, and CO-DRIFT, we found that Pd atoms exhibit in partially positive electronic state. The operando ESR and in-situ Uv-vis spectra indicated that dioxygen was readily activated on single Pd atoms and the active oxygen species behaved chemically like singlet  $O_2$ . Hopefully, this research will provide potential inspiration for the design of highly active novel catalysts for aerobic oxidation reactions.

## Ceramic composites with zero-thermal-expansion property

#### Ikuo Yanase\*

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#### Abstract

Zero-thermal-expansion materials are important for various fields requiring high precision materials. Negative-thermal-expansion materials in a wide temperature range are effective for fabrication of zero-thermal-expansion materials when fabricating composites. In this study,  $Zr_2WP_2O_{12}$  (ZWP) and  $ZrV_{0.6}P_{1.4}O_7$  (ZVP) sintered bodies were fabricated and their linear thermal expansion coefficients (TEC) were investigated. Thermomechanical analysis confirmed that the TECs of ZWP and ZVP sintered bodies were found to be  $-2.92 \times 10^{-6} \, ^{\circ}C^{-1}$  and  $3.27 \times 10^{-6} \, ^{\circ}C^{-1}$  in the range of 25 to 500 °C, respectively. Sintered ZWP/ZVP composites with ZVP/ZWP volume ratios of 0.5/0.5, 0.53/0.47, 0.55/0.45, and 0.6/0.4 were fabricated to cancel out the negative thermal expansion of ZWP by the positive one of ZVP. ZVP/ZWP composites with various composition were sintered and the relative density of the composite was approximately 82% when fabricating at a ZVP/ZWP volume ratio of 0.53/0.47. Energy dispersive X-ray analysis

spectroscopy analysis clarified that the ZVP/ZWP composite mainly consisted of ZWP and ZVP grains. The ZVP/ZWP composite exhibited very low thermal expansion with a TEC was  $-0.29 \times 10^{-7}$  °C<sup>-1</sup> in the range of 25 to 500 °C.

#### Biography

Dr. Yanase has been graduated from Saitama University in Japan, and later on he obtained his post-graduation from National Research Institute of Science and Technology Agency in Japan and then started working at Saitama University where he has continued his research.

# Gelcasted solid-state-sintered SiC ceramic foams with excellent permeability

#### Haibo Wu<sup>\*</sup>, Zhengren Huang

*State Key Laboratory of High Performance Ceramics and Superfine Microstructure, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai 200050, China* 



#### Abstract

Pressureless solid-state-sintered SiC (S-SiC) foams possess the advantages of both S-SiC ceramics and cellular materials, including outstanding high-temperature strength, excellent chemical stability, high heat-exchange efficiency, large specific surface area, etc. These unique features enable them to withstand harsh physicochemical environments and have numerous potential applications in the energy and environment fields, such as catalyst supports, high-temperature filters for flue-gas, and volumetric absorbers of solar radiation. As a simple and representative preparation method, direct foaming-gelcasting process has been been widely applied for the production of various ceramic foams, and shows its simplicity and high efficiency in tailoring pore microstructures (porosity, pore size, etc). However, the gelcasted ceramic foams through single foaming mechanism normally displayed inferior connectivity between bubble-derived pores, because of the limited amount and size of windows in the struts of bubble-derived pores. Unfortunately, the connectivity between pores shows its extreme importance for the above-mentioned applications to supply fluid channels. In this study, we utilized direct foaming-gelcasting process to fabricate S-SiC ceramic foams, and another poring mechanism (solid poreforming agent or partial sintering) was also introduced to further improve the gas permeability. Moreover, rheological behaviors of slurries, microstructures, compressive strength, and gas permeability of sintered bulks were systematically

investigated, and the relationships between the microstructures and properties were revealed as well.

#### Biography

Dr. Haibo Wu has been graduated from Shanghai Institute of Ceramics, Chinese Academy of Sciences (SICCAS) as a doctor of materials science, with the specialties of high-performance structural ceramics. Later on he started working at State Key Laboratory of High Performance Ceramics and Superfine Microstructure in SICCAS where he has continued his research. Presently he has been working as associate professor at the Shanghai City in China.



# Recycled AA6111 Al alloys manufactured by melt conditioned direct chill casting and thermomechanical forming processes

## Isaac Chang, Dan Luo, Kawther Al-Helal, Jayesh B Patel, Yan Huang, Geoff Scamans, Zhongyun Fan

Brunel Centre for Advanced Solidification Technology (BCAST), Brunel University London, Uxbridge, UB8 3PH, UK

#### Abstract:

Recycling of scrap Al requires 5% of energy and saves 95% of CO2 emission as compared to the production of primary Al. Hence, there is an increasing demand to exploit the use of recycled Al alloys to reduce energy consumption and carbon footprint associated with the manufacturing processes. However, a major technical challenge to the widespread use of recycled Al is the presence of high impurity content such as Fe, which can severely deteriorate its mechanical performance. Hence, the development of a new technology is crucial to the production of good quality recycled Al alloys from the metal scrap. A melt conditioned direct chill (MC-DC) technology has been developed at BCAST which is based on the application of a high shear dispersive mixer in the molten alloy prior to solidification to produce a fine as-cast microstructure with reduced segregation in the absence of any grain refiners. This study is concerned with the microstructure/properties of recycled AA6111 Al alloy billets produced from two different metal scraps including Incinerator Bottom Ash (BA) and Old Rolled Taint Tabor (TT), using a combination of the novel MC-DC, together with hot extrusion and cold rolling processes. A combination of OM, SEM, XRD, DSC, hardness and tensile testing methods were used to characterise the microstructures and mechanical properties of recycled AA6111 Al alloys processed from scrap metals. This contribution presents detailed studies of the microstructures and tensile properties of recycled AA6111 Al

alloys as a function of scrap Al feedstock, melt conditioning and thermomechanical processing conditions.

#### Biography

Isaac completed his DPhil studies in 1991 and continued his postdoctoral research at Department of Materials, University of Oxford. Since 1996, he held a Faculty position at the School of Metallurgy and Materials, University of Birmingham. He took up the Professorship of Metallurgy at Brunel University London in 2016.



He has over 127 publications and is serving as an editorial board member of Journal Materials Physics and Chemistry. He specializes in the field of physical and powder metallurgy. His research is focussed on the understanding of the relationship between processing, microstructure and properties of alloys and composites.

## Improving thermal stability of aluminum alloys through additions of rare earths

#### Frank Czerwinski

CanmetMATERIALS, Natural Resources Canada, Hamilton, Ontario L8P 0A1, Canada

#### Abstract

Aluminum alloys represent an important segment of structural lightweight engineering materials with a wide range of industrial applications. A substantial expansion of Al alloys is hindered by their limited structural stability at increased temperatures over extended service time. The paper presents an opportunity in improving thermal stability of Al alloys created by rare earths. Among rare earths a particular interest in cerium is assessed due to a combination of its physical and chemical characteristics as well as economic factors. Examples of binary Al-Ce and ternary Al-Ce-X alloys are presented with cerium contents reaching up to 20 wt.%. In addition to solidification characteristics, determined by thermal analysis, detailed microstructural characteristics are presented along with their changes during thermal exposures. Results are compared with improvements in thermal stability of Al achieved after micro alloying with a number of transient elements.

#### Biography

Dr. Frank Czerwinski holds two Ph.D. degrees: in metallurgical engineering from McGill University, Montreal, Quebec, Canada and in materials science from the University of Mining and Metallurgy, Cracow, Poland. He has also completed post-doctoral studies at McMaster University, Hamilton and McGill University, Montreal.

At present he is a senior research scientist at CanmetMATERIALS, materials research center of Government of Canada. During his professional career, Dr. Czerwinski was a university professor of materials and metallurgical engineering, and before joining CanmetMATERIALS, for over a decade, he was with industry, working for Husky Injection Molding Systems Ltd., the largest brand name supplier of injection molding equipment and services to the plastics and metal industry.

Dr. Czerwinski is the author of 2 books, editor of 3 books as well as the author and co-author of 16 patents and over 200 research papers.

## PM production of tungsten and its alloy: A multi-scale numerical study

#### Xizhong An\*, Yi Zou, Qian Jia, Fan Xu, Meng Li

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#### Abstract

Tungsten (W) and its alloys have wide applications in many key industrial areas due to their superior properties. However, the high melting point of W ( $\approx$ 3410°C) or its poor compatibility with many elements makes it difficult to fabricate high performance pure W and its alloys by using conventional methods like melting and casting. In comparison, the powder metallurgy (PM) method is more promising and has been proved to be very effective in producing refractory metals and their alloys with isotropic or anisotropic properties owing to its advantages like high accuracy, low cost, easy operation, and mostly importantly the net shape or near net shape forming. In present work, the whole PM process including die filling, compaction and sintering of pure W and its composite powders (e.g. W-Cu) was numerically reproduced by multi-particle finite element method from particulate scale. All the stages in PM process were considered and coupled to reduce the assumptions and increase the simulation accuracy. Meanwhile, the initial packings of pure W or W-Cu composite powders with different structures were firstly generated by discrete element method, then they were imported into FEM model for compaction and subsequent sintering. The effects of various factors such as the initial packing structure, compaction method/pressure and temperature on macroscopic/microscopic properties of the powder mass were investigated, and the densification dynamics and mechanisms in each PM stage were analyzed and identified. The obtained highlighted results can provide theoretical and practical references for the PM production of high-performance W and its alloys.

#### Biography

Dr. Xizhong An has completed his PhD from the University of Science and Technology Beijing, China and postdoctoral studies from the University of New South Wales, Australia. He is currently a full professor and the director of Process Metallurgy and Powder Engineering Research Center in School of Metallurgy, Northeastern University. He has published more than 100 papers where >70 are in reputed SCI journals and applied more than 20 patents where 6 have been authorized. He is the director of many academic organizations and has been serving as the editorial board member of many International journals.



## **Refractories; An essential evil?**

#### Michael Walton <sup>a</sup>, Wayne Wright <sup>a</sup>

<sup>a</sup> RefMet, PO Box 126, Prahran, Victoria, Australia 3181

#### Abstract

The high temperature processing industry depends almost entirely on Refractories, for process vessel integrity and longevity. Refractory failures, during operation, cost the business orders of magnitude more than to value of the installed materials, and thus it is essential that the operator invests sufficiently in QA/QC during maintenance periods to ensure longevity. Most companies no longer have dedicated specialists, and rely heavily on installation companies. Given the dearth of well trained tradesmen, QA is becoming more important for successful completion of shuts, and achieving acceptable campaign lives. This paper describes the most common modes of refractory failures, important aspects of refractory installation, and the essential QA requirements.

#### Biography

Michael is Principal Engineer and Founder of RefMet. He has over 45 years of experience in the high temperature industries, gained in roles in production, Technical Sales support and consulting, working on 3 continents. Although primarily a pyrometallurgist, he has extensive experience in Refractories' applications, in the Metallurgical, Cement/Lime and Power Generation industries. Michael is a metallurgy graduate of Imperial College, and was awarded an MBA by RMIT. He is a Fellow of the IoM<sup>3</sup>, and a member of the Institute of Refractories Engineers. He is also a Registered Professional Engineer-Queensland.



## Acousto-microfluidic one-step synthesis and activation of metal-organic frameworks (MOFs)

#### Heba Ahmed

RMIT University, Australia

#### Abstract

Metal- organic frameworks (MOFs)- highly ordered three-dimensional coordination networks- have recently garnered significant attention, particularly in sensing and gas separation, because of their exceptionally high Brunauer–Emmett–Teller (BET) surface areas (~104 m2/g), porosities and limitless compound and network combinations. Nevertheless, the current techniques for scalable preparation of these materials can however be lengthy and tedious, and the build-up of successive layers can compromise crystal orientation. Further, the need for additional post-synthesis steps to obtain vacant pores, a process known as activation, and release them from the substrate, presents a considerable production challenge. Here, we report a high frequency, megahertz, acoustically driven microcentrifugation platform that facilitates fast convective solutal transport, allowing the synthesis of MOF crystals in as short as five minutes. We demonstrate this with two MOF systems, HKUST-1 and MIL 88-B. Interestingly, we observed that the acoustically- synthesised MOFs exhibited a high degree of out-of-plane orientation parallel to the vertical {222} crystal plane. The crystals are not only oriented due to long-range out-of-plane superlattice ordering aided by molecular dipole polarization under the acoustoelectric field, but also simultaneously activated during the synthesis process with BET surface area of 1600 m2/g, which is close to that reported for activated commercial HKUST-1 crystals and more than double the surface area for HKUST-1 crystals produced in the absence of SAW. Moreover, the SAW chips can be fabricated at low costs (about US\$1 per device) allows them to be easily scaled in large numbers for efficient, large-scale, environmentally friendly production of this exciting class of materials.

#### **Biography**

Dr. Heba Ahmed graduated with a BSc pharmacy from Alexandria University, Egypt (2002). Besides being a trained pharmacist, she

worked in the R&D department in both Sigma Pharmaceuticals and Pfizer Inc., Egypt. In 2016, she obtained a MSc. Biotechnology from the American University in Cairo. She was awarded a PhD in Chemical Engineering from RMIT University in Melbourne (2018), for using high frequency sounds waves for material engineering. Besides being a trained pharmacist, she worked in the R&D department in both Sigma Pharmaceuticals and Pfizer in Egypt. Dr. Ahmed worked as a visiting researcher in Massachusetts Institute of Technology (MIT) (2011-2012) and also as a researcher in Youssef-Jameel Research and Technology Centre, in Egypt. She also held the position of lead scientific investigator in D-Kimia Diagnostic Solutions, the first start-up company in Egypt. Dr. Ahmed is currently a post-doctoral researcher in RMIT University under professor Leslie Yeo with a focus on engineering new materials and composites for sensing, and optoelectronic applications.



## Effect of chicken feather and its carbon derivatives on the compressive strength of cement mortar

## B. B. Pajarito<sup>1+</sup>, A. J. B. Belarmino<sup>1</sup>, R. M. R. Calimbas<sup>1</sup>, J. R. B. Gonzales<sup>1</sup>, and M. N. Acda<sup>2</sup>

<sup>1</sup>Department of Chemical Engineering, University of the Philippines, Diliman, Quezon City 1101 Philippines <sup>2</sup>Department of Forest Products and Paper Science, University of the Philippines, Los Baños, Laguna, Philippines

#### Abstract

Chicken feathers (CFs) contribute to the pollution of the environment through their accumulation as solid waste. In an effort to address environmental issues, construction materials such as concrete and mortar have utilized CFs as additives and reinforcing fillers. However, the incorporation of CFs reduces the compressive strength of cement-based materials due to the inherent polymeric characteristics of CF. To improve the compressive strength, we first transformed CF into carbon before adding into the cementitious material. This study reports the compressive strength of cement mortars blended with 3 different types of CFderived carbon particulates (carbonized CF, non-exfoliated and exfoliated graphitized CF) at varied loadings and cement curing times.

After 28 days of curing, cement mortars blended with carbon particulates have higher compressive strength than unfilled mortar and mortars filled with CF. Non-exfoliated (0.015 wt% of cement) and exfoliated (0.1 wt%) graphitized CF significantly improved the compressive strength of unfilled mortar by 32.6 and 29.1%, respectively. This demonstrates the potential of CF carbon as reinforcing additives in cement-based materials.

#### Biography

Bryan B. Pajarito is an associate professor at the Department of Chemical Engineering, University of the Philippines – Diliman. He earned his doctorate degree from Tokyo Institute of Technology, Japan in 2012. He was a visiting research fellow at the College of Engineering and Computer Science, Australian National University in 2018. His current research interest is on modification of polymers into functional materials.



# **Oral Presentations**

# Development of a 3D printed scaffold allowing multiple drug delivery for the treatment of bone metastasis in breast cancers

#### Habib Belaid\*<sup>a,b</sup>, Catherine Teyssier<sup>b</sup>, David Cornu<sup>a</sup>, Vincent Cavailles<sup>b</sup>, Mikhael Bechelany<sup>a</sup>

<sup>a</sup>Institut Européen des Membrane UMR535, Place Eugene Bataillon, F-34095 Montpellier, France <sup>b</sup>Institut de recherche en cancérologie U1194, 208 rue des apothicaires, F-34298 Montpellier, France

#### Abstract

Breast cancer is the most common invasive cancer in women. Metastatic breast cancer, most frequently localized in bone, is causing considerable pain and high patient morbidity. The treatment of bone is challenging, and patients are often treated by surgery in addition to a systemic chemotherapy treatment.

