2019 International Symposium on Frontier Materials

Workshop on $Li_4Ti_5O_{12}$ Materials and Supercapacitor Fabrication

November 17-18, 2019
University of Technology Sydney, Australia

Topics:

Lithium Batteries
Electrocatalysts
Electrochemistry
Operando Characterisation
Supercapacitors
Biomaterials
Materials Chemistry

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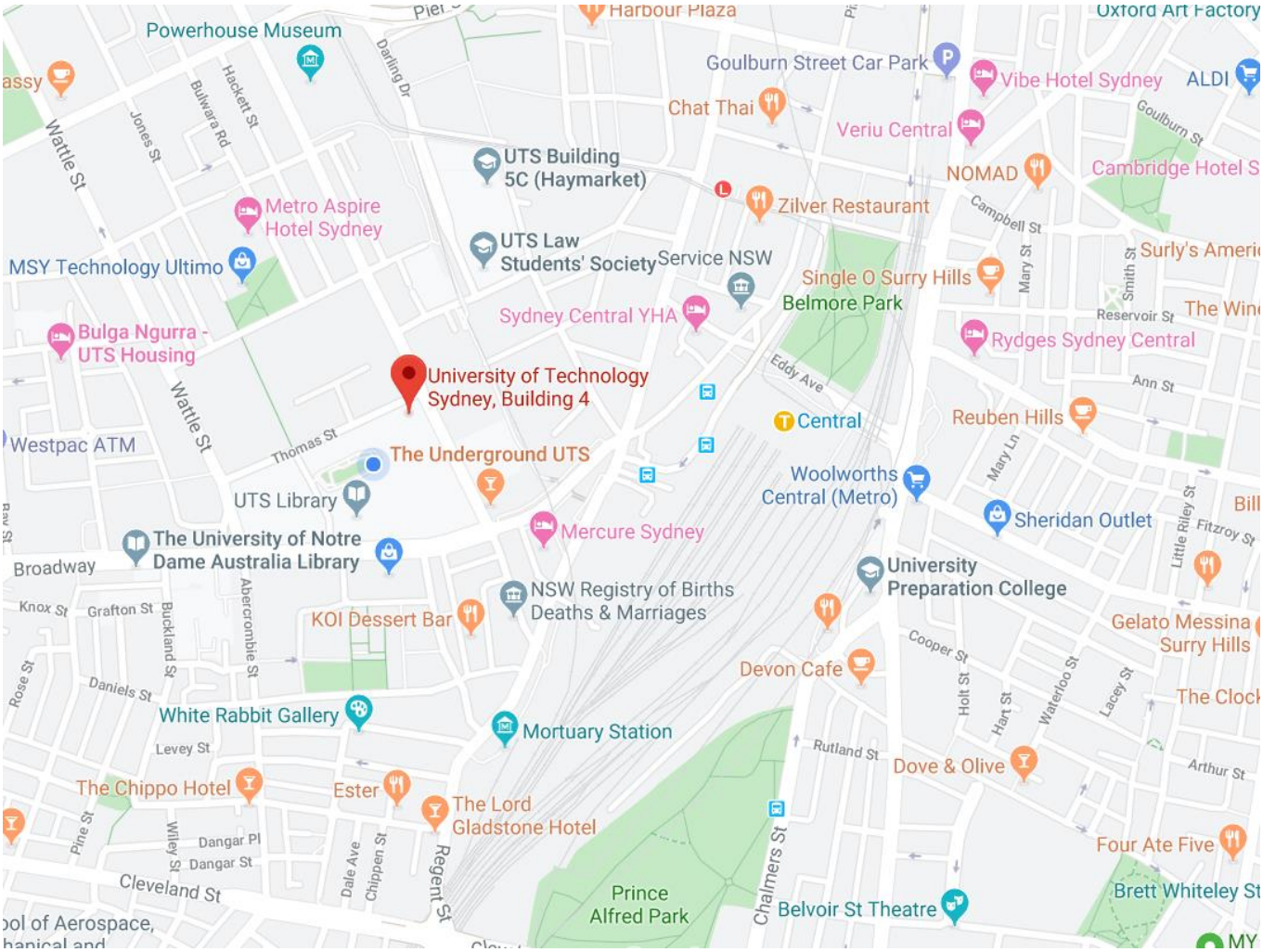
Program of 2019 International Symposium on Frontier Materials

Workshop on $Li_4Ti_5O_{12}$ materials and supercapacitor fabrication

17th November 2019	
18:00	Registration and Reception dinner *Emperor's Garden Restaurant, 96-100 Hay St, Haymarket NSW 2000* (Tel: 02 9211 2135)

