Hong Kong Symposium of Batteries

17-18 December 2018

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The Hong Kong Polytechnic University

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Welcome Speech

Professor P.K. Alex Wai

Vice President (Research Development)
The Hong Kong Polytechnic University

Good morning, Ladies and Gentlemen!

On behalf of the Hong Kong Polytechnic University, I welcome all of you, distinguished speakers and participants, to this Hong Kong Symposium of Batteries.

With 7.5 million people, five world renowned universities and GDP per capita of about 38,000 USD, Hong Kong scientists and engineers have the responsibility to advance the frontiers of knowledge while enhancing the well-being of the local, mainland and international community. In fact, we have been doing this in the past couple of decades. Take PolyU for example, be it pioneering fibre optic railway technologies that have been applied in Hong Kong, Singapore MTR, investigational new drugs (IND) granted by US FDA for anti-cancer, robotics or food safety, we are marching forward with the leading experts in the world in a number of applied research areas.

Energy is known to be the top challenge humanity faces currently. Smart and sustainable energy is the must for a sustainable development of the society. For effective usage of sustainable energy, especially solar, wind energies, the effective energy storage is essential. The electrification of urban transportation calls for the supply of high capacity batteries with safe operation at low cost. All such challenges need collective efforts from scientists and engineers to meet them.

This symposium serves as a great meeting place for our battery researchers to exchange ideas and disseminate research findings with international eminent colleagues. It is the first of its kind in Hong Kong, thanks to the generous sponsorship from GP Batteries, wishing Hong Kong become a recognized battery R&D hub in the world. I am sure that our sponsor’s wish will be realized because of your active participation in the symposium, and because of the collaboration with top researchers around the world, because of the increased R&D support pledged by the Chief Executive Officer of Hong Kong, and also the opportunities made available from Mainland China through the Greater Bay Area development, and the direct participation of Hong Kong researchers in National Key Projects administered through Ministry of Science and Technology (MOST), etc.

I would like to invite you to visit campus of HK PolyU, to visit the university facilities we have established including materials characterization facility, and to talk with our faculty and students. We encourage and welcome collaborations. In order to facilitate such collaborations, I am pleased to inform you that the Research Committee of HK PolyU has just approved the establishment of “Research Centre of Advanced Materials for Batteries”, with Prof. Guohua Chen, this Symposium Chairman, being the founding director.

Ladies and gentlemen, you are working in an exciting field and making great impact on the sustainable development of the world. Congratulations! I would like to take this opportunity to wish you a joyful and fruitful symposium.

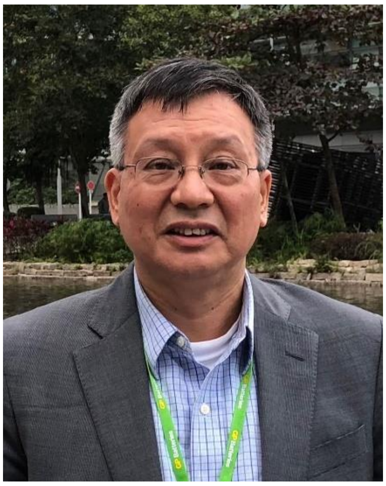
Wish you all a very Merry Christmas and Happy New Year!

Opening Remarks

Dr. Mingde Wang

Head of Center of Excellence-RD (Acting)
Head of Strategic Business Unit-Lithium,
GP Batteries International.

Ladies and Gentlemen:



First of all, on behave of GP Batteries International, I'd like to thank the Organizing Committee for their very well putting together of the symposium for the batteries in Hong Kong PolyU and thank all the speakers and participants for attending this event.

I believe this symposium is the first one held in Hong Kong, joined by mostly Hong Kong academia, research and development institutions and companies. A good portion of the program also consists of research and development from Hong Kong. This is exciting for us, because this is the first time which we, at GPI, can meet, hear and learn from professors and researchers here locally in Hong Kong and explore opportunities for cooperation to make Hong Kong a spot on the global map of batteries and related materials.

This excitement is further enhanced by the excellent speakers and topics from other countries and regions, which I believe, represent the most updated and forefront research in the areas of batteries and related materials. We are also glad to see the scopes of the topic covers a wide range of battery systems, materials and ways for analysis and modeling. This truly shows that the programs reconcile quite well with the theme of Hong Kong Symposium of Batteries.

I hope all of us enjoy the symposium by hearing, interacting and learning. I wish a great success of the symposium.