3D printing is a powerful tool providing the ability to print bone substitute materials or "scaffolds" designed to mimic the extracellular matrix. For patients with bone metastasis, the scaffold may also allow the controlled and local release of anticancer drugs.

The aim of this work is the development and characterization of novel biomimetic biodegradable 3D printing scaffolds allowing both bone regeneration and inhibition of breast cancer cell proliferation. To this aim, Poly (lactic-co-glycolide) or PLGA microspheres have been loaded with Raloxifene Hydrochloride (RH) and Alendronate (AL). These microspheres have been incorporated into a 3D scaffold fabricated using a Stereolithography 3D printer system with a Poly (propylene fumarate) (PPF) photopolymer. The physicochemical properties of the nanocomposites scaffold have been fully characterized. Biological testing has been carried out in order to confirm the effects of encapsulated drugs on MCF7 cells proliferation. Cell viability, adhesion and differentiation test using MG63 cells has been conducted to determine the scaffold biocompatibility and its effects on cell proliferation. Altogether, our data showed that PLGA microspheres incorporated in PPF scaffolds could be suitable for the treatment of bone metastasis in breast cancer.

#### Biography

Mr Habib Belaid obtained a degree in Chemistry in 2014 from University of Aix-Marseille. Then he obtained a M.Sc. in Material science in 2014 from the University of Toulouse. He is currently working as a doctoral researcher between the European Institute of Membranes of Montpellier and Research Institute of Cancerology of Montpellier, where he focuses his work on a new generation of 3D scaffolds for multiple drug delivery in the treatment of bone metastasis of breast cancers.



## Uptake, permeability and diffusion of multifunctional mesoporous silica nanoparticles in 3D cell assemblies

#### Indra Van Zundert<sup>1</sup>, Beatrice Fortuni<sup>1</sup>, Matteo Giovanni Maria Boretto<sup>2</sup>, Hugo Vankelecom<sup>2</sup> and Hiroshi Uji-i<sup>1,3</sup>

#### <sup>1</sup>KU Leuven, Celestijnenlaan 200F, 3001 Leuven, Belgium

<sup>2</sup>KU Leuven, Department of Development and Regeneration, Cluster of Stem Cell and Developmental Biology (SCDB), Unit of Stem Cell Research, Laboratory of Tissue Plasticity in Health and Disease, Campus Gasthuisberg, Herestraat 49, B-3000 Leuven, Belgium <sup>3</sup>RIES, Hokkaido University, Sapporo, 001-0020, Japan

#### Abstract

Over the last years, mesoporous silica nanoparticles (MSNPs) became highly popular drug nanocarriers in cancer therapy because they offer many advantages such as high drug loading capacity, easy surface functionalization and high biocompatibility. A full understanding of their behavior inside the tumor is vital knowledge for their further translation towards the clinic. Unfortunately, nanoparticle uptake and efficacy studies often remain at the single cell level, hardly being representative for an actual in vivo tumor. In this research, we investigate the permeability of MSNPs into 3D cell assemblies called organoids, directly originating from cancer patient's biopsies. These "tumoroids" recapitulate key features of the real tumor and therefore serve as a near-physiological model to study the behavior of drug delivery systems. We test uptake, permeability and diffusion of MSNPs with different polymer coatings, being polyethyleneimine and hyaluronic acid. Depending on the charge and characteristics of the polymer coatings, the uptake and penetration of the MSNPs inside the tumoroid will be altered. In addition, the polymers chosen in this research each have an their specific cellular function. As such, this research will provide valuable information about the action of this multifunctional drug delivery system which can be also applied to other nanocarriers.

#### **Biography**

Indra Van Zundert (PhD Student) has been Graduated from KU Leuven with a degree in biochemistry. I started my PhD also at the chemistry department (affiliation molecular imaging and photonics) where I already performed my master thesis. Currently, I am in the middle of my second year PhD.

## Development of antimicrobial and biocompatible fluorescent Hydroxyapatite-chitosan nanocomposite films for biomedical applications

#### Somtirtha Kool Banerjeea, Dr. Biswajoy Bagchib\*, Dr. Arpan Koolc, Dr. Kaustuv Dasa, Prof. Sukhen Dasa\*.

<sup>a</sup>Physics Department, Jadavpur University, Kolkata 700032, India.

<sup>b</sup>Present Address: Department of Medical Physics and Biomedical Engineering, University College London, W1W 7TS, United Kingdom <sup>c</sup>Department of Physics, Techno India University, Sector V, Salt Lake, Kolkata 700092, India

#### Abstract

Fluorescent erbium doped hydroxyapatite (eHAp)-Chitosan nanocomposite film is developed. Nanocrystalline eHAp has been synthesized via hydrothermal assisted precipitation method using erbium (III) ions as dopant. The films were characterized by UV-Visible spectroscopy, X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), photoluminescence

spectroscopy (PL), and field emission scanning electron microscopy (FESEM). Physicochemical characterization results confirmed incorporation and uniform distribution of eHAp in chitosan films. High antimicrobial activity was observed using eHAp incorporated chitosan films against E. coli and S. aureus by contact inhibition on agar plates. The films also showed

excellent biocompatibility with human lung fibroblast cells (WI-38) which showed strong attachment and proliferation on the chitosan films with negligible cytotoxicity. The doped films also have great biodegradation and mineralization behaviour after 2 weeks

in stimulated body fluid. Thus the doped fluorescent chitosan films with multifunctional characteristics can be used as strong candidate for diverse applications in antimicrobial treatment, wound healing, tissue scaffolds and bioimaging.

#### Biography

Mrs. Somtirtha Kool Banerjee has received her M.Sc and B.Sc degree in Microbiology from University of Calcutta, India in 2014 and 2012 respectively. I am pursuing PhD from Department of Physics, Jadavpur University, India. My research work is based on therapeutic application of ceramic and polymer materials.

# Polybutylene succinate porous scaffold prepared by fused deposition modeling and salt leaching techniques for drug delivery application

#### Kasidis Teerasuchaia, Bussarin Ksapabutra and Nattawut Chaiyuta\*

<sup>a</sup>Department of Materials Science and Engineering, Faculty of Engineering and Industrial Technology, Silpakorn University, Nakhon Pathom, Thailand. 73000

#### Abstract

The scaffold is an innovation of creating a suitable environment for the restoration of tissues or can be used to achieve drug delivery and efficiency to specific sites. Since, polybutadiene succinate (PBS) is one of the magnificent biocompatible and biodegradable polymers, it was choosen to study in this research. The Fused Deposition Modeling (FDM) and salt-leaching technique were combined to prepare the PBS scaffold that purposely designed with two specific structural alignments, as well as, the scaffolds with and without porous obtained from salt leaching were fabricated in this study. The scaffold alignments, which were  $0/90^{\circ}$  and  $0/60^{\circ}/120^{\circ}$  lay-down patterns, and the scaffold porosity which was created from salt-leaching technique have expected to affect the efficiency of drug encapsulation and release. Scanning electron microscopy and Contact angle analysis were carried out to characterize the morphology and surface properties of the scaffolds. The fabrication technique led to produce the scaffolds with two different pore sizes, which were  $5-20 \mu m$  and  $45-70 \mu m$ . Moreover, the alignment of the scaffold showed no significant effect on the porosity. The

Water contact angle testing revealed that these porous scaffolds were low hydrophilic (nearly 90°). The porosity of the porous scaffolds was about 71% on average.

#### Biography

Kasidis Teerasuchai completed his bachelor's degree from department of Material Science and Engineering, faculty of Engineering and Industrial Technology, Silpakorn University in 2016. Presently, he has been studying a master's degree in Polymer Science and Engineering at Silpakorn University.

## Charcterization of calceined waste shells

## Wiranchana Srichanachaichok<sup>a,b\*</sup>, Dakrong Pissuwan<sup>b,c</sup>

<sup>a</sup>Materials Science and Nano Engineering Undergraduate Program <sup>b</sup>Nanobiotechnology and Nanobiomaterials Research Laboratory (N-BMR), School of Materials Science and Innovation <sup>c</sup>Materials Science and Engineering Program Faculty of Science, Mahidol University, 272 Rama VI Poad, Ratchathewi, Bangkok 10400, Thailand





#### Abstract

Due to a high consuming of shellfish meat, it can produce a high amount of waste from shells. It is well-known that calcium carbonate (CaCO<sub>3</sub>) is a major component in mussel shells. In Thailand, farmers have crushed the shells and used them as a natural fertilizer. However, it was reported that this waste shells can be a good source of calcium oxide (CaO). CaO can provide a lot of benefits in various applications such as being catalysts or antibacterial substances. In this study, the conversion of CaCO<sub>3</sub> to CaO by calcination at different temperatures was investigated. The mixture of crushed shells from a local market in Thailand was used in this study. The crushed shells were heated in a furnace at temperatures 800 °C, 900 °C, and 1,000 °C. After calcination, the calcined shells were characterized by using X-ray diffraction (XRD), X-ray fluorescence (XRF) analyzer, Fourier-transform infrared spectroscopy (FTIR), and scanning electron microscope (SEM). The crushed shell powder heated at 1,000°C was the best condition that could well transform CaCO<sub>3</sub> to CaO. This work demonstrates the potential of the waste shell conversion to CaO.

#### **Biography**

Ms. Wiranchana Srichanachaichok is the 3rd year undergraduate student of Materials Science and Nano Engineering Undergraduate International Program, Faculty of Science, Mahidol University, Thailand.

#### The influence of thermoplastic nonwovens containing multi-walled carbon nanotubes on CFRPs properties

#### Kamil Dydek<sup>1</sup>, Paulina Latko-Durałek<sup>1</sup>, Anna Boczkowska<sup>1</sup>, Michał Sałaciński<sup>2</sup>, Rafał Kozera<sup>1</sup>

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#### Abstract

One of the latest trends in the development of new materials in order to improve the electrical conductivity of Carbon Fiber Reinforced Polymers (CFRPs) is to use of carbon nanotubes(CNTs). There are known at least several methods to increase electrical resistivity of CFRP using CNTs: spraying CNTs with epoxy on dry CFs, growing CNTs on CFs or application of Bucky Paper. A new idea developed by our team, is modification of CFRP by implementation of thermoplastic nonwovens containing CNTs. Such nonwovens can be produced by two methods: the melt-blown process or extrusion and pressing thermoplastic fibers containing CNTs. Nonwovens can be placed on a top or as interleaves between layers of a carbon fabric or prepreg. In order to investigate the effect of CNT-doped nonwovens on the electrical, mechanical and thermal properties of CFRP, laminates were made using commercial epoxycarbon prepreg by out of autoclave method. In each case, the nonwovens were placed between the prepreg layers. Surface and volume electrical conductivity of fabricated panels were measured. The results were supported by microscopic observations. The mechanical properties of the CFRP composites were measured in a short-beam shear test. In addition, the influence of thermoplastic nonwovens on the thermal properties of laminates was analyzed by Dynamic Mechanical Analysis.

The studies were carried out within grant no. DOB-1-3/1/PS/2014 financed by the National Centre for Research and Development.

#### **Biography**

Mr. Kamil Dydek has been graduated from Faculty of Power and Aeronautical Engineering of Warsaw University of Technology in 2015, after which he started PhD studies in the Faculty of Materials Science and Engineering. In his PhD thesis he works with improving the electrical conductivity of CFRP. In the last 5 years he participated in 7 projects, including 3 international ones. In addition, he completed studies in Project Management at Warsaw School of Economics in 2019.

## 3D printed PLA/BN scaffolds for bone tissue engineering application

Materials Oceania-2019 | September 16-18, 2019 | Melbourne, Australia

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#### Abstract

Contaminated or infected bone defects remain serious challenges in clinical trauma and orthopedics. The aim of this work is the



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development and characterization of novel biomimetic biodegradable implants called « scaffolds » obtained by 3D printing. Scaffolds that possess adequate biodegradability, interconnectivity, and mechanical properties in accordance with the injured tissue are required.

Polylactide (PLA) is a currently used bioresorbable, biodegradable and biocompatible synthetic polymer that has been widely investigated and approved by FDA for biomedical applications. However, PLA is a typical hydrophobic polymer. It has poor mechanical properties for tissue engineering applications. One of the strategies to improve these properties is to incorporate nanofillers inside this polymer.

During this study, PLA scaffolds reinforced with different quantities of Boron Nitride (BN) nanosheets were prepared by Fused Deposition Modeling 3D printing. Morphology and surface of the scaffolds were observed by Scanning Electron Microscopy. The physicochemical analysis by X-ray Diffraction and Raman spectroscopy were performed in order to confirm the presence of the nanofillers. Improved mechanical properties by tensile test have been demonstrated.

Scaffolds have been tested on osteosarcoma cells (MG63) in order to evaluate their enhanced mineralization ability. Biocompatibility, cell attachment and proliferation results showed that the scaffolds are nontoxic. Moreover, MG63 cells grown on the scaffolds were induced in differentiation as shown by alizarin red staining. Altogether, our data showed that BN nanosheets reinforced PLA scaffolds and these materials could be suitable for bone tissue engineering.

#### Biography

Mr Habib Belaid obtained a degree in Chemistry in 2014 from University of Aix-Marseille. Then he obtained a M.Sc. in Material science in 2014 from the University of Toulouse. He is currently working as a doctoral researcher between the European Institute of Membranes of Montpellier and Research Institute of Cancerology of Montpellier, where he focuses his work on a new generation of 3D scaffolds for multiple drug delivery in the treatment of bone metastasis of breast cancers.



# Effect of co-solvent on the properties of non-woven porous neomycin-loaded poly(lactic acid)/ polycaprolactone fibers

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#### Abstract

In this research, the model drug neomycin was loaded into biodegradable fibers containing Poly(lactic acid) (PLA) blended with Polycaprolactone (PCL) as a matrix using the rotational jet spinning (RJS) technique. The mixed polymer solution of PLA and PCL in dichloromethane and a co-solvent of dichloromethane and ethanol was prepared. The effect of the spinning condition such as a rotational speed (1000-4000 rpm), a ratio between PLA and PCL (80:20, 75:25 and 70:30) and a ratio between dichloromethane and ethanol (90:10 and 80:20) as a co-solvent on porosity percentage and morphology were investigated. The results demonstrated that when the PLA concentration increased, the fibers diameter increased but the porosity percentage decreased due to the low mobility of PLA. Upon increasing the rotational speed, the fibers diameter decreased because of highly developed jet, which overcomes the intermolecular forces between polymer chains and polymer-solvent interaction. When incorporating the higher concentration of PCL into PLA matrix, the porosity percentage tended to increase. The results also showed that the rougher surface fibers prepared by RJS technique due to the evaporation of the anti-solvent compared to the fibers spun using only dichloromethane as a solvent. The porous structure of the fibers changed when using a co-solvent due to the phase inversion before the solvent evaporated and the different evaporation rates between dichloromethane and ethanol. The porosity percentage increased upon adding ethanol into the polymer solution. In vitro drug release studies concluded that the higher porosity increases the efficiency of drug release and drug loading of fibers.

#### Biography

Thiphathai Hongthipwaree completed her Bachelor's Degree in Petrochemicals and Polymeric Materials at the Silpakorn University, Thailand in 2016. At present, she received a master's degree at Silpakorn University in Polymer Science and Engineering, Faculty of Engineering and Industrial Technology. Her research topic is the preparation of Poly(lactic acid)/ Polycaprolactone blend fibers using rotational jet spinning for wound dressing application.