18th November 2019 *Room 430, Level 5, Building 4, University of Technology Sydney, 745 Harris St, Ultimo. NSW 2007*	
9:00 – 9:10	Welcoming and Opening Opening Address: Prof. Anthony Dooley Chair: Prof. Guoxiu Wang
9:10 – 10:00	Plenary talk –Yi Cui (*Stanford University)*
10:00 – 10:30	Morning tea
10:30 – 11:10	Plenary talk - Dmitri Golberg (*Queensland University of Technology)*
	Chair: Prof. Yuan Chen
11:10 – 11:30	Keynote talk – Patrick Howlett *(Deakin University)*
11:30 – 11:50	Keynote talk – Mega Kar (*Monash University)*
11:50 – 12:05	Oral talk– Bing Sun (*University of Technology Sydney)*
12:05 – 13:30	Group photo & Lunch
	Chair: Prof. Patrick Howlett
13:30 – 14:10	Plenary talk – Justin Gooding (*University of New South Wales)*
14:10 – 14:30	Keynote talk – Marlies Hankel (*The University of Queensland)*
14:30 – 14:50	Keynote talk – Chuan Zhao (*University of New South Wales)*
14:50 – 15:20	Afternoon tea
	Chair: Prof. Chuan Zhao
15:20 – 15:40	Keynote talk – Qinghong Yuan (*The University of Queensland)*
15:40 – 16:00	Keynote talk – Yuan Chen (*The University of Sydney)*
16:00 – 16:15	Oral talk– Jinqiang Zhang (*University of Technology Sydney)*
16:15 – 17:00	Lab tour
18:00	Conference dinner *Marigold Restaurant, 683 George St, Sydney NSW 2000 (Tel: 02 9281 3388)*

Location of the conference (Room 430, Level 5, Building 4, University of Technology Sydney, 745 Harris St, Chippendale, Ultimo NSW 2007):



Accommodation:

Novotel Sydney Central

Address: 169-179 Thomas St, Sydney NSW 2000

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Plenary Abstracts

MATERIALS AND INTERFACE DESIGN FOR BATTERIES

Yi Cui

Department of Materials Science and Engineering, Stanford University.
Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory.

Abstract

The fast growth of portable power sources for transportation and grid-scale stationary storage presents great opportunities for battery development. How to increase energy density, reduce cost, speed up charging, extend life, enhance safety and recycle are critical challenges. Here I will present more than a decade long research from my lab to address many of these challenges including: 1) Materials design to enable high capacity Si and Li metal anodes and S cathodes. 2) Interfacial design to enhance cycling efficiency of battery electrodes; 3) Battery safety study and strategy; 4) Nanoscale composite solid electrolyte; 5) New battery chemistries for grid scale storage; 6) A breakthrough tool of cryogenic electron microscopy applied to battery materials research, leading to atomic scale resolution of Li metal dendrite and solid electrolyte interphase (SEI) for the first time.

Biography

Yi Cui is a Professor in the Department of Materials Science and Engineering at Stanford University. He received B.S. in Chemistry in 1998 at the University of Science and Technology of China (USTC), Ph.D in 2002 at Harvard University. After that, he went on to work as a Miller Postdoctoral Fellow at University of California, Berkeley. In 2005 he became an Assistant Professor in the Department of Materials Science and Engineering at Stanford University. In 2010 he was promoted with tenure. He has published ~450 research papers and has an H-index of 187 (Google). In 2014, he was ranked NO.1 in Materials Science by Thomson Reuters as "The World's Most Influential Scientific Minds". He is a Fellow of Materials Research Society, Electrochemical Society and Royal Society of Chemistry. He is an Associate Editor of *Nano Letters*. He is a Co-Director of the Bay Area Photovoltaics Consortium and a Co-Director of Battery 500 Consortium. His selected awards include: Dan Maydan Prize in Nanoscience (2019), Nano Today Award (2019), Blavatnik National Laureate (2017), MRS Kavli Distinguished Lectureship in Nanoscience (2015), the Sloan Research Fellowship (2010), KAUST Investigator Award (2008), ONR Young Investigator Award (2008), Technology Review World Top Young Innovator Award (2004). He has founded three companies to commercialize technologies from his group: Amprius Inc., 4C Air Inc. and EEnovate Technology Inc.

NANOMATERIAL PROPERTIES AND FUNCTIONS UNCOVERED USING STATE-OF-THE-ART *IN SITU* TEM METHODS

Dmitri V. Golberg

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

E-mail: dmitry.golberg@qut.edu.au

Abstract

Unveiling properties and functions of a nanomaterial is of key value for its smart integration into modern nanotechnologies. However, in many cases these are measured by means of instruments with no direct access to the material atomic structure, its crystallography, spatially-resolved chemistry and existing defects. Therefore, the acquired results cannot be straightforwardly linked to a particular structure and defect networks. Thus a wide scatter of experimental data has commonly been observed between various samples and research groups. This problem has largely confused engineers and led to many uncertainties with respect to real nanomaterials' application potentials.

In my talk I will demonstrate how modern in situ transmission electron microscopy (TEM) techniques can be effectively employed for a detailed property and function analysis of advanced nanomaterials, e.g. individual nanotubes, graphene-like nanosheets, nanowires, nanoparticles, heterostructures and nanocomposites.1-4

Young's moduli, fracture strength and toughness, plasticity, electrical conductance, thermal gradients, photocurrents and spatially-resolved luminescence of any nanomaterial are now precisely determined inside TEM, while employing piezo-driven probes, sensors, nanomanipulators and/or optical fibers inserted into the microscope column.

Acknowledgements

In situ TEM Project at QUT is supported through an Australian Research Council (ARC) Laureate Fellowship FL160100089 and QUT Projects 322170-0355/51 and 322170-0348/07.

References

1) Golberg D. et al. Adv. Mater. 24, 177 (2012).
2) Kawamoto N., Golberg D. et al. Nano Energy 52, 323-328 (2018).
3) Zhang C., Golberg D. et al. Nano Lett. 18, 7238-7246 (2018).
4) Zhang C., Golberg D. et al. Adv. Mater. (2019); doi: 10.1002/adma.201904094.