Plenary Lecture 1

Advances in NiMH Battery Technology for Energy Storage

Michael A. Fetcenko
President, Ovonic Battery Company

Abstract

Li-Ion battery chemistry dominates consumer and electric vehicle applications due to extremely high energy and impressive commercial cost reduction since introduction in 1991. NiMH was introduced at the same time and became an industrially important battery chemistry in consumer applications due to drop-in replacement of primary alkaline and hybrid electric vehicles due to exceptional safety, power, cycle life, cost and recycle capability. Stationary energy storage applications are presently dominated by lead-acid chemistry due to low cost and that specific energy and energy density are not as critical. Advantages of NiMH technology for energy storage applications will be presented.

Biography:

Michael Fetcenko is President of Ovonic Battery Company, the inventor and licensor of Nickel-Metal Hydride batteries worldwide with over 40 licensees. Ovonic was acquired by BASF in February 2012 where he became Managing Director of BASF Battery Materials North America and Director of Global Licensing. He has over 35 years of experience in the battery industry and has led the R&D, scale-up and commercialization efforts of NiMH batteries with over 70 patents and 100 publications in the NiMH and Li-Ion battery field. His inventions are used in all NiMH batteries for consumer, stationary, and hybrid vehicle applications such as the iconic Toyota Prius with over 10 million vehicles on the road. Mr. Fetcenko directs commercial battery activities in North America for all battery chemistries such as NiMH, Li-Ion, Li-S and solid state including R&D, manufacturing, sales and marketing. He directs battery intellectual property activities globally. He serves on the Board of Directors and Technical Steering Committee for Sion Power, a leader in advanced Lithium systems including Li-S and protected metallic anodes for Li-Ion batteries.

Plenary Lecture 2

Using Synchrotron X-ray and Neutron Based Scattering combined with TEM and TXM imaging Techniques to Study the New Cathode Materials for Batteries

Enyuan Hu[1], Seong-Min Bak[1], **Xiao-Qing Yang[1*]**, Xiqian Yu[1, 2], Yong Chu[3], Zulipiya Shadike[1], Ruoqian Lin[1], Hung-Sui Lee[1], Yuguo Guo[4], and Yijin Liu[5]

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Abstract

The new results of using *in situ* and *ex situ* synchrotron based x-ray techniques, such as x-ray diffraction (XRD), x-ray absorption spectroscopy (XAS), transmission electron microscopy (TEM), transmission x-ray microscopy (TXM), *in situ* X-ray fluorescence (XRF) microscopy combined with X-ray absorption spectroscopy (XAS), as well as x-ray pair distribution function (XPDF) and neutron pair distribution function (NPDF) on advanced battery materials will be discussed. Studies on several new materials, such as high nickel content layer structured materials, Li-rich and Mn-rich materials as high energy density materials for Li-ion batteries and Li-metal batteries will be presented.

Acknowledgement

The work at Brookhaven National Laboratory was supported by the Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Vehicle Technologies of the U.S. Department of Energy through the Advanced Battery Materials Research (BMR) Program, including Battery500 Consortium under Contract No. DE-SC0012704.

Biography:

Dr. Xiao-Qing Yang is the group leader of the electrochemical energy storage group in the Chemistry Department of Brookhaven National Laboratory (BNL). He is the Principal Investigator (PI) for several Battery Material Research (BMR) programs including the Batter500 consortium at BNL funded by the Office of Vehicle Technologies, EE&RE, U.S. Department of Energy (USDOE). He has been invited to give presentations at international conferences, as well as at DOE organized workshops in battery research. He has served as organizer and Co-Chairman of many international conferences on lithium battery research, such as the IBA2007 (International Battery Material Associate meeting 2007 in Shenzhen, China), and the IMLB2008 (International Meeting of Lithium Battery 2008 in Tianjin, China). He received the "2012 Vehicle Technologies Program R&D Award" from the Vehicle Technologies Office of EE&RE, USDOE in May, 2012. In January 2015, he received the 2015IBA Research award from the International Battery Association (IBA). He is one of the leading principal investigators (PIs) of the USDOE funded Battery500 project.