## Properties of nonwoven polylactic acid fibers from prepared by simple rotational jet spinning method

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#### Abstract

This research focused on the preparation of nonwoven polylactic acid fiber from rotational jet spinning (RJS) method in the melting system due to that easy method, high productivity and applicable to all polymers. The viscosity of polymer was an important factor that preparation the nonwoven fiber. A commercial grade and synthesized PLA were used to preparation for nonwoven fiber. The nonwoven PLA were produced at 180-250 °C with rotational speed 1000-4000 rpm. The morphology of nonwoven PLA was investigated by scanning electron microscopy (SEM). The effect of temperature and shear degradation was investigated by gel permeation chromatography (GPC), comparison between melting and solvent system at the same rotational speed. The temperature or rotational speed increased the fiber diameter was decreased. The nonwoven PLA had a smooth surface along the fiber. The necessary speed for produced nonwoven PLA was below 2000 rpm that could be seen from the fiber's distribution (16-61 µm), the rotational speed above 2000 rpm the fiber's distribution (14-185 µm) because the polymer jet was unstable due to centrifugal force and aerodynamic forces was excessively high. The GPC result, the molecular weight of nonwoven PLA was decreased to 30-50 % after spinning due to the effect of temperature degradation wasn't affected. The wettability of the samples was determined by mean of the water absorption. The results showed the increase in the samples weights with time, indicating more

hydrophilic nature of the fibers obtained at the high rotational speed and temperature.

#### **Biography**

Worapon Rodchanasuripron graduated with a bachelor's degree from department of Material Science and Engineering, faculty of Engineering and Industrial Technology, Silpakorn university in 2016. At present, he received a master's degree at Silpakorn University in polymer Science and Engineering, Faculty of Engineering and Industrial Technology.

## Magnetic nanoparticles for monocyte separation

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#### Abstract

Breast cancer is the most cancer that found in the woman. In metastatic stage, breast cancer cell can spread out from primary tumor in breast to bloodstream (circulating tumor cells or CTCs) and form the tumor in another organ. This stage has become a serious problem that can cause of death. Therefore, the detection of cancer at an early stage could increase the survival rate of patient. There are many techniques that have been developed to enhance the efficiency of detection of CTCs circulated in blood. The difficulty is that many red blood cells (RBCs) and white blood cells (WBCs) are also in the blood. Therefore, it is challenge to separate these non-

target cells out from the blood sample first. In this work, we have used magnetic nanoparticles that can target monocytes to separate monocytes out from the model sample. THP-1 monocyte cells were used as a model cell for our study. This proposed technique could help separate non-cancer cells out from the test sample.





Porntida Wattanakull is a Ph.D. student of Materials Science and Engineering Program, Faculty of Science, Mahidol University, Thailand. She has worked under supervision of Assist. Prof. Dakrong Pissuwan and be a member of Nanobiotechnology and Nanobiomaterials Research Laboratory.



## Doped ZnO in hybrid nanostructure for lighting and solar cell applications

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## Abstract

Zinc oxide (ZnO) is a wide bandgap semiconductor possessing excellent optical properties due to different types of intrinsic defects, for instance, O vacancy ( $V_o$ ) and Zn interstitial (Zn<sub>i</sub>). The visible photoluminescence (PL) of ZnO originating from deep-level defects makes it a promising candidate for applications such as white light emitting diodes (WLEDs) and down-shifting layer for solar cells. Although it is still a controversial issue attributing visible emissions to specific defects, the environmentally-friendly nature of ZnO keeps driving the research in ZnO, in view of its potential to replace rare-earth-based phosphors as WLEDs material. <sup>[1]</sup> In our previous study, a hybrid sphere structure of ZnO nanoparticles and polyacrylic acid (PAA) matrix synthesized through a hydrolysis method has proven a noble material emitting intensively in the visible range. <sup>[2]</sup> Herein, we present a general and in-depth study of the effect of dopants in ZnO hybrid structure. Various dopants are introduced into ZnO hybrid structure in order to optimize the PL of ZnO nanoparticles. Effects of dopant nature, size and valence are investigated at different doping concentrations. The emission colour of doped ZnO nanoparticles can be tuned in visible range between yellow and green and the photoluminescent quantum yield (PL QY) can be improved by specific doping. The present work facilitates the synthesis and control of doped ZnO nanocrystals emitting from cold to warm white light.

#### References

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## Biography

Mr. Yu ZHANG received his bachelor degree (2013) and master degree (2016), both in materials science and engineering, from Central South University in Changsha, China. Financially supported by China Scholarship Council (CSC), he is currently a PhD candidate under the direction of Prof. Bruno Masenelli and Dr. Aleksandra Apostoluk at INSA Lyon, France. His thesis is on fabrication, structural and spectroscopic studies of ZnO nanoparticles and his specialties include spectroscopy and nanomaterials.



# Polyethyleneimine (PEI) impregnated bimetallic MIL-101 metal organic frameworks (MOF) for CO2 capture study

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## Abstract

In this study we report PEI impregnated Cr and Mg bimetallic MOF (MIL-101 (Cr, Mg) by using a wet impregnation method to enhance  $CO_2$  capture performance. MIL-101(Cr, Mg) was synthesized by a solvothermal method (Fig. 1). MIL-101(Cr, Mg) possesses relatively large surface area of 3274 m<sup>2</sup>/g, excellent stability to chemical, heat and moisture, and increased  $CO_2$  sorption capacity compared to parent MIL-101 (Cr) due to open metal site and alkaline group. The pore volume of MIL-101 (Cr, Mg) (1.61 cm<sup>3</sup>/g) was higher than the parent MIL-101(Cr) (1.39 cm<sup>3</sup>/g). We expect that the Cr-OH and Mg-OH groups in MIL-101(Cr, Mg) can interact strongly with the amine groups of the PEI and more PEI will be distributed on the surface of the MIL-101 (Cr, Mg) due to the large surface area and pore volume.

The pore size distribution of MIL-101(Cr, Mg) after PEI loading was measured using DFT method from  $N_2$  adsorption-desorption isotherms. The pores were in the range of 0.5 – 1.5 nm and the pore

volumes decreased significantly with increase of PEI amount (Fig. 2). Series of MIL-101 (Cr. Mg)-PEI adsorbents exposed to humid air and acid gases to confirm the stability. $CO_2$  capture capacities were reduced 35% while crystallinity of the adsorbents remain unaffected and confirmed by XRD data. It is clear that humid air, SOx and NOx affected the PEI materials while crystallinity of MIL-

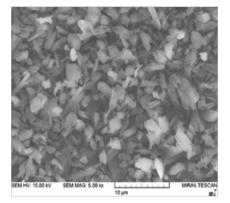
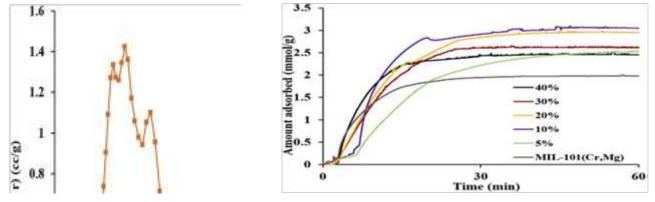


Fig 1. SEM image of MIL-101 (Cr,Mg) PEI



**Fig 2.** Pore size distribution of MIL-101(Cr, Mg) after PEI loading

Fig 3. CO2 adsorption curves at 28°C and 1bar for PEI-MIL-101(Cr, Mg) with different PEI loading amounts.

TGA was used to measure  $CO_2$  capacities and calculate diffusion coefficients for  $CO_2$  and  $N_2$  based on micropore diffusion model, showing that  $CO_2$  capacities increased with increase of PEI amount. With up to 20% PEI loading, the adsorbents showed the enhanced adsorption capacity about 3 mmol/g compared to 2.0 mmol/g of the parent MIL-101(Cr, Mg) (Fig. 3). As percentage of PEI further increases, pore volume and  $CO_2$  adsorption capacity decreased, showing that more PEI resulted in negative effects due to the diffusion barrier. Stability of PEI impregnated MIL-101(Cr, Mg) was analyzed by exposing it in humid air and acid gases and comparing adsorption capacities with samples before the exposure.  $CO_2$  adsorption capacity reduced by 30%–35%. The reported methodology can be applied to other porous adsorbents such as activated carbons and zeolites.

## Biography

Mr. Sanjit Gaikwad has been graduated with major chemistry from Atpadi College Atpadi Kolhapur University, Maharashtra India. Later on, he obtained his post-graduation from Pune University with subject Organic chemistry. After receiving her M.Sc. (Organic Chemistry) degree he has taken up a research position at the Changwon National University, South Korea Presently he has been working under the supervision of Prof. Sangil Han at the Department of Chemical Engineering Changwon National University, South Korea. His research group is interested in the catalyst and surface chemistry of MOFs, as well as their materials properties and applications.



# Generation of charged Ti nanoparticles and their deposition behaviour under the applied bias during RF magnetron sputtering

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## Abstract

It is well known that charged as well as neutral species are generated in the plasma during the sputtering process. We studied the effect

of charged Ti nanoparticles (NPs), which are present in the gas phase, on the thin film deposition during RF magnetron sputtering using a Ti target. The charged Ti NPs were captured on the membrane of a TEM grid (Ted Pella, Inc.) for 30 sec under the biases of -70V, 0V, +5V, +15V, and +30V. The TEM grid was placed on the conducting plate to which the bias was applied and a grounded copper mesh was placed above the TEM grid for preventing the interference from the plasma. The TEM analysis showed that the number density of Ti NPs on the TEM membrane at biases of -70V and 0V applied to the conducting plate was higher than those at biases of +5V, +15V, and +30V. This result indicates that the majority of Ti NPs should be positively charged, considering that when the negative bias is applied, positively charged NPs would be attracted to the TEM membrane whereas negatively charged NPs would move away from the TEM membrane. In order to investigate the effect of these NPs on the thin film deposition, Ti films were deposited for 30 min on Si substrates under biases of -70V, 0V, and +30V. SEM and XRR analyses showed that both thickness and density of the films deposited at -70V were higher than those deposited at +30V. These results are attributed to the fact that positively charged Ti NPs are accelerated by the applied bias during thin film deposition.

#### Biography

Ph.D. candidate Ji Hye Kwon have studied at department of Materials Science and Engineering Seoul National University with subjects of high-quality thin film growth by charged nanoparticles during CVD (hot filament CVD) and PVD (RF magnetron sputtering) system.



## Development of a self-charged photo-power cell based on in situ synthesized Electroactive and large dielectric SrF2/PVDF nanocomposite film

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#### Abstract

In the modern society, clean energy (mechanical, solar, chemical etc.) investigation and its application to the global development is one of the most intense research topics for overall environmental security. So the present researchers are highly interested to resolve this critical issue for the entire energy demand by establishing new development in the technologies and devices for clean energy conversion, storage and conservation. So our intention is to develop such a self-charging energy storage system capable for both solar energy conversion and its simultaneous storage. A self-charged photo-power cell has been fabricated in a very simplistic way that can be used as a portable photo-charged power bank and it is named as a self-charged photo power bank (SCPPB). To fabricate the device we have assembled a photoelectrode (FTO) involving an organic dye phenosafranine-polyvinyl pyrrolidone (PSF-PVP) film, zinc oxide (ZnO) and titanium dioxide (TiO2) NPs solar part as photo-electrons generator in combination with the electroactive and high dielectric SrF2-PVDFNC film as storage unit. The maximum open circuited voltage 1.48 V is obtained under visible light illumination (~110 mW /cm2) with a constant discharge current density ~1.64 mA/cm2 and power density ~ 24.3 W/m2. The maximum areal specific capacitance is obtained ~ 1600 F/m2 with 92 % energy storage efficiency and ~ 2.57 % overall efficiency. The charging-discharging behaviour of the device is verified for almost 3 months. The longevity and efficiency of SCPPB is also demonstrated by lighting up 24 commercially available blue light emitting diodes for 10 days with same intensity.

#### **Biography**

Mrs. Farha Khatun has obtained her M.Sc and B.Sc degree in physics from University of Calcutta, India in 2009 and 2011 respectively. Thereafter she has started PhD research work at Department of Physics, Jadavpur University, India. The PhD work is focussed on electroactive and high dielectric polymer composite based self-charging photo power cell.



## Role of colossal dielectric Cu impregnated $\alpha$ -MnO2 nanoparticles in highly durable asymmetric solid state supercapacitor

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#### Abstract

High dielectric Cu incorporated α-MnO2 nanoparticles have been synthesized successfully through the improved chemical synthesis

technique. Tetragonal tunnel type  $\alpha$ -MnO2 crystalline structure has been identified using X-ray diffraction (XRD) analysis and Raman spectroscopy (RS) measurement. Obtained nanocrystalline size and crystallinity from XRD have been further confirmed with the high-resolution transmission electron microscope (HRTEM) images. Doping induced size modulation along with micro structural defect inside the host material has been identified by XRD and photoluminescence spectroscopy (PL) measurement. With the increase of Cu doping percentage, band gap decreases from 1.385 eV to 1.272 eV. Defects lead to achieve a giant scale of dielectric constant 1.6 × 106 with skimpy tangent loss at 20 Hz frequency. Finally, a high charge storing hybrid asymmetric supercapacitor with high durability has been designed and fabricated in a modified fashion where the performance of the optimized Cu impregnated  $\alpha$ -MnO2 nanoparticles as high dielectric mediator with non-aqueous electrolyte medium (PVALiClO4) is found to improve the cycling stability of the device. Cyclic voltammetry and galvanostatic charge-discharge performance of the fabricated device show the excellent pseudocapacitive electrochemical activity with maximum capacitance of 564.28 Fg-1 and energy density of 259.6 Wh kg-1 for 1 Ag-1. With the load of 90 LEDs (each of 1V) for 10 minutes, the device dissipated 13.29% of its initial charge. Therefore our present work reveals the development of an advance charge storage materials for improving energy storage efficiency can be increased to a greater extent.

## Biography

Dheeraj Mondal is a research scholar at Jadavpur University, India. I have completed bachelor degree from Calcutta University and Master degree from Jadavpur University, India. I have published 8 International research articles in my research topic. My scientific interests are mostly focused on the fabrication of non-toxic, nonconventional energy harvesting and storing device. In my research strong emphasis is put on the understanding of the quantum dot particle characteristics, as well as functionalities in charge storing device and photocatalytic activity. I am very much pleased with my joint-supervisor Prof. Sukhen Das and Dr. kaustuv das, Jadavpur University, India.



# Homochiral metal-organic frameworks functionalized SERS substrate for atto-molar enantio-selective detection

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#### Abstract

The brand-new concept of this work includes the utilization of unique properties of a homochiral metal-organic framework (HMOF) in combination with nonchiral plasmon-active nanograting for the unprecedented chiral detection of biomolecules. The plasmon-active gold grating functionalized by homochiral metal-organic frameworks (L- or D-MOF-6) was proposed as unprecedent tool for enantio-selective SERS-based discrimination. The gold grating surface possesses the homogeneous distribution of plasmon intensity along the active sample area, responsible for excitation of consistent SERS signal. L- and D- lactic acids enantiomers were used for the preparation of enantio-selective surface grafted MOF layer with opposite chiral-entrapping selectivity. The chiral MOFs films, grafted onto gold gratings provide the selective enantiomers entrapping from solution and contribute to the chemical enhancement of SERS. Obtained SERS substrates were able to selectively entrap the (R)-(+)- and (S)-(-)-methylphenylsulfoxide (model analyte) from solution and recognize them with atto-molecular concentration limits and perfect reproducubility. Moreover, the possibility of enantioners detection and recognition in their mixtures was also demonstrated with similar recognition limits. The unprecendent detection and enantioselective recognition were further demonstrated on the biorelevant analytes. Reported concept paves the way for the application of chiral porous materials in combination with nonchiral plasmonic materials, expand and significantly improve the analytical toolbox for enantioselective detection.

## Biography

Guselnikova Olga is 4th year Ph. D. student of University of Chemistry and Technology Prague (Czech Republic) and Tomsk Polytechnic University (Russia). She received her bachelor and master degree from TPU. She is the author of 26 scientific papers (H-index 7) and holds several patents. During her Ph. D. she is focused on the design of advanced SERS sensors for the ultra-sensitive detection in the fields of environmental pollutants and bio-objects; preparation of polymer materials with tuneable functional properties, especially switchable wettability; plasmon induced transformations and organic reactions.