Biography

Dmitri Golberg is an Australian Laureate Fellow, Professor and Head of "Inorganic Nanomaterials" Laboratory, Queensland University of Technology (QUT), Brisbane. He joined QUT in 2017 after more than 20 years of his career development in Japan, at the National Institute for Materials Science (NIMS), Tsukuba, where he served as a Nanotube Group Leader and Principal Investigator of the International Center for Materials Nanoarchitectonics (MANA). In 2005 he was also appointed as an adjunct Professor of Tsukuba University. His main research is focused on the synthesis, structural analysis, and physical property measurements of diverse inorganic nanomaterials, e.g. nanotubes, nanowires, nanoparticles and graphene-like nanostructures, in particular, using state-of-the-art methods of in situ transmission electron microscopy. With more than 700 published articles (19 highly cited papers, Web of Science), and more than 42.000 citations (h-109; Scopus), Dmitri is currently ranked within top 250 most-cited world materials scientists.

HOW NANOMATERIALS ARE TAKING US TOWARDS QUANTITATIVE SENSORS BY MONITORING MANY SINGLE MOLECULES

Yanfang Wu, Padmavathy Bakthavathsalam, Roya Tavallaie, Sharmin Hoque, Manish Sriram, Bijan P. Markhali, J. Justin Gooding

School of Chemistry, Australian Centre for NanoMedicine and ARC Centre of Excellent in Convergent Bio-Nano Science and Technology, The University of New South Wales, Sydney, 2052, Australia

E-mail: Justin.gooding@unsw.edu.au

Abstract

Advances in measurement science have seen a progressive reduction in sample size to the point that single-molecule measurements are today relatively common. A new generation of sensors is expected that perform quantitative analysis by measuring many single-molecule events. This talk discusses the challenges and opportunities presented by quantitative single-molecule sensors[1]. It will then cover three technologies developed in out laboratory that allow the detection and quantification of very low numbers of analyte molecules and down to single molecules. In all cases nanomaterials are the key to achieving this. The first is using gold coated magnetic nanoparticles (Au@MNPs) as dispersible electrodes which allow the development of ultrasensitive sensors for proteins and microRNA, even down to just a few thousand molecules [20. The theme of magnetic nanoparticles will then be combined with solid state nanopores for the second development of single molecule protein sensors that can operate in whole blood [3]. The second looks at the application of solid state nanopores and magnetic nanoparticles for the quantitative analysis of rare protein species to give devices with ultralow sensitivity but rapid response time. The final technology that is described is using single molecule localisation microscopy to monitor bioaffinity reactions between surface bound proteins and antibodies [4].

References

[1] J.J. Gooding, K. Gaus, Single molecule sensors: challenges and opportunities for quantitative analysis, *Angew. Chem. Int. Ed.* **55** 11354-11366 (2016).

[2] R. Tavallaie, J. McCarroll, M. Le Grand, N. Ariotti, W. Schuhmann, E. Bakker, R.D. Tilley, D.B. Hibbert, M. Kavallaris, J.J. Gooding, DNA-programmed electrically reconfigurable network of gold-coated magnetic nanoparticles enables ultrasensitive microRNA detection in blood, *Nature Nanotech.* **13** 1066-1071 (2018).

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[4] X. Lu, P. Nicovich, K. Gaus, J.J. Gooding, Towards Single Molecule Biosensors using Super-Resolution Fluorescence Microscopy, *Biosensors Bioelectronics* **93** 1-8 (2017).

Biography

Scientia Professor J. Justin Gooding, FAA, FTSE, FISE, FRSN, FRACI, FRSC

Scientia Professor Justin Gooding is currently an ARC Australian Laureate Fellow, the co-director of the Australian Centre for NanoMedicine and the co-director of the New South Wales Smart Sensing Network. He is a Fellow of the Australian Academy of Science and the Australian Academy of Technology and Engineering. He is the inaugural editor-in-chief of the journal ACS Sensors.

He has published over 400 research papers including Nature Nanotechnology, Nature Biotechnology, Nature Immunology, Nature Communications and Science Advances. He has also authored 14 patents and one text book. His papers have been cited more than 20000 times and his H-index (Scopus) is 68. He has won numerous awards including Eureka Prizes in Scientific Research and Mentoring of Young Researchers, the Faraday Medal of the Royal Society of Chemistry, the Elsevier Biosensors and Bioelectronics Award and the Katsumi Niki Prize in Bioelectrochemistry from the ISE. He has been part of the commercialization teams for a glucose biosensor that is sold worldwide and sustains a company of 200 employees and an Australian based 3D bioprinting company of over 50 employees. He leads a research team of over 40 researchers interested in surface modification and nanotechnology for biosensors, biomaterials, electron transfer and medical applications.

Representative papers

T.M. Benedetti, C. Andronescu, S. Cheong, P. Wilde, J. Wordsworth, M. Kientz, R.D. Tilley*, W. Schuhmann*, J.J. Gooding*, Electrocatalytic nanoparticles that mimic the three dimensional geometric architecture of enzymes: Nanozymes, *J. Am. Chem. Soc.* **140** 13449-13455 (2018).