Plenary Lecture 3

Tackling Challenges in Flow Cells Using Thermo-fluid Sciences

T.S. Zhao
Cheong Ying Chan Professor of Engineering and Environment
Chair Professor of Mechanical & Aerospace Engineering, HKUST
Director of the HKUST Energy Institute
Senior Fellow of the HKUST Institute for Advanced Study

Abstract

The combination of energy shortage and climate change is one of the most complex challenges the world, as a whole, has had to face. The next 50 years is a vital period for human civilization and it is imperative that we revolutionize the way we produce and store energy and incorporate renewables as our primary source of energy. This talk will provide a snapshot of the future of the sustainable energy landscape and identify several game-changing technologies that will facilitate the widespread deployment of renewables. In particular, we will highlight our recent advances in redox flow batteries, fuel cells, and lithium-oxygen battery technologies achieved through an interdisciplinary approach that combines thermal-fluid science and electrochemistry. The scientific issues and practical challenges pertaining to this advanced battery will be discussed, with a particular emphasis on how the challenges can be addressed using thermos-fluid sciences.

Biography:

T.S. Zhao is an elected Fellow of the American Society Mechanical Engineers (ASME), Fellow of the Royal Society of Chemistry (RSC), and a Highly Cited Researcher by Thomson Reuters (2014, 2015, 2016, 2017, 2018).

Professor Zhao combines his expertise in research and technological innovation with a commitment to creating clean energy production and storage devices for a sustainable future. He has made seminal contributions in the areas of fuel cells, advanced batteries, multi-scale multiphase heat and mass transport with electrochemical reactions, and computational modeling. In addition to 5 edited books, 9 book chapters and over 70 keynote lectures at international conferences, he has published 331 papers in various prestigious Journals. These papers have collectively received more than 14,000 citations and earned Prof Zhao an h-index of 62 (Web of Science). In recognition of his research achievements, Prof Zhao has in recent years received many awards, including the 2014 Distinguished Research Excellence Award (HKUST), two State Natural Science Awards, Ho Leung Ho Lee Scientific and Technological Advancement Award (2018), the Croucher Senior Fellowship award, the Overseas Distinguished Young Scholars Award (NSFC), and the Yangtze River Chair Professorship, among others.

In the international community, Prof Zhao serves as Editor-in-Chief of *Applied Thermal Engineering,* Executive Editor of *Science Bulletin,* and Editor of RSC's *Energy & Environmental Science*. He has served as an editorial board member for *Energy & Environmental Science*, *Journal of Power Sources*, and other 10 prestigious international Journals.

Plenary Lecture 4

Material-Gene and Structure Electrochemistry of Li-ion battery

Feng Pan (National 1000-plan Professor，Founding Dean)

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Abstract

Insight into relationship between Crystal/Interface structure and properties of capacity, stability and rate capability are important for developing advanced Li-ion batteries. Using theoretical calculations combined with experimental in-situ tests, we did extensive studies on the kinetic of Li-ion diffusion for two representative cathode materials: layered $Li(Ni_xMn_yCo_z)O_2$ (NMC) ($x + y + z = 1$) and $LiFePO_4$. We not only focus on the bulk kinetics, but also the kinetics across electrode/electrolyte solid-liquid interface and in the electrolytes. For example, we first proposed that "Janus" solid-liquid interface would facilitate the Li-ion transport in battery and introducing some disordering in non-active cathode materials would activate them for Li-ion storage.（**Ref. 1**）

For high energy and power density applications (e.g., EVs), the safety becomes especially important. Using ab initio calculations combined with experiments, we clarified how the thermal stability of NMC materials can be tuned by the most unstable oxygen, which is determined by the local coordination structure unit (LCSU) of oxygen ($TM(Ni, Mn, Co)_3$-O-$Li_{3-x'}$): each O atom bonds with three of transition metal (TM) from the TM-layer and three to zero of Li from fully discharged to charged states from the Li-layer. Under this model, how the lithium content, valence states of Ni, contents of Ni, Mn, and Co, and Ni/Li disorder to tune the thermal stability of NMC materials by affecting the sites, content, and the release temperature of the most unstable oxygen is proposed. In NMC, insight of Ni/Li disorder has be investigated by theory and experimental e.g. neutron powder diffraction experiments and magnetization measurements. The spins of TM ions construct a two-dimensional triangular networks, which can be considered as a simple case of geometrical frustration. Remarkably, the frustration parameters of these compounds are estimated to be larger than 30, indicating the existence of strongly frustrated magnetic interactions between spins of TM ions, which give rise to lattice instability, the formation of Li/Ni exchange in NMC will help to partially relieve the degeneracy of the frustrated magnetic lattice by forming a stable antiferromagnetic state in hexagonal sublattice with nonmagnetic ions located in centers of the hexagons. Moreover, Li/Ni exchange will introduce 180° superexchange interaction, which further relieves the magnetic frustration through bringing in new exchange paths. Thus, the variation of Li/Ni exchange ratio vs. TM mole fraction in NMC with different compositions can be well understood and predicted in terms of magnetic frustration and superexchange interactions. **(Ref. 2)**