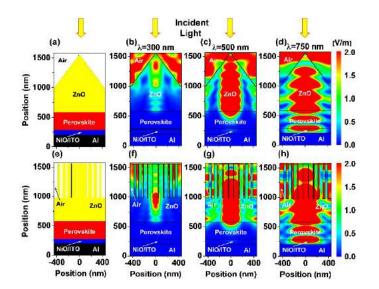
## A route to reach the absorption limit of perovskite solar cells by using metal-oxide front contacts

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#### Abstract

The front contact of a perovskite solar cell has a significant impact on short circuit current density and energy conversion efficiency. The short circuit current and energy conversion efficiency of single junction perovskite and perovskite/silicon tandem solar cells can be increased by photon management. In this study, metal oxide front contacts have been investigated as potential light trapping structures to realize high short circuit current and energy conversion efficiency of a perovskite solar cell. The zinc oxide pyramid texture and non-resonant metasurface structures are experimentally realized from metal organic chemical vapor deposition and templated growth electrodeposition techniques, which are used as front contact of perovskite solar cell leading to approach the absorption limit. In the current study, a potential perovskite solar cell device structure is introduced where materials with the comparable reflective index are utilized, which reduces the reflection losses significantly. The zinc oxide pyramids are used to scatter and diffract the incident light where non-resonant metasurfaces change the phase of the incident light. The optical path length is increased for both cases (pyramid and metasurface), which improves the light trapping through the solar cell structure. Perovskite solar cell with zinc oxide non-resonant metasurfaces and pyramids are compared, providing almost identical performance in terms of quantum efficiency and short circuit current. As compared to the device on a smooth substrate, the solar cells with metasurface and pyramid textured perovskite solar cells provides a 10-25 % improvement of the short circuit current density. Detailed guidelines for the design of the metal oxide front contacts and the solar cell will be provided.



#### Biography

Mohammad ismail hossain is currently pursuing his Ph.D. in Photonics, Plasmonics, and Optoelectronicsmaterials and devices under Hong Kong Government Fellowship Scheme (HKPFS) in the Applied Physics Department, The Hong Kong Polytechnic University. His current research mainly focuses on Perovskite and silicon photovoltaic materials to make the high-efficiency solar cell. He is also working as a research specialist at Computer Science and Engineering Department, University of Connecticut, U.S.A. His research activities are jointly performing between The Hong Kong Polytechnic University, Hong Kong and Stanford University, USA. His research interest includes optics, thin-film material deposition (spin coating, CVD, ALD, etc.), nanophotonic device design and simulation, and characterization. He has achieved a very good number of



publications during his Ph.D. study. He is an Assistant Professor (currently on study leave) of Electrical and Electronic Engineering Department in American International University Bangladesh (AIUB). Hossain received his master's in electrical engineering degree from Jacobs University Bremen (JUB), Germany in 2013 and completed his bachelor's in electrical and Electrical Engineering in 2010 from AIUB, Bangladesh. He was working with Prof. Dr. Werner Henkel at Transmission Group and Prof. Dr. Dietmar Knipp at Electronic Devices and Nanophotonics Lab as a Graduate Research Assistant. He was also a teaching assistant at JUB, Germany and conducted lab courses.

# Capacitive organic anode based on fluorinated-contorted hexabenzocoronene: Applicable to lithium-ion and sodium-ion storage cell

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<sup>b</sup>Institute of Advanced Composite Materials, Korea Institute of Science and Technology (KIST), Jeonbuk 55324, Republic of Korea

#### Abstract

Conducting polymer-based electrochemical capacitor materials have attracted attention because of their high conductive nature and highly reversible redox reaction on the surface of electrodes. However, owing to the poor stability in the aprotic electrolyte, organic electrochemical capacitive electrodes research field pursues to find alternatives. Herein, we introduce fluorine atoms into contorted hexabenzocoronene (cHBC) to achieve the first small-molecule-based organic capacitive energy storage cells that operate at high current rate with decent specific capacity of ~160 mA h g<sup>-1</sup> also provide a superior cycle capability (> 400) without significant alteration. This high capacitive behavior in the P2<sub>1</sub>/c crystal phase of fluorinated cHBC (F-cHBC) is caused mainly by the fluorine atoms at the end of each peripheral aromatic ring. The most electronegative fluorine atoms accelerate ion diffusion on the surface to promote fast Li<sup>+</sup> ion uptake and release by applied current. Moreover, the F-cHBC has potential applications as the capacitive anode in Na-ion sodium storage cell. The fast dynamics of the electric double layer on the surface of F-cHBC enables to deliver specific capacity of 65 mA h g<sup>-1</sup> at a high current of 4000 mA g<sup>-1</sup>.

#### Biography

Jaehyun Park received his B.S. degree in Energy Engineering and Chemistry from Ulsan National Institute of Science and Technology (UNIST), South Korea in 2016. He is currently pursuing his combined Master's – Doctoral Program in the School of Energy and Chemical Engineering at UNIST under the supervision of Prof. Seok Ju Kang. His research interests include the contorted organic polycyclic aromatic hydrocarbon molecules for lithium– and sodium ion secondary battery anode.



# Deterministic growth of a sodium metal anode on a pre-patterned current collector for highly rechargeable seawater batteries

#### Jaeho Jung, Dae Yeon Hwang, Imanuel Kristanto, Sang Kyu Kwak<sup>\*</sup> and Seok Ju Kang<sup>\*</sup>

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#### Abstract

Anode-free seawater batteries have emerged as prospective candidates for the next-generation energy-storage cells because of their unique discharge and charge characteristics. To fulfill this purpose, reliable Na metal plating on the current collector surface is an important requirement for improving electrochemical properties. Here, we developed a strategy for deterministic growth of Na metal on a pre-patterned current collector. The different surface energies of the Cu and Al metal surfaces enable the growth of patterned Na islands during electrochemical deposition, which efficiently form a film-like layer of Na metal. In particular, determining an optimum ratio between the metal-pattern diameter and the distance between adjacent pattern edges is the critical factor for producing a decent Na metal pattern array that can facilitate the enhancement of coulombic efficiency and cycling capability of a half-cell structure. Moreover, patterned growth of Na metal is highly beneficial for enhancement of the electrochemical performance of seawater batteries. By using a Na super-ionic conductor separator with a Cu/Al pre-patterned current collector, well-patterned growth of Na islands with improved cycling stability for over 200 cycles can be obtained for anode-free seawater batteries.

#### **Biography**

Jaeho Jung received his B.S. degree in Energy Engineering and Chemistry from Ulsan National Institute of Science and Technology (UNIST), South Korea in 2018. He is currently working his combined Master's – Doctoral Program in the School of Energy and Chemical Engineering at UNIST under the supervision of Prof. Seok Ju Kang. His research topics include the anode system of seawater battery and Na-O<sub>2</sub> battery for stable cyclability.



## $GdBaCo_{2,v}Mn_vO_{5+\delta}$ layered perovskites as cathodes for solid oxide fuel cells

## Anna Olszewska, Konrad Świerczek

Department of Hydrogen Energy, AGH University of Science and Technology, Poland

#### Abstract

Co-based oxides with  $\text{ReBaCo}_2\text{O}_{5+\delta}$  composition (Re = Rare Earth Element) and layered ordering in the Re-Ba sublattice are of special interest considering application as cathode materials in Solid Oxide Fuel Cells. This is due to their excellent physicochemical properties, including high mixed ionic-electronic conductivity and very good catalytic activity toward oxygen reduction [1]. However, their high thermal expansion is problematic, because it leads to thermal stresses in the cells and may result in faster degradation. Nature of the increased thermal expansion is well-known: oxygen release at high temperatures, consequent reduction of Co<sup>4+</sup> to Co<sup>3+</sup> and spin transitions of Co<sup>3+</sup> [2]. This issue can be partially resolved through substitution of Co with other 3d metals, such as iron, nickel, copper, but also, as lately shown, with manganese.

In this work studies of physicochemical properties of cation-ordered  $GdBaCo_{2-x}Mn_xO_{5+\delta}$  are presented. The conducted research allowed to establish influence of the introduced manganese on the crystal structure, oxygen content, charge state of the transition metals, total electrical conductivity, thermal and chemical expansion, as well as chemical compatibility in relation to commonly used lanthanum gallate-based solid electrolyte. Reduced thermal expansion in Mn-containing samples accompanied by high electrical conductivity and good compatibility toward the electrolyte allowed to successfully manufacture cathodes exhibiting low polarization resistance.

Acknowledgements: The project was funded by the Ministry of Science and Higher Education (MNiSW) on the basis of the decision number 0128/DIA/2016/45.

[1] J.-H. Kim, J. Mater. Chem. A, 3 (2015) 24195.

[2] D. S. Tsvetkov, Dalt. Trans., 43 (2014) 15937.

#### Biography

Anna Olszewska is a 3<sup>rd</sup> year PhD student of Power Engineering at Department of Hydrogen Energy at AGH University of Science and Technology in Krakow, where I am participating in researches on materials for advanced energy technologies, particularly on electrodes and electrolytes for fuel cells and ceramic membranes for gases separation. To be more specific, my studies are focused mainly on Co-based oxides with double-perovskite structure, which can successfully work as cathode materials for Solid Oxide Fuel Cells. Those research are conducted within the project financed by Polish Ministry of Science and Higher Education, of which I am the manager.



## A statistical and systemic study of the interaction between lubricin (LUB) on different substrate surfaces

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<sup>b</sup>Institute for Frontier Materials, Deakin University, Geelong, Victoria, Australia

#### Abstract

Lubricin (LUB), a mucin-like glycoprotein, plays a significant role in the boundary lubrication and wear protection system in human joints. Most lubricin researches have focused on its biotribological and biochemical properties in joints, LUB's unique combination of self-assembly, electrochemical, and anti-adhesive, properties are now being applied to solve many problems in a diverse range of different fields including microfluidics, electrochemical sensors, contact lenses, and bionic neural interfaces. Each of these applications requires lubricin to be adsorbed via self-assembly onto a range of non-biological surfaces. However, an understanding of how lubricin adsorbs and adheres to these physically and chemically different surfaces is lacking. This research aims to bridge this knowledge gap by directly quantifying repulsion force on separation for self-assembled LUB layers on different substrates with the help of AFM. In this report, we investigate the interaction between LUB and different substrates including 2D-nanosheets, microfluidic substrate surfaces and bimetallic substrate surfaces by measuring the adhesion energy of LUB on different substrates with the help of AFM. The results show that the adhesion energy of LUB varies with different substrates and the values for boron nitride is the highest (~8\*10<sup>-16</sup> J) which is almost 31 times higher than the value for mica that was frequently used in the LUB related studies. Meanwhile, the RMS of LUB coated substrates is incredibly low which indicates that the LUB layer on the substrate is fairly smooth. This work provides a systemic method and data prior to the potential combination of LUB with different materials for various applications such as bioimplant, anti-adhesive coating, bioimaging, biosensor and biolubricant.

#### Biography

Mr Mingyu Han received his bachelor degree in polymer material and engineering at the Harbin University of Technology, China, then the dual master degree in polymer technology with the track of biomaterials at both Chalmers University of Technology, Sweden and Aalto University, Finland. Mr Mingyu Han is currently a PhD student at Deakin University, Australia, working with Dr George W. Greene, focusing on the development of optical sensor and biolubricant based on lubricin and 2D-nanomaterials.



## Bulk deformation and toughness behavior of titanium alloys comprising the C15-type laves and beta phase

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#### Abstract

Laves phases are effective in tailoring the mechanical properties of alloys used for structural engineering applications. Therefore, it is an emerging research significance to investigate the deformation features of alloys comprising a Laves phase. In the present work, the Ti-33Zr-xFe-yCr (x = 5, 7 wt% and y = 2, 4 wt%) alloys were designed in a such a way that a Laves phase would form in the investigated alloys and then the Ti-33Zr-xFe-yCr alloys were cast by cold crucible levitation melting. Consequently, all the as-cast alloys exhibit a face-centered cubic C15-type Laves phase along with a dominant  $\beta$  phase. Amongst all the investigated alloys, Ti-33Zr-5Fe-2Cr shows the highest plastic strain (24.8 ± 2.5 %) in compression testing and the lowest yield strength (1128 ± 13 MPa) and hardness (359 ± 16 HV). Vickers micro-indentation technique was employed at the three different loads to examine the deformation features (around the indentations) of the as-cast alloys. The volume fraction of C15-Laves phase influences the size of the deformation zone around the indentations and hardness of the investigated alloys. Consequently, Ti-33Zr-7Fe-4Cr demonstrates the highest hardness (417 ± 19 MPa) and the lowest size of the deformation zone around the indentation-based fracture toughness of Ti-33Zr-7Fe-2Cr and Ti-33Zr-7Fe-4Cr were estimated based on the Shetty-model, Laukford-model, Laugier-model, Casellas-model and Nihara-model proposed in the established literature.

#### Biography

Mr. Chirag is pursuing his final year of PhD in the School of Engineering at Edith Cowan University. Before starting his PhD, Mr. Chirag has worked as Assistant Professor in Marwadi University, India for 6 years from 2010 to 2016. His current research interest mainly focuses on investigating the microstructure, mechanical and fracture properties of metallic materials used for structural and biomedical applications. Mr. Chirag has published four first author papers including three in "Materials & Design" and one in "Materials Science and Engineering A". He has also published a second author paper in "Journal of Alloys and Compounds".



## Cyclic deformation behaviors of a nickel based superalloy: Potential competing failure mechanism

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## Abstract

The cyclic deformation behaviors of a nickel based superalloy at room temperature (RT) and 973 K were investigated, including low cycle fatigue (LCF) under higher strain amplitude level with strain ratio of -1 and high cycle fatigue (HCF) under lower stress amplitude level with stress ratio of 0.1. The alloy shows a typical necklace structures, which contains large fibrous grains and fine equiaxed grains. The samples exhibit two types of competing failure mechanisms including surface initiated and internal initiated

failures. For strain controlled LCF, the fatigue cracks initiate at surface defects no matter at RT or 973 K. For HCF, however, both surface initiated and internal initiated failures mechanisms are observed. Cracks initiation sites are gradually changed from surface defects to internal large crystallographic facets with temperature increasing. The probability of occurrence of surface initiated for strain controlled LCF is higher with maximum stress amplitude level applied which is more than 1100 MPa at 1.0% strain amplitude no matter at RT or 973 K. Simultaneously, the probability of facet initiated is increasing with lower stress amplitude level applied for HCF. However, the lower plasticity also increases the possibility of surface defects initiated at RT for HCF. That means both lower plasticity and higher stress amplitude level could aggravate the degree of stress concentration near surface defects, resulting in surface crack initiation. It is worth noting that crystallographic facets initiate from large fibrous grains rather than fine equiaxed grains at 973 K for HCF, which is attributed to the better collaborative deformation ability of fine equiaxed grains.

#### Biography

Mr. Wei-Wen Kong obtained his B.S. Degree at Nanchang University in China in 2016, and completed his M.S. Degree at University of Science and Technology of China in 2018. Now, he is doing Ph. D. research at University of Science and Technology of China under the guidance of Pro. C. Yuan and is excepted to graduate in 2022. His current research is focused on the study of microstructure, properties and service behavior of Superalloys, including fatigue and creep. If the application is approved, Mr. Wei-Wen Kong would complete the oral presentation as the presenting author.



# Preparation of inorganic porous adsorbent by gasification fly ash and adsorption behavior for Cr(VI) removal

#### Yang GUO<sup>[1,2,3]</sup>, Lu ZHOU<sup>[1,2,3]</sup>, Jianjun WU<sup>[1,2,3]</sup>, Yixin ZHANG<sup>[1,2,3]</sup>

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#### Abstract

The innovation of this paper is to synthesize inorganic porous adsorbent under mild conditions by using solid waste gasification fly ash from chemical plants as raw materials, and then used for the adsorption of Cr(VI).

The gasification fly ash used in this paper comes from Shenhua Ningdong Coal-to-Oil Company. Preparation of inorganic porous adsorbent by alkali fusion hydrothermal synthesis method. The cation exchange capacity of inorganic porous adsorbent prepared under different ash to alkali ratio, aging time, crystallization temperature and crystallization time was determined by formaldehyde method. Analysis of properties of inorganic porous adsorbent by XRD, SEM, FTIR, BET and MIP methods. The adsorption equilibrium experiment of Cr(VI) solution was carried out on inorganic porous adsorbent under different conditions, and the adsorption characteristics were analyzed by kinetic and

thermodynamic models. The results show that when the ratio of ash to alkali is 1:1, the aging time is 15h, the crystallization temperature is 120oC, and the crystallization time is 10h, the cation exchange capacity of the inorganic porous adsorbent prepared is the highest, reaching 1.81meq/g. Quasi-secondary kinetic model and intraparticle diffusion model can well describe the adsorption behavior of inorganic porous adsorbent on Cr(VI). In addition, the adsorption process of Cr(VI) by inorganic porous adsorbent is more consistent with Langmuir model, which indicates that the adsorption is single-layer coverage.