R. Tavallaie, J. McCarroll, M. Le Grand, N. Ariotti, W. Schuhmann, E. Bakker, R.D. Tilley, D.B. Hibbert, M. Kavallaris, J.J. Gooding*, DNA-programmed electrically reconfigurable network of gold-coated magnetic nanoparticles enables ultrasensitive microRNA detection in blood, *Nature Nanotech.* **13** 1066-1071 (2018).

S.G. Parker, Y. Yang, S. Ciampi, B. Gupta, K. Kimpton, F.M. Mansfeld, M. Kavallaris, K. Gaus, J.J. Gooding*, A unique photoelectrochemical platform for the capture and release of rare single cells, *Nature Comm.* **9** Art. No. 2288 (2018).

E. Hinde, K. Thammasiraphop, H.T.T. Duong, J. Yeow, B. Karagoza, C. Boyer, J.J. Gooding*, K. Gaus*, Pair-correlation microscopy reveals the role of nanoparticle shape in intracellular transport and site of drug release, *Nature Nanotech.* **12** 81-89 (2017).

Y.H. Zheng*, A. Soeriyadi, L. Rosa, S.H. Ng, U. Bach, J.J. Gooding*, Reversible gating of smart plasmonic molecular traps using thermoresponsive polymers for single-molecule detection, *Nature Comm.* **6** Art. No. 8797 (2015).

X. Cheng, E. Hinde, D.M. Owen, S.B. Lowe, P.J. Reece, K. Gaus*, J.J. Gooding*, Enhancing Quantum Dots for Bioimaging using Advanced Surface Chemistry and Advanced Optical Microscopy: Application to Silicon Quantum Dots (SiQDs), *Adv. Mater.* **27** 6144-6150 (2015).

Keynote abstracts

ALKALI ELECTRODES AND INTERPHASES IN SUPERCONCENTRATED IONIC LIQUID ELECTROLYTES AND THE ROLE OF INTERFACIAL STRUCTURE

P.C. Howlett[a,c], M. Armand[a,d], D.R. MacFarlane[b,c], R. Kerr[a,c], M. Hilder[a,c] and M.Forsyth[a,c]

a. Institute for Frontier Materials, Deakin University, Geelong, VIC 3217, Australia. b. School of Chemistry, Monash University, Clayton, VIC 3800, Australia. c. ARC Centre of Excellence for Electromaterials Science (ACES), Deakin University, Burwood, 3125 d. CIC Energigune, Alava Technology Park, Albert Einstein 48, 01510 Miñano Àlava, Spain

Abstract

Alkali metal electrode batteries based on lithium and sodium offer the promise of abundant high-energy battery technologies with the requisite safety, power and energy density performance to meet current and future application demands. Research to develop a safe and reliable metal anode is an important challenge within the field, as is the design and development of safe and stable electrolyte alternatives, both of which may be addressed through the use of Ionic Liquid (IL) based electrolyte systems. Electrolyte advances are also critical for enabling high capacity and high voltage cathodes.

Superconcentrated IL electrolytes have long been at the core of our research for their beneficial device and cycling performance.[1] Thus, we have focused on gaining an understanding of the fundamental aspects of bulk electrolyte transport and interfacial transport in these systems, with the addition of Li or Na salts.[2]

We have demonstrated IL based electrolytes which enable high efficiency Li and Na metal cycling and enhanced cycling stability with a variety of cathode materials.[3-5] This presentation will cover our recent progress in understanding of the role of electrolyte structure and composition on cell performance and on the nature of the SEI.

References

[1] H. Yoon, P. C. Howlett, A. S. Best, M. Forsyth, D. R. MacFarlane, *J. Electrochem. Soc.* **2013**, *160*, A1629.

[2] M. Forsyth, G. M. A. Girard, A. Basile, M. Hilder, D. R. MacFarlane, F. Chen, P. C. Howlett, *Echim Acta* **2016**, *220*, 609.

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Biography

Professor Patrick Howletts' research relates to electrochemical devices (e.g., batteries) and surface engineering through the manipulation of electrode interphases using novel materials approaches. The materials focus of Prof Howlett's research includes ionic liquids, polymer electrolytes, plastic crystal electrolytes as well as their composites and reactive metals such as lithium and sodium. His work also includes the use and development of advanced surface characterisation techniques including synchrotron based sources.

He has published over 180 refereed journal papers and 8 patents, with over 8000 citations and h-index of 44 (Google Scholar). He is a Chief Investigator within both the ARC Centre of Excellence for Electromaterials Science and within StorEnergy where he is a platform leader.

IONIC LIQUID-BASED ELECTROLYTES FOR RECHARGEABLE MAGNESIUM BATTERIES

Mega Kar[*], **Douglas R MacFarlane**[1]

[1] Monash University, Wellington Road, Clayton, Victoria, 3800, Australia

*Email address: mega.kar@monash.edu

Abstract

The current demand for alternative energy storage technologies has inspired many researchers to investigate rechargeable batteries based on low cost, highly abundant and safe metals such as magnesium (Mg). However, one main challenge lies in designing a stable and compatible electrolyte to achieve reduction/oxidation of (Mg) in rechargeable Mg batteries (RMBs). Recently we have reported the synthesis of a weakly-coordinating closo-boron-cluster-based room temperature ionic liquid (RTIL), $[N_{2(20201)(20201)(20201)}][CB_{11}H_{12}]$, with high oxidative stability (Figure 1a), which supports Mg deposition/stripping, [1] making them immensely attractive for high-voltage cathodes and the development of high-energy density RMBs.