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Biography:

Prof. Feng Pan, National 1000-plan Professor, Founding Dean of School of Advanced Materials, Peking University Shenzhen Graduate School, Director of National Center of Electric Vehicle Power Battery and Materials for International Research, got B.S. from Dept. Chemistry, Peking University in1985 and PhD from Dept. of P&A Chemistry, University of Strathclyde, Glasgow, UK,with "Patrick D. Ritchie Prize" for the best Ph.D. in 1994. With more than a decade experience in large international incorporations, Prof. Pan has been engaged in fundamental research and product development of novel optoelectronic and energy storage materials and devices. As Chief Scientist, Prof. Pan led 8 entities in Shenzhen to win the 150 million RMB grant for the national EV-battery innovation project in 2013-16. As Chief Scientist, Prof. Pan led 12 entities to win National Key project of Material Genomic Engineering (MGI) for Solid State Li-ion Battery in China in 2016. He has led his group to achieve outstanding research vs. MGI on electrochemistry, battery and materials by combination of comprehensive experimental tests and theoretical calculations, e.g. developing novel cathode materials and methods to study related electrochemical mechanism, and exploring new generation of solid state batteries. He has published more than 250 peer-reviewed papers in international journals and book chapters and 80 patents for inventions. He has been selected as one of the 2016 winner of Outstanding Research Award of Advanced Lithium Batteries for Automobile Applications (ABAA) and the 2018 winner of ECS Battery Division Technology Award.

Plenary Lecture 5

Advanced Energy Storage systems for enabling electrification of vehicles “lithium ion & beyond”

Dr. K. Amine
Argonne Distinguished Fellow and Manager
Advanced battery technology team
D. Director, US/China Clean energy research center
Argonne National Laboratory

Abstract

To meet the high-energy requirement that can enable the 40-miles electric drive Plug in Hybrid Electric Vehicle (P-HEVs), long range electric vehicle (EV) and smart grid, it is necessary to develop very high energy and high power cathodes and anodes that when combined in a battery system must offer 5,000 charge-depleting cycles, 15years calendar life as well as excellent abuse tolerance. These challenging requirements make it difficult for conventional battery systems to be adopted in P-HEVs and EVs. In this talk, we will present a next generation lithium ion battery that include Ni rich full gradient cathode, a high voltage and nonflammable electrolyte and Silicon-graphene composite anode including a novel pre-lithiation technology to overcome the irreversible loss of this anode in the first cycle. We will then show how Se doping of Sulfur (S) can overcome the conductivity issue of S and eliminate the dissolution of poly-sulfide using an advanced electrolyte system. We will also show that by incorporating Li_2S in graphene cages, we increase the electrode loading significantly to 10mg.cm^{-2} and eliminate the issue of cathode swelling that impact performance.

Biography:

Dr. Khalil Amine is an Argonne Distinguished Fellow and the leader of the Advanced Battery Technology team at Argonne National Laboratory, where he is responsible for directing the research and development of advanced materials and battery systems for HEV, PHEV, EV, grid, satellite, military and medical applications. Dr. Amine is also the Deputy Director of the US/China clean energy research center and serves as a committee member of the U.S. National Research Consul at US Academy of Sciences on battery related technologies. He is an adjunct professor at Stanford University, Hong Kong University of science & Technology, and Peking University. Among his many awards, Dr. Amine is a 2003 recipient of Scientific America’s Top Worldwide 50 Researcher Award, a 2008 University of Chicago distinguished scientist award, a 2009 recipient of the US Federal Laboratory Award for Excellence in Technology Transfer, 2013 DOE Vehicle technologies office award and is the five-time recipient of the R&D 100 Award, which is considered as the Oscar of technology and innovation. In addition, he was awarded the ECS battery technology award and the international battery association award. Dr. Amine holds over 189 patents and patent applications and has 549 publications with google h-index of 106. From 1998-2017, Dr. Amine was one of the most cited scientist in the world in the field of battery technology. He serves as the president of IMLB. He is also the chairmen of the international automotive lithium battery association, ECS fellow and associate editor of the journal of Nano-Energy.