#### Biography

Yang GUO was born in February 1995 and is now a PhD candidate in chemical engineering and technology at China University of Mining and Technology(CUMT). He has published two academic papers, two invention patents and participated in three research projects funded by the Ministry of Science and Technology of China. In addition, he is a member of Hong Kong Chemical, Biological& Environmental Engineering Society (HKCBEES) and Hong Kong Society of Mechanical Engineers



(HKSME).

# Enhanced electrochemical properties of ultrathin Ni(OH)2-MnO2 hybrid nanosheets by plasmaInduced grafted MWCNTs as binder-free electrode for high performance supercapacitor

#### Ai-Wen Chai

National Cheng Kung University, Taiwan

#### Abstract

The utilization of nickel hydroxide and manganese(II) oxide solely as high performance supercapacitive materials are hindered by their low capacitance retention and electrical conductivity. As Ni(OH)2 and MnO2 give synergistic effect, ultrathin Ni(OH)2-MnO2 hybrid nanosheets with thickness (about 18nm) are successfully grown on carbon fiber via a single-step hydrothermal co-deposition method, named CF-Ni(OH)2-MnO2, is presented. Different ratios of Ni(OH)2-MnO2 hybrid nanosheets (Ni0Mn100, Ni40Mn60, Ni50Mn50, Ni60Mn40, Ni100Mn0) are fabricated, where Ni40Mn60 hybrid nanosheets exhibited highest capacitance behavior. Influence of various surfactants are studied, cetyltrimethylammonium bromide (CTAB) exhibited uniform porous nanosheets and strong adhesion on carbon fiber which is useful for ions transport and prolonged cycle life. Multiwalled carbon nanotubes (MWCNTs) are grafted with maleic anhydride(MA) through plasma-induced grafting process, followed by thiol-ene reaction to synthesis MWCNTs-MA-S. Electrochemical properties of Ni(OH)2-MnO2 are further enhanced by dip-coating MWCNTs-MA-S on hybrid nanosheets. Composition and morphology of MWCNTs-MA-S and Ni(OH)2-MnO2 hybrid nanosheets are characterized by using FESEM, FTIR, ESCA, TEM, TGA, NMR, XRD, ICP, and Raman spectroscopy. Electrochemical characteristics of fabricated electrodes are evaluated by using cyclic voltammetry and chronopotentiometry methods. CF-Ni(OH)2-MnO2/MWCNTs-MA-S electrode is successfully synthesized without using any binder, exhibited ultrahigh specific capacitance (2049 F/g at current density of 1 A/g) and excellent capacitance retention (>80%) at 2 A/g charge/discharge rate after 1000 cycles.

#### Biography

Ai-Wen Chai, a second year PhD. candidate who's studying in Chemical Engineering Department, National Cheng Kung University, Taiwan. I have my Chemical Engineering degree with first class honor at the same university and received offer to pursue PhD. study with a scholarship sponsored. My PhD. study focuses on supercapacitor and electrochemical sensor. Our project related to supercapacitors are currently funded by Ministry of Science and Technology (MOST) in Taiwan. With this funding, our lab wish to eventually come out with a large scale grid energy storage system as an alternative to battery system.



## Thermolysis behavior of microcrystalline cellulose at low heating rates

## Mohamed Rashid Ahmed-Haras\*, Nhol Kao<sup>a</sup> and Liam Ward<sup>a</sup>

Chemical and Environmental Engineering, School of Engineering, RMIT University, VIC 3000, Australia

#### Abstract

The main objective of this work was to gain a better understanding of the thermolysis (thermal decomposition) behavior of microcrystalline cellulose (MCC) under low heating rates (5°C/min and 15°C/min). In this study, the micro-structured cellulose was subjected to slow thermal decomposition in inert gas (nitrogen) atmosphere. The heating rates were adopted in order to study the effect of varying low heating rates on MCC weight loss, maximum decomposition temperature and char yield. It was found that a higher maximum decomposition temperature at 346 °C and a lower char yield of 3 % were observed with MCC thermolysis at 15°C/ min heating rate. The FTIR microscopy showed hydroxyl and glycosidic functional groups characteristics of cellulosic materials. The crystal size, detected by XRD, of MCC was measured at 5 nm, while its crystallinity was recorded at 76 %.

#### Biography

Mr. Mohamed Rashid is current PhD student at School of Engineering, RMIT University. He worked as a research officer in industrial chemistry section, and later in the innovation and commercialization office at Universiti Sains Malaysia (USM). He has considerable experience of nanomaterials, material chemistry, advanced materials, oilfield chemistry and polymer science.



## **Poster Presentations**

## Synthesis and drug binding properties of recombinant canine serum albumin

#### Tomomi Hasegawa, Yoshitsugu Morita, Teruyuki Komatsu

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#### Abstract

There is no blood bank for pet animals. Consequently, veterinarians themselves must obtain blood for transfusion therapy. Among the blood components, serum albumin is the most abundant plasma protein and plays two major roles, (i) maintaining colloid osmotic pressure and (ii) transporting a great variety of metabolites and drugs. If it is possible to produce recombinant canine serum albumin (rCSA) using genetic engineering procedure, rCSA is anticipated for use as a plasma expander for dogs. In this paper, we report the synthesis, structure, and drug binding properties of rCSA. First, rCSA was produced using Pichia yeast as a host cell and purified using affinity chromatography. The protein showed identical feature to that of the native CSA derived from canine plasma. Furthermore, we ascertained the crystal structure of rCSA at 3.2 Å resolution. The overall structure and the shape of drug binding property of rCSA using a site II fluorescent probe. The site II drugs for HSA, such as diazepam and ibuprofen, bind to the site II of rCSA. The linear relation between the fluorescence decreasing ratio and the binding constant was determined. The rCSA can be used widely for various clinical and pharmaceutical applications.

#### Biography

Ms. Tomomi Hasegawa graduated from Department of Applied Chemistry, Faculty of Science and Engineering, Chuo University. She has studied recombinant protein chemistry under the guidance of Prof. Teruyuki Komatsu. She continues the research on synthesis, structure analysis, and ligand binding properties of recombinant canine serum albumin in the Graduate School of Science and Engineering, Chuo University.



## Insulin receptor binding aptamer and milk exosome conjugates as promising therapeutic agents for Diabetes

## Gna Ahn<sup>1\*</sup>, Ga-Young Park<sup>1,2</sup>, Yang-Hoon Kim<sup>1</sup> and Ji-Young Ahn<sup>1</sup>

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#### Abstract

Insulin is used to control blood sugar in people who have type 1 diabetes. Patients may have a bit of trouble getting used to the process of preparing and administering their own insulin injection shots. Thus, there is a need for new therapies as an adjunct to insulin injection, to better manage blood sugar levels. Aptamers are short single-stranded oligonucleotides that are capable of binding various molecules with high affinity and specificity. Exosome, cell-secreted nanovesicle, contains many biological materials such as miRNA, protein and metabolites. We studied insulin receptor binding aptamer (IRapt) and milk exosome complexes (IRapt-miExo) as an oral therapeutic reagents for diabetes. IRapt was isolated from a pool of random sequences with a process called systematic evolution of ligand exponential enrichment (SELEX). MiExo was purified by ultracentrifuge method. IRapt were efficiently conjugated by cholesterol-PEGmalemide polymer on the surface of milk exosomes and the results were further confirmed by electrophoresis methods. To validate the differentially expressed genes related to insulin signaling, we performed qRT-PCR. IRapt was selected to SPR and its affinity was 0.92 pM. We present an optimized ultracentrifugation approach for highly reproducible isolation for 50–150 nm exosomes. IRapt-miExo

conjugates were also confirmed by IRapt complementary DNA probe. IRapt-miExo was sufficient to induce the insulin signaling transduction that controls the glucose uptake and glycolysis key factors, IRS-1, GLUT-4, C/EBPβ and PDK4. IRapt-miExo conjugates are sufficient to induce the insulin signal transduction levels. Overall, the contribution of IRapt-miExo to sustain insulin signaling and glucose metabolism is modest.



Gna Ahn is integrated M.D/Ph.D course student in the School of Biological sciences at the Chungbuk National



University since 2015. She completed her undergraduate studies at Chungbuk National University. Her interests are currently focused on the therapeutic use of nanovesicles (exosome and outer membrane vesicle and so on).

## Protection layer/semiconductor structure of photoelectrode for photoelectrochemical water splitting

#### Jianyun Zheng<sup>1,2</sup>, San Ping Jiang<sup>1</sup>, Shuangyin Wang<sup>2</sup>

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#### Abstract

Silicon (Si) has required a protection layer to maintain stable and long-time photoanodic reaction. However, the trade-offs between photoelectrode efficiency and stability significantly hinder the practical application of silicon-based photoelectrochemical devices. Here, we firstly reported a simultaneous enhancement of charge separation and transfer in Nb-doped NiOx/Ni/black Si photoanodes induced by plasma treatment. The optimized photoanodes yields the highest charge-separation efficiency (nsep) of ~81% at 1.23 V versus reversible hydrogen electrode, corresponding to the photocurrent density of ~29.1 mA·cm-2. The concentration and species of oxygen defects in the NiOx-based layer are adjusted by synergistic effect of Nb doping and plasma treatment, which are the dominating factors for forming suitable band structure and providing favorable hole-migration channel. In addition, we used a facile approach to decouple the trade-offs of silicon-based photocathodes by employing crystalline TiO2 with graded oxygen defects as protection layer. The crystalline protection layer provides high-density structure and enhances stability, and at the same time oxygen defects allow the carrier transport with low resistance as required for high efficiency. The silicon-based photocathode with black TiO2 shows a limiting current density of ~35.3 mA cm-2 and durability of over 100 hours at 10 mA cm-2 in 1.0 M NaOH electrolyte, while none of photoelectrochemical behavior is observed in crystalline TiO2 protection layer. These results elucidate the important role of oxygen defects on the protection layer/Si-based photoelectrochemical systems and is encouraging for application of this synergistic strategy to other candidate photoelectrodes.

#### Biography

Jianyun Zheng received his Ph.D. degree in Physical Chemistry from Shanghai Institute of Ceramics, Chinese Academy of Sciences in 2015. He currently works in Hunan University and Curtin University as a united postdoctoral researcher. His main interests focuses on the preparation of semiconductor materials, design and assembly of photoelectrode, and their performance in photo(electro)catalysis.



## Bacterial nanofibrial polymer (BNP) for wound-healing application

#### Seon Hyung Lee, Yang-Hoon Kim and Ji-Young Ahn

Department of Microbiology, Chungbuk National University, Cheong-Ju, Korea

#### Abstract

Wound healing requires conditions such as humid, aseptic conditions. Bacterial Nanofibrial Polymer (BNP) had high water holding capacity, high-surface-area, non-toxicity that meets requirements for wound healing. Thus, BNP is suitable for use as a wound healing material and our studies have been intensively carried out to improve the BNP to applying to wound healing. BNP was produced from Gluconacetobacter hansenii. UV mutagenesis was performed to screen the high-yield strain of BNP. Fifteen colonies were randomly selected and separately inoculated into 2 ml of HS medium in 12-well culture plate, and grown under static conditions at 28°C. To optimize the production conditions, the yield of BNP was assessed by varying the pH under the 3 different carbon source medium. In-vitro wound healing assay and qRT-PCR analysis were performed to find out the wound healing ability of BNP. Through the UV mutagenesis, the mutant strains with increased BNP production yield were obtained. The 2% glucose medium led to the highest yield of hydrated mass ( $0.88 \pm 0.18$ g/L) at 28°C for 5 days. FESEM image displayed highly interconnected and porous structure composed of web-like continuous, nanopolymer with an average diameter of <300 nm. We confirmed that the endo/epithelial cell growth and migration was accelerated during BNP treatment by in-vitro wound healing assay. Finally, several scar-free healing genes were affected (activated/repressed) by BNP. Skin treatment of BNP can accelerate the gene expression level. BNP is a highly porous and mechanically stable nanopolymer, has excellent potential as a material in many novel applications.

Seon Hyung Lee is integrated M.D/Ph.D course student in the School of Biological sciences at the Chungbuk National University since 2017. She completed her undergraduate studies at Chungbuk National University. Her interests are currently focused on the therapeutic use of bacterial nanofiber as a wound dressing material.



## Super tough, thermally conductive composite hydrogel and its biomedical applications

#### Yi Wang<sup>∗</sup>, Jinrong Wu, Jing Zheng, Guangsu Huang

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#### Abstract

While hydrogels with both high mechanical properties and thermal conductivity hold great promise for applications in artificial cartilages, actuators, antipyretic pastes and so on, it is still challenging to fabricate such hydrogels. Here, we report a class of mechanically robust, ultrastretchable and thermal-conducting composite hydrogels by in situ polymerizing acrylamide monomers in the presence of vinyl-functionalized boron nitride nanosheets (v-BNNS). In this way, v-BNNS with vinyl functional groups serve as multifunctional cross-linkers for the polymerization of acrylamide monomers, yielding a denser and stronger hydrogel network and promoting the interfacial interactions between v-BNNS and PAM chains. As a consequence, the composite hydrogels with 4 wt‰ v-BNNS show about 700% and 680% increases in compressive stress and tensile strength, respectively, and simultaneously possess ultrastretchability of 2000%. Meanwhile, the composite hydrogels are highly anti-fatigue, as dynamic loading-unloading tests show that they have outstanding load-bearing and shape recovery properties even after 820 cycles. Moreover, due to the high thermal conductivity of v-BNNS and the covalent interaction facilitating phonon transfer between v-BNNS. We further demonstrate that the composite hydrogels have good biocompatibility, and thus can be applied as antipyretic pastes with

excellent ability to relieve fever and potentially as artificial cartilages due to their anti-fatigue performance.

#### Biography

Yi Wang is pursuing his Ph.D. in Polymer Materials Science at Sichuan University, China (2015 to present). He received his B.E. in Polymer Materials and Engineering from Sichuan University, China (2011-2015). Currently, his research interest includes the functionalization and applications of high-performance hydrogels.



## Highly stretchable and self-healing "solid-liquid" elastomer with strain-rate sensing capability

#### Qi Wu\*, Xiancheng Ren, Guangsu Huang, Jinrong Wu

State Key Laboratory of Polymer Materials Engineering, College of Polymer Science and Engineering, Sichuan University, 24 Nanyi Section, Yihuan Road, Chengdu, China, 610065

#### Abstract

Polyborosiloxane (PBS), nicknamed as "bouncing putty" or "silly putty", is a well-known "solid-liquid" material because of its fascinating viscoelastic properties. It behaves as a viscous liquid at a low strain rate but like an elastic solid at a high strain rate under room temperature. While mimicking the capabilities of the human skin to detect temperature, pressure and touch has been of a great success in wearable devices and artificial robots, fabricating a skin-like velocity-sensitive device is still challenging. Herein, we fabricate a class of "solid-liquid" elastomers (SLEs) by interpenetrating PBS with polydimethylsiloxane (PDMS). PBS forms a dynamic network through boron/oxygen dative bonds, while PDMS is covalently crosslinked to form a permanent network. The permanent network affords a scaffold for the dynamic network, imparting SLEs with high elasticity and structural stability, thereby overcoming the inherent drawbacks such as fluidity and irreversible deformation of conventional solid-liquid materials. Meanwhile, the dissociation and association of dynamic network is time dependent. Thus, the modulus of SLEs varies with strain rates, and if the SLEs contain carbon nanotubes their electric conductivity is also responsive to strain rates. This property can be utilized to fabricate skin-like sensors with the ability to distinguish different contact velocity. Moreover, the dynamic network can dissipate energy and be repaired, leading to the high stretchability and self-healing performance of SLEs.

Qi Wu is pursuing his Ph.D. in Materials Science at Sichuan University, China. He received his B.E. in Polymer Science and Engineering from Zhejiang University, China (2014). Later on, he obtained his M.S. in Inorganic Chemistry from University of Chinese Academy of Sciences, China (2017). Presently His research interest includes the functionalization and applications of self-healing elastomers.