The ongoing challenge of common impurities, such as water, which can have a significant effect on the cycle life of Mg, is also addressed in our recent publications. [2][3] Herein we demonstrate the use of trace amounts of a dehydrating agent, $Mg[BH_4]_2$, to achieve stable magnesium deposition/stripping in a mixture of RTIL/organic solvents (**Figure 1b**). [3]

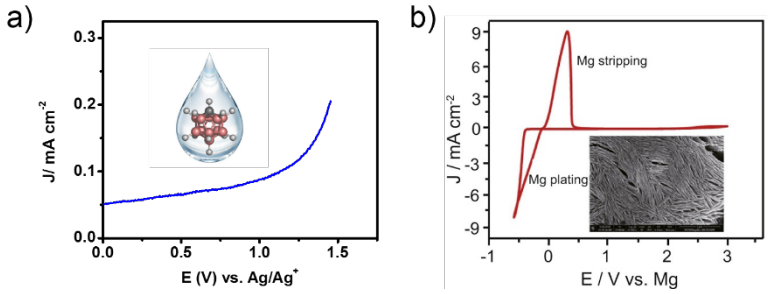

Figure 1: Cyclic Voltammetry illustrating **a)** Anodic stability of $[N_{2(20201)(20201)(20201)}][CB_{11}H_{12}]$ (Substrate: Glassy carbon)[2] and **b)** Mg deposition/stripping from a mixture of RTIL/organic solvent in the presence of $Mg[BH_4]_2$ (Substrate: Platinum). [3]

References

[1] Kar Ma, Tutusaus O, MacFarlane DR, Mohtadi R. Novel and versatile room temperature ionic liquids for energy storage. *Energy and Environmental Science.* 2019; 12:566-571.

[2] Ma Z, Kar M, Ciao X, Forsyth M, MacFarlane DR. Electrochemical cycling of Mg in $Mg[TFSI]_2$/tetraglyme electrolytes. *Electrochemistry Communications.* 2017; 78:29-32.

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Biography

Dr. Mega Kar
Research Fellow[a]
[a]Monash University, Wellington Road, Clayton, VIC, 3800, Australia

Dr. Mega Kar completed her undergraduate degree with honours at The University of Melbourne in 2008. She then went on to study her doctor of philosophy (PhD) at Monash University (2012-2015) in Professor Douglas MacFarlane's group, funded by the *Australian Research Council (ARC), Centre of Excellence for Electromaterials Science (ACES)*. Dr. Kar is currently a Laureate Research Fellow at Monash University, lecturing and specializing in IL synthesis and electrochemistry, working on electrodeposition and metal batteries. Her main research is aimed at designing novel ionic liquids for application in rechargeable magnesium batteries, a collboration project with Toyota Motor Engineering & Manufacturing, North America (TEMA). In 2015, Dr. Kar received ***The Most Promising Woman Scientist*** award at the *6th International Congress on Ionic Liquids*. Recently, Dr Kar has also been awarded the *Faculty of Science Advancing Women's Success Grant* to design workshops or other activities to help overcome cultural and practical barriers with the aim of increasing retention of women in energy science. Along with Professor Douglas MacFarlane and Associate Professor Jennifer Pringle, she has co-authored a textbook titled "*Fundamentals of Ionic Liquid Science – From chemistry to applications*", published in 2017. Dr Kar has also been awarded the Australian-India Early Career Research Fellowship grant (2018) to undertake to undertake further research to investigate new materials for next-generation energy storage.

SYNTHETIC CHEMISTRY OF MULTIFUNCTIONAL STRUCTURAL SYSTEMS

Dan Wang

State Key Laboratory of Biochemical Engineering, Institute of Process Engineering, Beijing 100190 China

danwang@ipe.ac.cn

Abstract

Our group developed a general and widely usable sequential templating approach (STA) to prepare hollow multi shelled structures (HoMSs) by utilizing carbonaceous spheres as templates to adsorb metal ions and heating them to remove the template and generate multiple shells[4,5]. Numerous HoMSs of oxides, sulfide, phosphide, nitride and also heterogeneous have been successfully prepared using STA. The geometric parameters of HoMSs could be controlled by controlling the burning reaction rate of template and crystallization reaction rate of the HoMS. The doping and compositing of graphdiyne (GD) as well as their applications in photorelated and electrorelated catalytic applications. This new carbon allotrope, i.e., GD, has excellent intrinsic electrical, mechanical, and optical properties. When combined with metal nanoparticles, semiconductors or doped with other elements, it can greatly enhance the charge separation and transportation during the photo- or electro- catalytic conversion processes, bridging the gaps between semiconductors or metal nanoparticles by providing good electrical contact and low interfacial resistance. Their excellent performance in photo- or electro-chemical conversion areas suggests they are a cost-effective and superior alternative to the prevalent carbon materials. As-synthesized materials have been applied for broad multi composition efficient electrodes systems.