Keynote Lecture 1

First Principles Based Multiscale Simulation for Fuel Cell and Lithium Ion Battery Design

Professor Che-Wun Hong
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Abstract

This talk will present a first-principles based multi-scale design simulation technique on the transport phenomena inside electrochemical devices, such as proton membrane exchange fuel cells (PEMFCs), direct methanol fuel cells (DMFCs), lithium ion batteries (LiBs), photoelectrochemical cells (PECs) and high temperature solid oxide fuel cells (SOFCs). Computational techniques integrate quantum mechanics (for catalytic process simulation and nano-structured electrode design), molecular dynamics (for membrane and electrolyte design), lattice Boltzmann dynamics (for bubble removal flow channel design), computational fluid dynamics plus electrochemistry (for fuel cell manifold and electrochemical performance design), and system dynamics (for fuel cell and hybrid vehicle design) into one design tool to study the reaction process on the catalyst surface and inside electrolytes, diffusion layers, flow channels and fuel cell stack systems. Several experiments, including electrochemical performance tests and flow visualization, have been carried out to validate the simulation results. This first-principles based multi-scale simulation tool is capable of screening conceptual design ideas, from nano-scale materials to meso-scale components to the macro-scale fuel cell systems, before a prototype is fabricated. It has been applied to the novel green energy engineering for both new system design and performance improvement.

Biography:

Professor Hong received his Ph.D. in Mechanical Engineering from Imperial College, London, UK in 1987. He is currently the Director of the Green Energy & Quantum Engineering Lab in the Department of Power Mechanical Engineering, National Tsing Hua University in Hsinchu, Taiwan. His research interests are mainly at molecular engineering in various green energy systems, such as: fuel cells, solar cells, LEDs, thermoelectric chips, combustion engines and automotive engineering, which are all based on academic fundamentals of Quantum Mechanics, Molecular Dynamics, Monte Carlo, Boltzmann Dynamics, Computational Fluid Dynamics, as well as System Dynamics/ Intelligent Control. Apart from academic researches, he has been actively conducting projects with the government, motor companies and various research institutes. In the year of 2011, he received the outstanding research award from the Ministry of Science and Technology (MOST) of the Taiwanese government. He was the general chairman of the International Symposium on Advanced Vehicle Control in 2006 (AVEC ’06) and the Asia-Pacific Conference on Energy Storage and Conversion (APEnergy 2016). He was elected as the Fellow of the ASME (American Society of Mechanical Engineers) in 2013. Currently, he serves as the scientific committee members and editors for many international conference organizations and academic journals. He has graduated 16 Ph.D. and 90 MSc. students in his academic career from 1987 until now and has published around 236 papers including journal articles and conference papers.

Keynote Lecture 2

Construction of Flexible Interfacial Layer for Solid-State Li Batteries

[1]Hongchun Wang, [2]Bizhu Zheng, [1]Yuanjun Shao,[2] Jianping Zhu[1], Zhengliang Gong[1], Yong Yang[1,2*]
([1]School of Energy, [2]State Key Lab of Physical Chemistry of Solid Surfaces and College of Chemistry and Chemical Engineering, Xiamen, 361005)

Abstract

There is a growing interest in all-solid-state lithium batteries(ASLBs) for their safety and high energy density. However, the power density for ASLBs is still far away from satisfactory on the account of high interfacial resistance at electrode / solid electrolyte interface. For example, Garnet-type solid-state electrolytes (SSEs) are considered as a good choice for solid-state batteries, yet the interfacial issues with metallic Li limit their applications. In my group, we propose an ultra-simple and effective strategy to enhance the interfacial connection between garnet SSEs and Li metal just by drawing a graphite-based soft interface with a pencil [1]. Both experimental analysis and theoretical calculations confirm that the reaction between graphite-based interfacial layer and metallic lithium forms a lithiated connection interface with good lithium-ionic and electronic conductivity. Compared to the reported interfacial materials, the graphite material provides a soft interface with better ductility and compressibility. With the improvement by this soft interface, the impedance of symmetric Li cells significantly decreases from 1350 to 105Ωcm^2 and the cell can cycle for over 1000hoursat a current density of 300 μA/cm^2 at room temperature. Moreover, a solid-state battery with Li-metal anode, ternary cathode NCM523 and graphite-based interface modified garnet SSEs is fabricated and displays excellent rate capability and long cycling performance.