## Characterizing the multi-scale energy dissipation mechanism of natural rubber

#### Cheng Huang\*, Junqi Zhang, Jingrong Wu, Xufu Cai, Guangsu Huang

State Key Laboratory of Polymer Materials Engineering, College of Polymer Science and Engineering, Sichuan University, 24 Nanyi Section, Yihuan Road, Chengdu, China, 610065

#### Abstract

As a biosynthetic material, natural rubber (NR) displays excellent mechanical properties owing to the existence of non-rubber components such as proteins and phospholipids. However, how these rubber chains and non-rubber components response to stress upon deformation is still unclear up to now. Herein, a multi-scale energy dissipating mechanism of NR at small and large strains has been proposed. The hydrogen bonds and ionic bonds within proteins and phospholipids serve as sacrificial bonds which break first to dissipate energy at small strains. By tracing the morphology of protein aggregates during deformation using laser scanning confocal microscopy, we found the aggregates break into smaller fragments with growing stress, which also plays crucial role on energy dissipation of NR at small strains. Additionally, the sacrificial bonds and aggregates can reconstruct once the small strain remove, endowing NR with good recovery capability to repeated small stress. What's more, the aggregates of proteins and phospholipids act as anchoring pivots for entanglements, which promotes the strain induced crystallization (SIC) behavior of NR at large strains. As a special self-reinforcement mechanism, the crystals act as physical crosslinking points, obviously improving the mechanical properties. Once the large strain removes, the crystals fade, also endows NR with good recovery capability to repeated large stress. Therefore, we proposed a multi-scale energy dissipating mechanism brought out by non-rubber components in NR at small and large strain regions.

#### Biography

Cheng Huang is now pursuing the Ph.D degree in Material Science at Sichuan University, China. He received his B.E. and M.S.in Polymer Science and Engineering from Sichuan University, China in 2014 and 2017. Presently he concentrates on the functionalization and the structure-property relationships of diene rubbers.

## Ultra-tough, defect-tolerant and humidity-responsive self-healing elastomers for intelligent actuators

#### Yong Zhu, Guangsu Huang, Jinrong Wu<sup>\*</sup>

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#### Abstract

It is highly desired yet challenging to develop robust soft actuators that can interface with human body and adapt to harsh environments. Herein, inspired by many living organisms that create tough stimuli-responsive materials by integrating soft and hard ingredients through delicate structural design, we report a facile latex-assembly method to fabricate a class of ultra-tough, defect-tolerant and humidity-responsive elastomers by constructing a microscopic honey-comb like skeleton of dynamically crosslinked chitosan within a continuous matrix of vulcanized natural rubber. Such structural design enables the load-bearing capability, sacrificial property and self-healing ability of the skeleton, the stress redistribution and extensibility of the matrix as well as the stiffness variation between hard and soft ingredients, thereby imparting the elastomers with outstanding mechanical strength and defect tolerance, as well as extremely high toughness of 122 KJ m<sup>-2</sup> which is even higher than that of the current state-of-the-art titanium alloys. Moreover, the elastomers show prominent humidity sensitivity due to the hydrophilic nature of chitosan skeleton. Harnessing these advantages, we fabricate a walking robot triggered by humidity variation and shoes that are able to regulate temperature and humidity. The concept of designing rigid sacrificial skeleton within soft continuous matrix on microscale is quite general, enabling the development of high-performance and intelligent materials for emerging applications.



Yong Zhu is currently studying for his PhD at the College of Polymer Science and Engineering in Sichuan University. He received his Bachelors degree in Polymer Science and Engineering at Sichuan University in 2016. His current scientific interests are focused on high-performance elastomers and Intelligent Materials.

## Ionic modified halogenated elastomers with the capabilities of self-healing and water insensitivity

#### Linjun Zhang, Xikui Liu, Guangsu Huang, Jinrong Wu\*

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#### Abstract

Although the covalent crosslinked elastomers obtain high performence, it cannot realise the requirements of recycling and self-healing and cause environmental pollution. Here, a self-healing halogenated elastomer modified by amine derivatives based on dynamic ion crosslinking was prepared by mechanical blending. The synthetic amine derivatives were mechanically mixed with halogenated elastomers at a certain temperature and then molded by plate vulcanizer. In the process of high temperature molding, amine derivatives grafted on the molecular main chain and free halogen negative ions, and then gather to form dynamic physical crosslinking points. The tensile results showed that the tensile properties and strain of the amine derivatives grafted on the different halogenated elastomers reached  $18 \sim 30$  MPa and  $1100 \sim 1300\%$  respectively. DMA test proved that the derivatives grafted with different structures had little effect on Tg of halogenated elastomers, but the temperature of physical crosslinking point changed on account of steric hindrance. The activation energy and binding energy of ion physical crosslinking points with different structures were obtained by combining DMA stress relaxation and DFT optimal calculation. The water-incensitive and self-healing experiments showed that the performance of the ionic modified halogenated elastomer was not affected by the water environment, and the self-healing efficiency was close to 100% at  $60 \sim 100\%$  in accordance with the different structure, which widens the application range of the ionic crosslinked elastomer and are expected to be used as engeering materials.

#### Biography

Linjun Zhang is pursuing his Ph.D. in Polymer Science and Engineering at Sichuan University, China. He received his B.E. in Polymer Science and Engineering from Sichuan University, China (2015). Now, His research fields mainly include the self-healing elastomers with high performence and multi-functionalizations.

## Synthesis of catalase microtube motors with controllable velocity and biodegradability

#### Natsuho Sugai, Teruyuki Komatsu\*

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#### Abstract

Considerable interest has arisen recently in self-propelled microtube (MT) motors because of their potential applications, such as bacterium removers, pollutant cleaners, and separation devices. The propulsion is typically O2 microbubble ejection from the terminal opening. Most MT motors comprise hard metal pipes with a platinum inner surface, where the O2 bubbles are generated by the disproportionation of H2O2. However, they do not have biodegradability. In this paper, we report the synthesis of new protein MT motors having an internal wall of catalase (Cat), which is a H2O2 decomposing enzyme, and highlight their controllable velocity of autonomous movement in water. The precursor MTs comprising human serum albumin as a wall material and avidin as an interior surface were prepared by alternating layer-by-layer assembly technique using a microporous polycarbonate membrane (1.2  $\mu$ m outer diameter and 24  $\mu$ m length). Cat MTs were self-propelled in aqueous H2O2 medium by jetting O2 microbubbles from the open-end terminus. The velocity of the MTs reached a maximum (120  $\mu$ m/s) at the optimum pH and temperature of Cat. To our surprise, the migration of O2 bubbles was readily visible in the center of the tube because the protein walls were transparent. Furthermore, Cat MTs were digested completely by proteases, showing sufficient biodegradability.





Ms. Natsuho Sugai graduated from Department of Applied Chemistry, Faculty of Science and Engineering, Chuo University. She has studied biofunctional material chemistry under the guidance of Prof. Teruyuki Komatsu. She continues the research on synthesis, structure, and applications of self-propelled protein microtube motors in the Graduate School of Science and Engineering, Chuo University.



# Structural and electrochemical properties of Li- and Mn-rich positive electrode materials exhibiting oxygen activity

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#### Abstract

Energy storage and conversion devices are currently one of the most important goals of the energy strategy. The most popular and most effective systems are Li-ion battery technologies. Ongoing intensive research works enhancing the quality of this technologies are mainly focused on improving the performance parameters of cathode materials [1].

Recently, Li- and Mn-rich positive electrode materials exhibiting oxygen activity are recognized as promising candidates for Liion technologies.  $xLi2MnO3 \cdot (1-x)LiMO2$ , also written as Li[LiyMn1-y-zMz]O2 (M= transition metal) offers access to much higher specific capacity (>250 mAh g-1) and wide voltage range (2.0 - 4.8 V). Additionally, in the electrochemical processes in high voltage region (above 4.5 V vs. Li0/Li+), both transition metal ions and oxygen might take part in a reversible way. However, there is observed an irreversible decrease of the capacity during the first charging cycle leading to partial structural changes. It seems that a promising way to reduce the capacity decrease is a partial Mn substitution with another 3d metal [2].

Herein, we report the structural and electrochemical properties of Li[LiyMn1-y-zMz]O2 layered oxides. Therefore to examine the structural properties XRD and XPS analysis were performed supplemented by SEM studies. Additionally, the Li/Li+/Li[LiyMn1-y-zMz]O2 cell was assembled with intention to make charge/discharge tests, CV and EIS measurements.

Acknowledgement: This work was supported by the Polish Ministry of Science and Higher Education (MNiSW) on the basis of the decision number 0197/DIA/2016/45.

Work was realized by using the infrastructure of the Laboratory of Conversion and Energy Storage Materials in the Centre of Energy AGH.

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W. Li, et al., Chem. Soc. Rev. 46 (2017) 3006–3059.

#### Biography

Katarzyna redel received her B.S. (2015) and M.S. (2016) degrees in Energy Engineering with major in Hydrogen Power Engineering (Graduation with honours) from AGH University of Science and Technology in Krakow, Department of Hydrogen Energy. She is presently a Phd student in the Faculty of Energy and Fuels at AGH University of Science and Technology in Krakow under the direction of professor Janina Molenda. Her primary research interests include fabrication and physicochemical measurements of high-voltage Li-rich cathode materials exhibiting oxygen activity for energy storage and conversion devices.



## Ecofriendly synthesis of gold nanoparticles using low-cost biosorbents from lower Silesia region

#### Dorota Jermakowicz-Bartkowiak, Piotr Cyganowski

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#### Abstract

Various methods of chemical and physical techniques for the syntheses of gold nanoparticles are known. They involve the use of hazardous chemicals that generate huge amounts of waste solutions. Biosorbents are green alternative for the removal and recovery of gold from aqueous solutions. Biosorption-based processes offer advantages including low operating costs, minimization of the volume of chemical sludge to be handled and high efficiency in detoxification of effluents.

We report a simple route for synthesis of gold nanoparticles (AuNPs) by simple mixing of flower of plants, available in Polish Lower Silesian District, with solutions of tetrachloroaurate acid. The studies covered research on reducing potential of Taraxacum officinale (dandelion), Trifolium pratense (clover), Malva sylvestris (mallow), Calendula officinalis (calendula), Forsythia europaea (forsythia). The colloids containing AuNPs were received as the result of combined process of gold Au(III) sorption and its reduction from water and 0.1M HCl solutions containing HAuCl<sub>4</sub>. Bio prepared AuNPs have been characterized using UV-Vis spectroscopy, TEM, XRD, DLS techniques, as well as dzeta-potential measurements. Application of the tested flowers allowed to synthesize "green" AuNPs under biologically-controlled conditions without using neither, harmful reducing agents nor stabilizers. The obtained colloidal suspensions were stable near 1 month after the process at 4°C. The present studies, reveal a triple role of the investigated flowers as they can serve as biosorbents of gold, as well as reducing and stabilizing agents of obtained gold colloids.

#### Biography

Dorota Jermakowicz-Bartkowiak Ph.D., DSc. received her M.D. and Ph.D. degree at the Wrocław University of Technology. She defended her dissertation (2000) titled "Anion exchange resins with guanidyl groups towards the sorption of gold". She is awarded by Polish Ministry of National Education and Sport. Since the 2013 she has been working as an Associate Professor at the Wrocław University Science and Technology. Her current research interests are nanoparticles, biosorbents, recovery of precious metals and rhenium, sorption processes, ion-exchange resins, biodegradable and oxodegradable polymers, microwave-assisted processes for resins preparation and sorption of metals.



# Investigation on mechanical and frictional properties of barium titanate and PVDF using atomic force microscopy

#### Zhiyong Wei, Yajing Kan, Wei Si, Yin Zhang, Yan Zhang\*

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#### Abstract

Electronic friction is an important energy dissipation mechanism in metals and semiconductors due to the coupling of atomic motions and electrons. In this work, the Atomic Force Microscopy (AFM) technique is used to investigate the frictional properties of barium titanate and the PVDF, which are two kinds of piezoelectric materials. Both them can generate polarized charge on the surface under pressure, and thus are ideal materials for studying electronic friction. Specifically, we discuss the effects of surface roughness and surface charge density on the friction. The experimental results show that the friction between the probe and barium titanate or PVDF increases expectedly with the increase of the adhesion or the scanning speed. Furthermore, for barium titanate substrate, the measured friction increases linearly with the positive normal load, which obeys the traditional Amontons law. In contrast, for the PVDF substrate, the relationship between friction and the normal load turns to be nonlinear when the normal load is further enhanced. This may be because the deformation of the piezoelectric substrate generates different surface roughness and surface charge density. Moreover, by applying an external voltage, it is found that the increase in the surface charge density contributes greatly to the increase of friction force observed on the PVDF substrate, while the surface roughness has little effect. Our results may provide helpful evidences for understanding the importance of electronic dissipation in friction.

Dr. Yan Zhang obtained his PhD in Mechanical Engineering from Southeast University in Nanjing, China in 2013. Currently she is an associate professor at School of Mechanical Engineering of Southeast University. Her research interests include nano-tribology and surface technology of 2D materials.



## Overview of the composite nanoceramics prepared by sintering of in-situ made multiphase nanopowders in the bimetallic system aluminum nitride AlN/gallium nitride GaN

## Jerzy F. Janik<sup>1a</sup>, Mariusz Drygas<sup>1a</sup>, Katarzyna Kapusta<sup>1a</sup>, Kamil Wojteczko<sup>1b</sup>, Miroslaw M. Bucko<sup>1b</sup>, Swietlana Stelmakh<sup>2</sup>, Stanisław Gierlotka<sup>2</sup>, Bogdan Palosz<sup>2</sup>

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#### Abstract

High-temperature and high-pressure nanopowder sintering is a viable route to useful materials compacts. Given the advantageous semiconducting/electronic properties of gallium nitride GaN and the electrically resistive/heat-conductive properties of aluminum nitride AlN and Al<sub>x</sub>Ga<sub>1,x</sub>N solid solutions, their composite nanoceramics may exhibit an unusual set of functional properties.

Ammonolytical reactions in a priorly equilibrated mixture of both metals tris(dimethylamides) by either (i) short mixing (SM) of hexane solutions at RT or (ii) in refluxing hexane (RH) resulted in molecularly mixed polymeric gallium imide, aluminum amideimide, and in some cases, bimetallic amide-imide. Nitridation of such bimetallic precursors at 800 and 950 °C resulted in the in-situ formed mixture of composite nanopowders Powd800 (SM and RH) and Powd950 (SM and RH) made of AlN ( $D_{av}$ =2-4 nm), GaN ( $D_{av}$ =25-27 nm) and, occasionally,  $Al_x Ga_{1-x} N$  ( $D_{av}$ =27-35 nm; x=0.5). Sintering of the nanopowders at 7.7 GPa and 650 or 1000 °C yielded ceramic pellets (D=4 mm). Their structural and close range ordering was examined by XRD,SEM, and <sup>27</sup>Al/<sup>71</sup>Ga MAS NMR. Sintering at 650 °C caused no nitride recrystallization/reactions whereas for Powd950\_RH sintered at 1000 °C the content of binary  $Al_{0.5}Ga_{0.5} N$  ( $D_{av}$  = 80 nm) increased from 33 to 85 wt%.

The mechanical properties were probed by the Vickers hardness test,  $H_v$ . For instance, sintering of NP950 at 650 °C yielded  $H_v$  in the range 10-14 GPa and at 1000 °C  $H_v$  dropped to 5-9 GPa. The former  $H_v$  values favorably compare to those for single crystals of AlN, 10-18 GPa, and GaN, 10-12 GPa whereas the latter ones are noticeably lower, possibly, due to recrystallization phenomena and formation of increased proportions of the nitrides solid solution  $Al_{0.5}Ga_{0.5}N$  at 1000 °C.

Acknowledgement: Funded by Polish NCN Grant No. 2017/25/B/ST5/01032.

#### **Biography**

Jerzy F. Janik graduated in 1987 from the University of New Mexico (UNM), Albuquerque, USA (Ph.D. in Chemistry). He spent several years as visiting professor at UNM (1990-1992, 2000-2002) and at Duke University, Durham, USA (1995-1998). Currently, he is a full professor at the AGH University of Science and Technology, Krakow, Poland. He has been involved in research on materials precursor chemistry and nanomaterials characterization of a range of semiconducting and ceramic compounds such as nitrides GaN, AlN, AlGaN, TiN, including sintering of pure GaN and magnetically doped GaN/Mn nanopowders, as well as silicon carbide SiC and SiC/C nanocomposites.