References

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Biography

Professor Dan Wang is a Professor in the Institute of Process Engineering at Chinese Academy of Sciences (China). He received his bachelor's degree of Science in Chemistry in 1994 and his master's degree of Science in 1997 from Jilin University and completed his PhD in 2001 at Yamanashi University. He received many awards of which in 2013 the National Science Fund for Distinguished Young Scholars award and in 2016 the "CAS Distinguished Research Fellow Program"Distinguished Talents award. His current research focuses on the synthesis of multi-shelled hollow structures and construction of mesostructures, energy conversion and storage, photocatalysis and photosynthesis, drug release and biological detection and bioseparation and bone substitutes. He has published more than 150 papers in peer-review journals with more than 13500 citations and an H-index of 50.

ELECTRODE DESIGN FOR RECHARGEABLE SODIUM-OXYGEN BATTERIES

Bing Sun

Centre for Clean Energy Technology, School of Mathematical and Physical Sciences, Faculty of Science, University of Technology Sydney, Broadway, Sydney, NSW 2007, Australia

Email: bing.sun@uts.edu.au

Abstract

Owing to the superior high energy density, alkali metal-oxygen (air) batteries have been considered as promising advanced battery systems to meet today's stringent requirements as the power source for electric vehicles (EVs). However, the development of metal-oxygen (air) batteries, such as sodium-oxygen batteries, is still constrained by several serious challenges, including low energy efficiency and poor cycle life. The electrochemical performance of sodium-oxygen batteries awaits a dramatic improvement in the design of oxygen cathodes and metal anodes. Herein, we present the synthesis of porous carbon materials and investigate their electrochemical performance as cathode catalysts in sodium-oxygen batteries. Furthermore, a 'sodiophilic' interlayer were designed for dendrite-free sodium metal anodes.[1-5]

References

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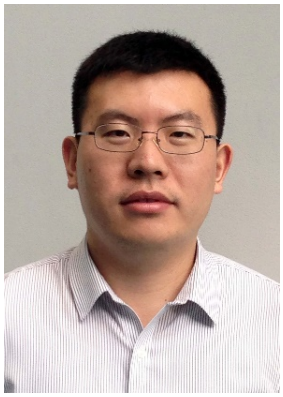
Biography



Dr Bing Sun is a senior research fellow in Centre for Clean Energy Technology at University of Technology Sydney (UTS). He received his bachelor's degree (2005) and master's degree (2007) from Harbin Institute of Technology (HIT) and completed his Ph.D. under the supervision of Prof Guoxiu Wang in 2012 at UTS. In 2018, he received Discovery Early Career Researcher Award (DECRA) from the Australian Research Council. His current research interests focus on the synthesis and characterization of nanomaterials and their applications in energy storage devices such as lithium/sodium-ion batteries, lithium/sodium-oxygen batteries, and potassium-ion batteries. He has published more than 60 papers in peer-reviewed journals with more than 4000 citations and H-index of 33.

ENABLING CARBON NITRIDE MATERIALS AS LITHIUM ION BATTERY ANODE MATERIALS THROUGH FUNDAMENTAL UNDERSTANDING

Marlies Hankel

Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, Brisbane, Australia

Abstract

Carbon structures have been extensively studied over recent decades as energy storage materials. One of the industry applications is as the anode of lithium (Li) ion batteries (LIBs). Graphite, a layered material consisting of sp2 bonded carbon sheets, is currently the predominant anode material offering a theoretical capacity of LiC6 with Li inserted between the layers.

Doping carbon materials with nitrogen has been shown to increase the storage capacity if used as an anode material. Graphitic C3N4 is a well-known and widely used material with a high nitrogen content. However, it is not suitable as a LIB anode material, as its interaction with lithium is too strong so that the lithium cannot be discharged again.

We have performed comprehensive studies of a range of carbon nitride materials to understand the mechanism of the interaction of the lithium with the carbon nitride material. We have modified graphitic C3N4, by breaking it into ribbon like structures and combining it with a carbon backbone, to increase its reversible storage capacity and to provide a path to harness carbon nitrides as lithium ion anode materials.

Density functional theory (DFT) calculations are employed to obtain the maximum lithium storage capacity. We also calculate diffusion barriers for the lithium movement from one site to another to determine their mobility. In addition to this we also show how the lithium binds to the material by consideration of the charge density distribution and the charge transfer from the lithium to and from the material. The volume change of the material on the insertion of lithium is determined by employing a bilayer or bulk configuration of the material. Our calculations are combined with experimental investigations. These interdisciplinary studies confirm that modified carbon nitrides could be suitability as LIB anode materials. They show that combining experiment with the fundamental understanding of calculations can provide a pathway to designing new LIB anode materials.

Biography

Dr Marlies Hankel is a computational scientist who's main research interest is in two dimensional (2D) materials for energy applications. These include lithium ion battery anode materials, aluminium ion cathode materials, gas sensing and capture. In her capacity as a eResearch analyst she also manages the AIBN high performance computer cluster, UQ's and QCIF's share of computer time on the national facilities (NCI) and access to UQ's FlashLite data and memory intensive cluster.

Dr Marlies Hankel is currently a Senior Research Fellow in the Theory and Computation group at the Australian Institute for Bioengineering and Nanotechnology at The University of Queensland. She obtained her Master degree in Mathematics from the University of Darmstadt (Germany). She then moved to Bristol (UK) and also changed her main subject to obtain her PhD in Chemistry which she achieved in 3 years. She was awarded a University of Bristol Scholarship. After a 2 year postdoc in Manchester (UK) she moved to UQ in 2004. At UQ she established an international profile as an expert in methodologies for atom-diatom reactions. In 2011 she started her position with QCIF and RCC and her work to promote computational resources to researcher and make computational resources more accessible. Her more recent work on lithium ion battery materials resulted in the award of a UQ Promoting Women Fellowship in 2014 and an ARC-DP grant in 2017. She is now an independent researcher in 2D materials for energy applications.