# Comparison of two different metal sulfide systems used in the mechanochemical synthesis of kesterite Cu2ZnSnS4 for photovoltaic applications

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#### Abstract

Kesterite  $Cu_2ZnSnS_{4^2}$  a complex metal sulfide is a prospective material considered for applications in modern photovoltaic cells due to its advantageous semiconductor and environment-friendly properties. The mechanochemical synthesis method of kesterite, which relies on high energy ball milling of precursors, is inexpensive and easy to perform adding to the potential success of kesterite-based solar cells.

This work presents results of research on the synthesis of kesterite using two different metal sulfide systems. The first one contains such sulfides as Cu<sub>2</sub>S, ZnS, SnS, and sulfur S, whereas the second one - CuS, ZnS, and SnS, all in the stoichiometrically required proportions. Initially, each of the precursor mixture was milled in xylene in the high energy ball mill Pulverisette 7 (Fritsch) for 4-20 hours at 900 rpm affording raw powders. In the second step, annealing of the raw powders at 500-550 °C for 6 hours under an argon flow was carried out. Both the raw and annealed powders were examined by XRD, SEM, UV-vis spectroscopy, and solid-state <sup>65</sup>Cu/<sup>119</sup>Sn MAS NMR. The major differences between the two precursor systems are (i) in the specific oxidation states of the elements, especially, copper and sulfur, and (ii) in the complexity of viable redox reactions, which all impact the efficiency of kesterite formation and its purity under applied conditions. Eventually, the final kesterite nanopowders differ in average crystallite size, residual magnetism/NMR resonance efficiencies and, what is very important in practice, the value of the band gap.

Acknowledgement: Study was supported by AGH-UST Research Subsidy No. 11.11.210.373.

#### Biography

Jerzy F. Janik graduated in 1987 from the University of New Mexico (UNM), Albuquerque, USA (Ph.D. in Chemistry). He spent several years as visiting professor at UNM (1990-1992, 2000-2002) and at Duke University, Durham, USA (1995-1998). Currently, he is a full professor at the AGH University of Science and Technology, Krakow, Poland. He has been involved in research on materials precursor chemistry and nanomaterials characterization of a range of semiconducting and ceramic compounds such as nitrides GaN, AlN, AlGaN, TiN, including sintering of pure GaN and magnetically doped GaN/Mn nanopowders, as well as silicon carbide SiC and SiC/C nanocomposites.



## Electrically colour tunable colloid in nonpolar solvents for the color reflective display film

#### Woo Jin Yim, Hyo Sun Bae, Dong Jin Lee and Chul Am Kim\*

NSPECTRA Co., Ltd., Republic of Korea

#### Abstract

The increasing demands for mobile and e-book devices with low power consumption and outdoor readability, reduced eye-fatigue have stimulated comprehensive research into full-color reflective displays that employ color-tunable photonic crystal technologies.<sup>1-3</sup> Photonic crystals (PCs)<sup>4</sup>, materials with a periodic modulation in refractive index, can be sources of exceptionally bright and brilliant reflected colors arising from coherent Bragg optical diffraction<sup>5-6</sup>. In this paper, we describe on the fabrication of a color reflective display film using photonic crystals materials. Monodispersed polystyrene (PS) nanoparticles are polymerized through typical emulsion polymerization process and are functionalized by negatively charged co-monomer to reduce the energy barrier of charge separation and improve the long-range electrostatic repulsive interactions. Then, those particles are successfully dispersed in the organic solvent tetrachloroethylene and manufactured microcapsule. The wall materials of microcapsule were made of gelatin and gum arabic by in situ polymerization. The surface morphology of the microcapsules was observed by optical microscopy. Polyurethane based aqueous solution were chosen as binder materials that support, disperse and protect the microcapsules. The mixture is coated onto the indium tin oxide (ITO) polyester film. The coated layer was dried, and then laminated with conductive adhesive of a patterned electrode plane. Therefore, we demonstrate highly stable colour switches over at least hundreds of cyclic operations, which exhibited changes in colour tunable by the applied voltage.

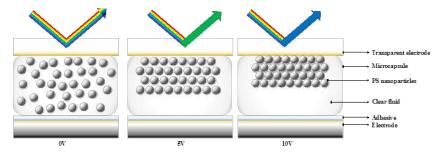
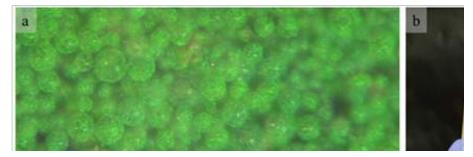


Fig. 1. Cross section of color-tunable photonic crystal reflective display.



**Fig. 2.** (a). Optical microscope photograph of the microcapsules, (b). Color reflective display film images using PS nanoparticles particles at 5 V dc voltage.

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## Quantum-dot microcapsule film for an oxygen and moisture problems

#### Jin seok Song, Hayoung Kim, Dong jin Lee and Chul Am Kim

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#### Abstract

The Quantum-Dot (QD) films use barrier films to solve the oxygen and moisture problems which reduce the optical properties and life times of the QD-LCD. We propose an encapsulation method to solve the oxygen and moisture problems without the barrier film. The QD colloids contain microcapsules were produced using complex coacervation in oil in water, emulsion system. The shells of the microcapsule consist of a gelatin and an acacia gum, which are crosslinked by the coacervation. The diameter of the microcapsules is about 20-25micromiter. The microcapsule were mixed with urethane binders onto PET film and dried. The Flame-s spectrometer was used to evaluate the optic of properties of the QD film with the UV light illumination. The encapsulation method can reduce the thickness of the QD films, the yield losses of the QD materials at a coating process, and the product cost. Also, the encapsulation method can improve the lifetime and the optical properties of the QD-LCD.

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Fig. 1. Optical microscope photography of QD colloid microcapsule

Nowadays one of the focusing issues in graphene technology is the development of functionalized graphene since it expands the range of application of this promising material. Here it is described a new methodology to obtain in situ  $\text{TiO}_2$  quantum dots functionalizing graphene. The oleothermal technique developed uses microwave assisted heating in oleic acid medium and a mild reduction agent to promote the exfoliation and the reduction of graphene oxide, and at the same time, the formation of  $\text{TiO}_2$  quantum dots attached to the graphene layers. The oil-based approach has the advantage to avoid the agglomeration that occurs in hydrophilic material, such  $\text{TiO}_2$ , when aqueous reaction medium is used (conventional hydrothermal process). The water graphene oxide nanodroplet dispersed using ultrasound in the oil medium promotes a close contact between the titanium precursor and the exfoliated graphene, originating quantum dots. It was observed that the temperature, pressure and time used during the oleothermal reaction

affected the degree of reduction, exfoliation and functionalization of the graphene oxide.

Felipe Amorim Berutti<sup>a\*</sup>, Allan R. A. Scharnberg<sup>a</sup>, João Vitor Braun<sup>a</sup>, Annelise Kopp Alves<sup>a</sup>

<sup>a</sup>Universidade Federal do Rio Grande do Sul: Av. Osvaldo Aranha 99/70, Porto Alegre, Brazil, 90035-190

#### Biography

Abstract

Dr. Felipe Amorim Berutti has been Graduated from the Universidade Federal do Rio Grande do Sul, in Brazil, as a Chemical Engineer, with the specialties including Catalysis and Materials Characterization. Later on he obtained his doctorate from the same university with subjects of Ceramic Materials and Characterization and started working at the Interdisciplinary Department of the university as a professor where he has continued his research in materials synthesis and characterization.

## NaLuGdF<sub>4</sub>:Yb<sup>3+</sup>/Er<sup>3+</sup> up-conversion nanoparticles as an optical sensor

## Bui The Huỵ, Yong-Ill Lee\*

Department of Chemistry, Changwon National University, Changwon 51140, Republic of Korea

## Abstract

Upconversion (UC) fluorescence is a process whereby a photon of higher energy is released following the absorption of two low energy photons. For the upconversion processes of the ion releasing light is called the activator. Besides an important part of upconversion materials is sensitizer, which are strong light absorbing ions and use to improve energy absorption process and transfer to a lanthanide based activator. The lanthanide based UC materials exhibit salient properties such as low harmfulness of low energy irradiation to analytes, high chemical stability, non-photobleaching, deep penetration, and non-autofluorescence interference. In this work, we developed novel optical sensor and imaging agent for detection of catecholamines and cell imaging based on NaLuGdF<sub>4</sub>:Yb<sup>3+</sup>/  $Er^{3+}$  (UCNP). The characterizations of the prepared materials were detailed. For sensing catecholamine, the different metals were

decorated on UCNP materials to use as "triggers" for the specific detection. Under the optimum conditions, the limit of detections for catecholamines, dopamine, and epinephrine are 2.8, 2.5, and 2.4 nM, respectively. Besides that, the prepared UC material was used for testing in vitro cell imaging on Hela cells to demonstrate as promising imaging agent. The upconversion and sensing mechanism were proposed.

## Biography

Dr. Bui The Huy has been graduated from Vietnam Academy of Science and Technology, Vietnam as Material

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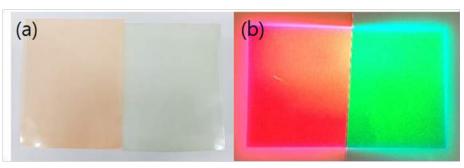


Fig. 2. (a) The QD Film image, (b) The QD Film image by UV light source

Effect of oleothermal synthesis parameters on TiO2 quantum dots functionalized graphene

Science Ph.D. He obtained his post-graduation from Changwon National University, Korea with subject of nanomaterial for biochemistry. He has continued his research as research professor in same university.

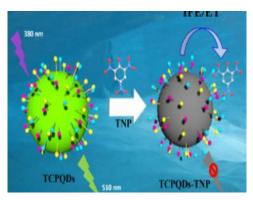
## Paper-based sensors coupled with smartphone for fluorescence detection of phenolic pollutants based on amphiphilic quantum dots

#### Salah M. Tawfik<sup>a,b\*</sup>, Yong-Ill Lee<sup>a</sup>

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#### Abstract

Trinitrophenol (TNP) is considered as a highly toxic material, which severely impacts soil and ground water and presents a considerable health hazard due to its strong solubility in aqueous media. Herein, we present paper-based sensors combined with amphiphilic quantum dots to detect phenolic pollutants. The proposed paper-based sensor could implement visual detection of TNP. The fluorescence of the amphiphilic quantum dots has been quenched by TNP via inner filter effect (IFE), electrostatic,  $\pi$ - $\pi$ , and hydrogen bonding mechanism. The limit of detection down to 0.56 nM during 60 s. Importantly, facile, portable, inexpensive, and easy to operate paper-based sensors have been successfully fabricated for visual detection of TNP (2.29 picogram). The potential of using a smartphone with a color-scanning application in the detection of TNP has also been developed. Furthermore, the detection of TNP in wastewater samples has been successfully described with good recoveries of 98.02–107.50%. This novel paper-based device shows great potential for portable and rapid detection of TNP pollutant in environmental real samples.



#### **Biography**

Dr. Salah M Tawfik has been Graduated from Assiut University as Chemist, with the specialties including Materials Science, Nanotechnology and Organic Chemistry. Later on, he obtained his Ph.D. from Ain Shams University with subjects Materials Science, Nanotechnology and Organic Chemistry and then started working at The Changwon National University, Changwon, South Korea where he has continued his research. His research interests include: New materials, nano materials for optical chemical sensing, for environmental, biochemical and industrial applications; Colorimetric and Fluorescence based sensing systems.



## Tuning the size and composition of nanohydrogels using a "phantom monomer" for biological applications

#### Gerardo Byk and Sarin Palakkal

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#### Abstract

We have designed series of monodispersed nanohydrogels (NHG's) size raging from 20 nm to 400 nm, generated from mixtures of N-isopropylacrylamide, di-block (hydrophilic-hydrophobic) and tri-block (hydrophobic-hydrophilic-hydrophobic) copolymer acrylamide macro-monomer. When the monomers are mixed at high temperature they collapse into well-defined self-assemblies, which can be further polymerized leading to particles with sizes matching the intermediate self-assemblies. The size of the self-assemblies can be tuned/calibrated by combining different ratios of the starting monomers mixtures at high temperature<sup>1</sup>.

Herein, we defined the concept of "phantom monomers" which are the closest structure that mimic a selected monomer but lacks the active function for polymerization. The phantom monomer co formulated with the other monomers will be present in

the intermediate self-assemblies due to their similarity with one of the active monomers, however, upon polymerization, different materials will be generated since the phantom will be excluded due to lack of reactivity. The comparative analyses of the classical systems (first generation) with those obtained with the phantom monomers (second generation) not only put in evidence the self-assembly mediated mechanism, but also prove the generation of new monodispersed NHG's. The second generation NHG's were found to be nontoxic based on the XTT assay. We have observed different loading and different phenotypes of the cells treated with the same amounts of DOX loaded into different NHG's or free as seen by confocal microscopy.

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#### Biography

Gerardo Byk received his PhD (summa cum laude) at the Hebrew University of Jerusalem. In his PhD work, he developed a new generation of peptidomimetic molecules by the introduction of the new concept of backbone cyclization. Since August 1992, he has been in AVENTIS, where he was involved in the development of novel non-viral gene delivery complexes for gene therapy. He joined Bar Ilan University/Israel in 1999, was promoted to Associate Professor in 2002, where he is currently associated with the Marcus Center of Pharmaceutical Chemistry. His main scientific interests: peptide, peptidomimetics, combinatorial chemistry and gene therapy. Lastly, his group entered the field of nanotechnology with the design and development of biocompatible nanoparticles suited both for peptide synthesis, and for in vivo applications.

## Development of selective hydrophilic/hydrophobic treatment towards future application to semiconductor substrate

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#### Abstract

Understanding and controlling wetting phenomena on liquid and solid surfaces is a very important thing not only from a chemical standpoint, but also industrially. Further, in recent years, hydrophobizing agents having various effects according to the application are being studied to meet the diversification of needs. The silane coupling agent is a kind of hydrophobizing agent, and the functional group in the molecule can be combined with the organic material or the inorganic material to modify the surface. In this study, various silane coupling agents were applied to various metal substrates, and control of hydrophobicity and grasp of phenomena were traced by contact angle measurement and XPS measurement.

Hexamethyldisilazane (HMDS) which is a common hydrophobizing agent was vaporized on the  $SiO_2$ , SiN, Cu, Co and W substrates. Moreover, the method in which substrates were immersed in HDMS solution diluted with organic solvents was also carried out. The number of hydroxyl group (-OH) was simply evaluated based on the water contact angle measurement, and the change in functional group was evaluated by XPS.

As a result, it was found that  $SiO_2$  surface became hydrophobic after HMDS treatment while W surface did not. Further, from the XPS, the proportion of -OH decreased after treatment with respect to  $SiO_2$  while -OH proportion in W did not change. Because HMDS reacts with the -OH and changing termination to -CH<sub>3</sub> group, this result suggests that HMDS selectively reacts only to  $SiO_2$ , and hydrophobized while W was not changed.



Mr. Hiroshi Ikari is doing studying for a Master's degree at Tokyo University of Science, with the specialties including Materials Science and Surface Treatment.



# Effective and stable heat modulation by smart window technology using advanced electrochromic and electrophoretic nanomaterials

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#### Abstract

Along with the development of renewable energy technologies, effective management of energy consumption is another key factor to address the increasing global energy demand coupled with the depletion of fossil fuel resources. In 2010, it is reported that more than 32% of global energy was spent in building industry, mainly for lighting as well as to conduct the room heating/cooling for indoor comfort [1, 2]. Recently, this energy consumption has been quickly growing as many modern buildings are commonly assembled with large scale glass window panels, where the effect of heat and light transfer through the windows is significantly enhanced. In this case, smart window technologies possess a huge potential for indoor energy savings due to the ability to modulate the transmittance of heat and light. However, the practical application of smart windows is restricted by the poor effectivity of heat modulation, low visible transparency, or short device lifespan. Our research recently has achieved two novel solutions to improve the performance of smart windows technology. Firstly, the electrochromic technology based on hybrid multilayered  $SnO_2$ -TiO<sub>2</sub>-WO<sub>3</sub> inverse opal nanostructure allows a highly transparent, effective and stable modulation of heat radiation through glass window. During colored state, this material can block approximately 90% of near infrared radiation while allows nearly 70% of visible transmittance. Secondly, the electrophoretic technology using graphene quantum dots thin film is able to control the heat conduction through glass window, with the minimal influence on the transparency. These advanced nanomaterials can significantly promote the application of smart window technology.