CARBON COMPOSITES FOR ONE-DIMENSIONAL SUPERCAPACITORS

Prof. Yuan Chen

School of Chemical and Biomolecular Engineering
The University of Sydney, Sydney, Australia

yuan.chen@sydney.edu.au, http://yuanchenlab.weebly.com/

Abstract

One-dimensional (1D) supercapacitors have arisen as a promising candidate to power emerging electronics in recent years, because of their unique advantages in energy storage and mechanical flexibility. Fiber electrodes are the most critical component in 1D supercapacitors, which enable efficient energy storage and provide suitable mechanical stability. Carbon nanomaterials with excellent electrical conductivity and large specific surface area, are ideal electrode materials for fabricating fiber electrodes. The challenge is to integrate nanoscale materials into macroscale fibers without losing their desirable properties. This talk will summarize our efforts in the synthesis of carbon composite fibers for 1D supercapacitors with tailored energy storage capacities, as well as innovative approaches for integrating multiple 1D supercapacitors into three-dimensional energy storage units to reduce device footprints.

Biography

Professor Yuan Chen received a bachelor's degree from Tsinghua University and a Ph.D. from Yale University. He joined the University of Sydney in 2015. His research focuses on carbon materials and their sustainable energy and environmental applications, including supercapacitors, batteries, electrocatalysts, membranes, and antibacterial coatings. He is a Fellow of the Institution of Chemical Engineers, the Royal Society of Chemistry (UK) and the Royal Australian Chemical Institute. He received the Australian Research Council Professorial Future Fellowship in 2016, an Excellence in Review Award from Carbon in 2015, a Young Scientist Award from the Singapore National Academy of Science in 2011. He is currently serving as an editor for Carbon (Elsevier). He also serves as Chair for Australian Carbon Society and Asian Association of Carbon Groups since August 2017.

THEORETICAL EXPLORATION ON THE STRUCTURE AND ELECTRONIC PROPERTIES OF TWO-DIMENSIONAL CARBON-NITRIDE MATERIALS

Qinghong Yuan1,2*, Saiyu Bu1,2, Nan Yao3, Debra Bernhardt1,4

[1] *Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, Brisbane, QLD, 4072, Australia*
[2] *State Key Laboratory of Precision Spectroscopy, East China Normal University, 3663 N. Zhongshan Road, Shanghai 200062, People's Republic of China.*
[3] *College of Teacher Education, East China Normal University, 3663 N. Zhongshan Road, Shanghai 200062, People's Republic of China.*
[4] *School of Chemistry and Molecular Biosciences, The University of Queensland, Brisbane, QLD, 4072, Australia.*

Email address: qinghong.yuan@uq.edu.au

Abstract

The lack of an intrinsic bandgap in graphene restricts its use as a field-effect transistor and consequently its applications in integrated logic circuit. [1] Incorporating nitrogen atoms into graphene lattice is a promising approach to tune the electronic properties of graphene. [2] However, precise control of the nitrogen doping remains a long-standing challenge because the incorporation of nitrogen atoms into the matrix of sp2-bonded carbon can lead to appearance of different kinds of nitrogen impurities, such as graphitic, pyridinic, and pyrrolic nitrogen.[3] By using Calypso and DFT calculations, we studied the structures and electronic properties of a series of two-dimensional (2D) carbon-nitride (CxNy) materials. It is found that the 2D CxNy materials with low N concentration (x/y>3) have honeycomb structure with only graphitic N. For materials with higher N concentration (x/y < l/3), structures with only pyridinic N and hexagonal or triangular holes are more stable. The 2D CxNy structures have variable bandgap, electron and hole mobilities, which may have potential applications in both electronic devices and catalysis.

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[3] Wang H.; Maiyalagan T.; Wang X. ACS Catal. 2, 781, 2012.

Biography

Qinghong Yuan received her Doctoral Degree in Theoretical Chemistry from the Chinese University of Hong Kong in 2010. After working in Hong Kong Polytechnic University as a postdoctoral researcher, she was appointed as an associate professor in 2012 and was promoted to a full professor in 2015 in the department of physics, East China Normal University. Qinghong Yuan got a DECRA fellowship from the ARC in 2016. Her research interest focuses on theoretical study of low-dimensional nanomaterials, including the mechanism of chemical vapour deposition growth of graphene and carbon nanotubes, theoretical design of new carbon nanomaterials, and catalysis. Her research, sponsored by the National Science Foundation, Shanghai Science and Technology Commission, ARC etc, resulted in over 40 peer-reviewed papers in high impact journals, including Nat. Mater., Nat. Commun., J. Am. Chem. Soc., Phys. Rev. Lett., Adv. Mater., Adv. Funct. Mater, Angew. Chem. Int. Edit., ACS Nano, and Adv. Sci. etc.