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#### Biography

Dr. Tam Nguyen obtained his bachelor degree in engineering physics and nanotechnology from Vietnam National University, Hanoi (VNUH) in 2012. He was also received the Temasek Foundation Leadership Enrichment and Regional Networking (TF-LEaRN) award from National University of Singapore (NUS) in 2012. Later on, he obtained his Ph.D. degree in materials science from Nanyang Technological University (NTU) in 2017. He is currently working as a Research Fellow at School of Materials Science and Engineering (MSE), NTU. His research interests include electro-catalysis and electrochemistry; materials for energy storage and conversion; semiconductor and electrochromic nanomaterials, carbon and graphene-based materials; membranes and polymer thin films.



## Effect of W loading on TiO2 electrochromic properties

## Annelise Kopp Alves <sup>a</sup>\*, Adaiane Parisotto <sup>a</sup>, Anne Esther R. T. P. de Oliveira <sup>a</sup>, Felipe Amorim Berutti <sup>a</sup>

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#### Abstract

Electrochromism is the reversible change in the light transmittance of a material due to an electrochemical redox reaction under the action of an applied potential. These phenomena are useful in applications such as smart windows, energy efficient buildings and displays. The electrochromism can be affected by the oxygen deficiency in the crystal structure of the electrochromic materials. In this context, this work studies the effect of W loading, an oxygen dislocation ion, in the structure of TiO<sub>2</sub> films. The metal-organic precursors materials was transformed in oxides at low temperature (150 °C) using the hydrothermal microwave assisted synthesis route. The obtained materials were deposited as a thin film over a glass substrate previously coated with FTO, using a spin-coater (1500 rpm). The films were characterized using XRD for the identification of the crystalline phases, SEM for analyzing the thickness and morphology of the films, photoluminescence (PL) for the evaluation of the oxygen vacancies, Raman spectroscopy for the identification of the bond structure, visible light transmittance, and color change using the CIELab patterns. A cyclic voltammetry analysis was used to evaluate the insertion/extraction of electrons and ions into/out of the films, causing the reversible color changes. The results indicate that the obtained films have excellent electrochemical reversibility since the values of charge densities are higher than 80%. The diffusion of hydrogen cations and the oxygen vacancies help to increase the optical switching times.

Dr. Annelise Kopp Alves has been Graduated from the Universidade Federal do Rio Grande do Sul, in Brazil, as a Materials Engineer, with the specialties including Materials Science and Ceramic Materials. Later on she obtained her doctorate from the same university with subjects of Nanotechnology and Catalysis and started working at the Materials Department of the university as a professor where she has continued her research in materials synthesis and characterization.



## Effects of phase structure on up-conversion photoluminescence and dielectric performance in Er3+ doped (Bi0. 5Na0. 5)TiO3-BaTiO3 lead-free ceramics

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#### Abstract

The effects of phase structure on up-conversion (UC) photoluminescence (PL) and dielectric properties of lead-free ceramics of  $Er^{3+}$ -doped  $x(Bi_{0.5}Na_{0.5})TiO_3-(1-x)BaTiO_3$  (xNBT-BT:  $Er^{3+}$ ,  $0.00 \le x \le 0.90$ ) were investigated. X-ray diffraction and Rietveld structural refinement analyses were conducted to characterize the phase structure. On increasing the NBT concentration, the crystal structure changes from tetragonal P4mm to P4bm phase. The UC emission is significantly enhanced with the increment of tetragonality, while it begins to decrease upon the occurrence of the P4bm phase. Temperature-dependent UC emission spectra have shown that the optimal emission sample of 0.70NBT-BT:  $Er^{3+}$  exhibits a high color-tuning performance (from green to red). Furthermore, an outstanding thermal stability of UC green emission (65.6% of the initial intensity at 483K) was achieved. The intensity ratio of UC green emission was adopted to reveal the temperature-sensing properties of xNBT-BT:  $Er^{3+}$  ceramics.

## A facile synthesis of supported metal nanoparticles with high dispersion by using the melt-infiltration method

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#### Abstract

The development of an effective synthesis method to prepare supported metal nanoparticles with a desirable structure is strongly demanded to utilize their possible applications as a catalyst because the activity and selectivity of active metal nanoparticles in the supported catalysts is significantly affected by their size and shape, particles dispersion, and nature of support materials.

Among various synthetic methods such as co-precipitation, chemical vapor deposition, microwaves, UV, etc., the melt-infiltration method (solid-state grinding method) has been interested of an easy and fast method to obtain various supported nanocatalysts, which is not including any use of solvents and complex synthetic processes.

In the present work, we report a new simple method for metal nanoparticles supported on porous materials such as  $SiO_2$ ,  $Al_2O_3$ , CMK-3, using melt infiltration process for hydrated metal salt and subsequent thermal reduction of the resulting metal-support complex. This method provided various nanocatalysts such as  $Fe_5C_2@CMK-3$ ,  $Fe_5C_2/Al_2O_3$ ,  $SiO_2@Cu_2O/SiO_2$ , and NiPd@CMK-3 nanocatalysts with well-defined structure and high metal dispersion, which contain highly active particles with the small crystalline sizes below 10 nm. Compared to conventional impregnation and drying method, these nanocatalysts showed high performance to various chemical reactions such as fischer-tropsch synthesis and C-C coupling reactions. [1-4]

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Dr. Shin Wook Kang received his Ph.D in chemistry under the supervision of Sang Woo Han from Korea Advanced Institute of Science and Technology (KAIST), Rep. of Korea in 2015. He is conducting research as a senior researcher in the clean fuel laboratory at Korea Institute of Energy Research (KIER), Daejeon, Rep. of Korea. His research interests are the synthesis of nanomaterials for the catalytic application and the development of chemical process.

## The utilization of nanocellulose as catalyst support for methanol steam reforming

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#### Abstract

Nanocellulose is an environmentally friendly and sustainable polymer material derived from natural resources (i.e. plants). It is five times lighter than iron but has high strength and does not expand even when heated. Due to its high binding force and strength, nanocellulose can be utilized in wide range of applications such as catalysis, sensors, building materials, fuel cells, and packaging materials.

This study will focus on the applications of nanocellulose as a metal catalyst support for methanol steam reforming reaction in order to support hydrogen economy transition. It is known that nanocellulose has several outstanding characteristics to be used as a catalyst support, including high surface area, thermal stability, and it has various natural surface chemistry. Therefore recyclable, more stable and efficient methanol steam reforming catalyst support than the commercial one could be obtained.

Several types of nanocellulose were prepared by freeze-drying and pyrolysis of its solution. The process was followed by dispersing Ni metal precursor by IWI method. The metal dispersion in each catalyst was confirmed by XRD, TEM, and ICP-MS. The performance of catalysts on methanol steam reforming reaction will be evaluated.

## Biography

Mrs. Soohyun Kim was been graduated from Green Energy Technology of Chungnam National University, as Master Degree, with the specialties including new energy process engineering and advanced catalyst material. She is working as a researcher engineer at the Korea Institute of Energy Research after graduated. Presently she has been working on catalytic research to produce hydrogen, especially using carbon-supported catalysts.

## Dipicolylamino quinoline derivative as novel dual fluorescent detecting system for Hg<sup>2+</sup> and Fe<sup>3</sup>

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#### Abstract

Novel quinolinyl oxazolidinonyl dipicolylamine derivatives (QOD) were synthesized via halo-induced cyclization of t-butyl allyl(quinolinyl) carbamate followed by substitution of dipicolylamine (DPA). One of the quinoline derivatives, 6QOD, shows a remarkable fluorescent enhancement in both  $Hg^{2+}$  in aqueous media and  $Fe^{3+}$  in  $CH_3CN$  over other metal ions with a detection limit of 1.01 and 0.22  $\mu$ M, respectively. Moreover, the complexation was proved to be a 1:1 stoichiometric binding by Job's plot and MS data. 6QOD was confirmed to form a bidentate binding with  $Hg^{2+}$  ( $K_a = 6,556 M^{-1}$ ) and  $Fe^{3+}$  ( $K_a = 27,700 M^{-1}$ ) as evidenced by the chemical shifts in <sup>1</sup>H NMR experiments of the DPA protons and the oxazolidinonyl protons in an excellent agreement with the most stable complex structures for both metal ions revealed by the DFT study. Both sensing mechanisms probably involve PET inhibition between the DPA unit and quinoline. The advantage of this 6QOD probe is that it can effectively be applied as a selective  $Hg^{2+}$  and  $Fe^{3+}$  chemosensor by adapting the proper dual-sensing system.





Dr. Waroton Paisuwan graduated in Ph.D. from Department of chemistry, Faculty of science, Chulalongkorn University, Thailand. His work involves methodology of the cyclization of allylcarbamate by using halogenating agent, synthesis of novel fluorescent sensors, and development of sensing materials to use in real sample. Later on he obtained the postdoctoral fund from Chulalongkorn University in 2019 to launch a new project involving the synthesis and development of benzodihydroquinoline and julolidine derivatives as fluorescent sensing materials. Currently, he has been working in Department of chemistry, Faculty of science, Chulalongkorn University, Bangkok, Thailand.



## Ultrasonic observation of H2 gas replacement in a pipe

#### Takuya Kido<sup>a</sup>, Mahjabin Taskin<sup>a</sup>, Ting Pan<sup>a</sup>, Yusei Yamamoto<sup>a</sup>, Masahiro Inoue<sup>b</sup>, and Yoshimine Kato<sup>a</sup>

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#### Abstract

Replacement of H2 (or He) gas from air (or N2) in a new gas pipeline was observed using ultrasound from exterior of a pipe. In this study, experiments of He gas replacement in a straight pipe was conducted under several conditions. It was found that the progress of replacement in the pipe depends on the inclination of the pipe, the flowing resistance and shapes of the pipes. Furthermore, it was also found that, depending on the exit resistance conditions, air or N2 may remain in the pipe. Measurement of gas concentration using ultrasound utilizes difference of sound velocity in various gases. In practice, air in the new pipe is replaced with N2, and then with H2 in sequence. Using the ultrasonic method, the gas concentration in the pipe can be safely monitored from the exterior of the pipe without making a hole. The required N2 amount before H2 gas replacement can be minimized. In the case of the upward inclining pipe, gas replacement is difficult, but comparison of experimental results with multiple types of

outlet attachments revealed an efficient replacement method. This study will help to establish a safe H2 gas concentration measurement and efficient gas replacement for the gas pipelines.

#### Biography



Takuya Kido was born in Hiroshima, Japan, in 1995. He received Bachelor's degree in Engineering from Kyushu University, Fukuoka, Japan in 2018. He has started pursuing his Master's degree in Automotive Science at Kyushu University since April 2018. His research interests are in the fields of gas sensors and ultrasonic technique.

## Performance and durability of flat-tubular solid oxide 3-cell stack in the reversible electrolysis-fuelcell operation

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#### Abstract

**Introduction** – Our study focused on the development of tube-type reversible solid oxide cells (RSOCs) for the mass production of hydrogen and energy storage. The cells employ a flat-tubular design, which have an active area of 100 cm<sup>2</sup>, and a ceramic interconnector in the body, i.e., an all-in-one type. We investigated the influence of the operating conditions, which included the working temperature, mass flow and sequence for mode change of electrolysis cell (EC) and fuel cell (FC), on the performance and durability of RSOC system. The test results of round trip operation of a FC mode and an EC mode for the in-house stacks composed of 3 flat-tubular cells are mainly discussed.

**Experimental** - NiO-YSZ cathode supports were prepared by the extrusion method in the shape of flat tubes [1,2]. YSZ electrolyte layers are coated on the pre-sintered anode supports by dip-conting and then sintered at 1400°C. LSCF cathode and ceramic interconnector are coated on the tubes by screen printing and co-sintered at 1050°C. The active area of the cell is 100cm<sup>2</sup>. The 3-cell stack is prepared by stacking on the metallic frame as can be seen in Fig. 1. The electrochemical performance were investigated including I-V test, long-term stability in FC mode, EC mode and reversible operation of EC-FC mode.



Fig. 1. Image of 3-cell solid oxide cell stack

**Results and Discussion** – Fig. 2 shows the current-voltage and current-power characteristics of the 3-cell stack. The stack's opencircuit voltage (OCV) was 3.5 V, and its power was 133 W at 60A, 2.2V and 700 °C. The long term performance of the stack was stable and showed no degradation during the early part of operation of 100h. The degradation rate of cyclic operation 3.9V (EC mode) and 2.1V (FC mode) also controlled in 5%/50cycle.

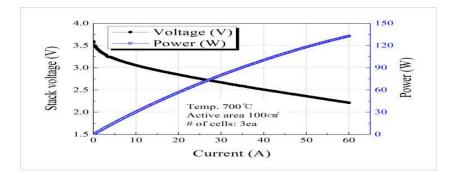


Fig. 2. I-V performance of 3-cell stack

**Conclusions** – The performance and durability of 3-cell stack were investigated in reversible operation mode of electrolysis and fuel cell. For long-term performance, the gas condition and sequence of operation mode should be optimized.

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## Biography

Dr. Sun-Dong Kim has completed his Ph.D. at the age of 31 years from Yonsei University in Korea (south). He worked for hyundai motor company from 2007 to 2010 at the fuel cell vehicle team, and now, he is a principal researcher of Korea Institute of Energy Research which is a government funding research institute in Korea. He has published more than 30 papers in reputed journals, and owned over 40 world wide patents in the field of energy research include fuel cells, high-temperature electrolysis and thermal-to electeic conversion.



# Effects of an inner coating of crystalline GDC nanosol in the porous metal support on the electrochemical properties of metal-supported SOFC cells

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## Abstract

Solid oxide fuel cells (SOFCs) are innovative power generation systems that directly convert chemical energy into electricity and heat without combustion. Recently, the 3rd generation metal-supported SOFCs (M-SOFC) has attracted interest, as it has structural robustness under thermal and mechanical stresses. The use of a metallic substrate provides many advantages, including fast start-up,

vibration resistance, redox cycle stability, sealing reliability, and cost-effectiveness. The improvement of the performance of SOFCs in low-temperature operating environments is necessary for the M-SOFCs. For this, in this work we tried to coat highly crystallized GDC nanosols on the inside of the porous metal-support. The GDC nanosols were synthesized by a sol-gel method using metal-alkoxide precursors. The obtained GDC nanosols were coated on the inside of the porous metal support based NiFe alloy and the Ni/Fe ratio of metal support was optimized. The synthesized GDC nanosols have a high crystallinity with particle size of 2–3 nm, evidenced by TEM. After the GDC nanosol coating, the I-V results show a remarkable improvement in the power density of the button cell (677 mWcm<sup>-2</sup>) compared to that of the uncoated cell (437 mWcm<sup>-2</sup>) at 650 °C. The total area specific resistance (ASR) after GDC nanosol coating significantly decrease from 0.226  $\Omega$  cm<sup>2</sup> to 0.125  $\Omega$  cm<sup>2</sup>. These results reflect that GDC nanosols play an important role in reducing the resistances due to the effective expansion of the triple phase boundary and the improved connectivity of the ionically conductive phase. The inner coating of porous metal supports using nanosized GDC sols led to the improved connectivity of the ionically conductive phase and the effective expansion of the triple phase boundary.

#### Biography

Tae Woo Kim earned his Ph.D. degree in the Department of Materials Science and Engineering at Yonsei University (South Korea) in 2011. He then worked as a postdoctoral researcher at Ewha Womans University in Seoul during 2011–2012 and at the University of Wisconsin-Madison (2012–2015), USA. He is currently a senior researcher in the Korea Institute of Energy Research (KIER). His research interests include the development of environmentally friendly metal oxide-based nanocomposites for use in energy storages (Li-ion battery, supercapacitor), Solid oxide electrolysis cell, photocatalysis, and photoelectrochemical cell.



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