EARTH ABUNDANT ELECTROCATALYSTS FOR HYDROGEN ENERGY CONVERSION AND STORAGE

Chuan Zhao

School of Chemistry, UNSW Sydney

chuan.zhao@unsw.edu.au

Abstract

The increasing demands for clean energy have triggered tremendous research interests on electrochemical energy conversion and storage systems with minimum environmental impact. Hydrogen holds the promise as energy carriers for global scale storage of renewable energy, e.g., solar and wind, enabling the continuous usage of these diffusive and intermittent energy sources when used together with fuel cells.1,2 Nevertheless, the widespread application of hydrogen technology has been severely constrained by the use of precious metal catalysts, such as oxides of ruthenium and iridium for the oxygen evolution reaction (OER), and platinum for the hydrogen evolution reaction (HER) and oxygen reduction reactions (ORR). Furthermore, electrochemical CO2 reduction reactions (CRR) and nitrogen reduction (NRR) provide alternative pathways for hydrogen storage and transport. These emerging technologies also call for highly efficient and selective catalysts to promote their industrial viabilities.

This presentation shows our efforts in developing non-precious metal-based, carbon-based and metal-organic framework (MOF)-based electrocatalysts for key hydrogen conversion reactions, as well as our strategies for enhancing these catalysts by nanostructuring to a level comparable to that of precious metal catalysts.[3-12] The commercialisation of some our catalysts in hydrogen industry also will be highlighted.

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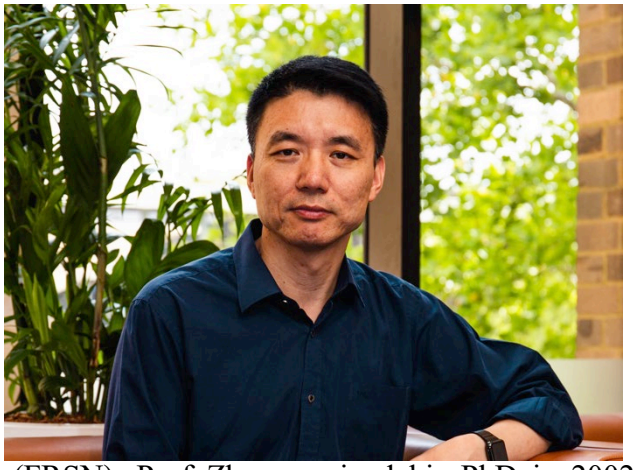
Biography



Chuan Zhao is a Professor at the School of Chemistry at the University of New South Wales (UNSW), and the Head of UNSW Nanoelectrochemistry Lab of ~30 researchers. He also holds a Future Fellowship from Australian Research Council. He currently is the Chair of the Royal Australian Chemical Institute (RACI) Electrochemistry Division, and elected the Fellow of Royal Society of Chemistry (FRSC), Fellow of RACI (FRACI) and Fellow of Royal Society of New South Wales (FRSN). Prof Zhao received his PhD in 2002 with an excellence award from Northwest University, then completed postdoctoral research at University of Oldenburg and Monash University. He started his independent research career as a Lecturer at UNSW in Oct 2010, and was promoted to full Professor in 2017.

Prof Chuan Zhao is interested in discovering novel electroactive nanomaterials and their implications to electrochemical energy storage and conversion, and sensors applications including water splitting, hydrogen fuel cells, CO2 & N2 reduction, and batteries. He has published more than 150 high impact research papers, and holds >10 patents of which 8 have been commercialised.

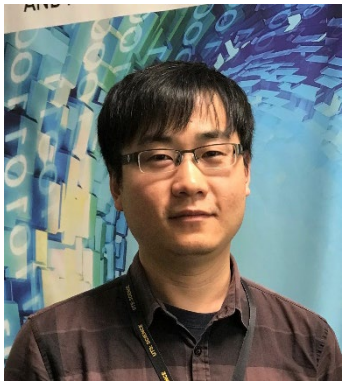
REFINING STRUCTURES OF ELECTROCHEMICAL CATALYSTS FOR LI-O_2 BATTERY AND ELECTROCATALYSIS

Jinqiang Zhang

Abstract

The development of highly efficient catalysts to improve the electrochemical performances is urgently needed due to the ever-increasing demand for energy storage and conversion devices in the last few decades. Lithium-oxygen (Li-O_2) battery and electrochemical water electrocatalysis are the two representatives respectively for the next-generation energy storage and conversion. However, the electrochemical performances are still not satisfying to be potentially used in industry applications. Here we present our recent research on developing redox-enabled small organic molecules for Li-O_2 battery and single-atom catalysts for electrocatalysis application. We show that by carefully designing and tailoring the molecular and electronic structures, the efficiency of the applied catalysts could be maximized which would be highly beneficial for the electrochemical performances in their individual applications. For instance, TEMPO-modified ionic liquid could stabilize the lithium anode and prolong the cycle life of Li-O_2 battery, while *in-situ* exfoliated MXene coupled with single Pt atoms show a mass activity more than 40 times higher than the commercial Pt/C. All these provide theoretical and experimental guidance to develop highly efficient catalysts for both Li-O_2 battery and electrocatalysis in the future.

Biography



Jinqiang Zhang Received his Master of Science at 2013 and PhD at 2018 from University of Technology Sydney. He is working as postdoctoral research associate at Centre for Clean Energy Technology (CCET), University of Technology Sydney. He works intensively on redox organic materials for lithium-oxygen batteries and single-atom catalysts for electrocatalysis, as well as their functional mechanisms.