In addition, LGPS-type materials show extremely high Li^+ conductivity. But when in contact to Li metal, they can be reduced to produce Li_2S, Li_3P and Li-M alloy and form a mixed ionic and electronic conducting layer at the interface, which hinders the application of Li metal in such solid electrolyte system. We report on a simple approach for the modification of the interface between Li and $Li_{10}SnP_2S_{12}$ sulfide solid electrolyte by utilizing ionic liquid [2]. Our study shows that the addition of 1.5M LiTFSI/Pyr_{13}TFSI ionic liquid can not only promote intimate contact but can in-situ form a stable SEI layer at the interface between Li and solid electrolyte as well. A stable SEI layer instead of mixed conducting layer can prevent sulfide solid electrolyte from further decomposition and improve the cycle performance of batteries.

References:

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2) B.Z. Zheng; J.P.Zhu, et al; *ACS Applied Mater. & Interfaces;* 2018, 10, 25473-25482

Biography:

Professor Yong Yang is the Distinguished Professor and Director of Research Institute of Electrochemistry and Electrochemical Engineering at Xiamen University. He received his PhD degree in Physical Chemistry at Xiamen University in 1992 and was an academic visitor at PTCL of University of Oxford, UK during 1997-1998. Now, he serves as IBA board member and advisory member of several leading international conferences. He published 290 peer-reviewed papers in the journals, 30 patents and 4 book chapters. He was awarded the IBA technology award in 2014. His major interests are research of novel electrode/electrolyte materials, reaction mechanism and interfacial studies for Li-ion and Li-metal batteries, development of in-situ characterization techniques for electrochemical energy system, new battery system such as Na-ion and solid state batteries. He is an Editor, Journal of Power Sources.

Keynote Lecture 3

Lithium-excess electrode materials with cation-disordered rocksalt structure for high-energy rechargeable lithium batteries

Naoaki Yabuuchi
Yokohama National University
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Abstract

In the past decade, lithium-enriched compounds, Li_2MeO_3 (Me = Mn^{4+}, Ru^{4+} etc.), have been extensively studied for high-capacity positive electrode materials of lithium batteries. Although the origin of high reversible capacities was a debatable subject for a long time, recently it has been evidenced that charge compensation is partly achieved by solid-state redox of non-metal anions, *i.e.*, oxide ions (anionic redox),[1] coupled with solid-state redox of transition metal ions (cationic redox), which is the basic theory used for classical lithium/sodium insertion materials. Competition between cationic and anionic redox reactions is often evidenced for the lithium-enriched materials because the energy level of oxygen 2p band is lowered by the presence of excess lithium ions with high ionic characters in the crystal lattice. Reversibility of anionic redox reactions is also influenced by ionic and covalent characters for chemical bonds of transition metal ions.[2, 3] In contrast, when the energy of metal 3d band is low enough than that of oxygen 2p, pure cationic redox is realized even for the lithium-excess system.[4, 5] Moreover, this concept is further extended to sodium battery applications.[6] From these findings, we discuss the stabilization and destabilization mechanisms and material design strategy with the concept of cationic and anionic redox reactions to develop new high-capacity lithium/sodium insertion materials for battery applications.

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Biography:

Dr. Nobuyuki Zettsu is currently a professor in the department of materials chemistry, Shinshu University (JAPAN). His expertise is utilizing liquid phase crystal growth for the shape, hyper-space, and surface-controlled lithium-ion conducting crystalline materials and their assembly toward the advanced lithium-ion batteries with superior performances. His research interest is the understanding of the intrinsic physicochemical properties of oxides and mixed anion materials to lithium-ion battery and solid-state batteries, driven by their morphological characteristics. He joined Prof. Younan Xia research group as a postdoctoral fellow at the University of Washington after acquiring a Ph. D in polymer science from Tokyo Institute of Technology in 2004. As an associate professor at Osaka University, as an associate professor at Nagoya University, He has joined at Shinshu University from 2013 as an associate professor. He has been named a 4th Rising star researchers in Shinshu University at 2017.

Keynote Lecture 4

Lithium-excess electrode materials with cation-disordered rocksalt structure for high-energy rechargeable lithium batteries

Naoaki Yabuuchi
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Abstract

In the past decade, lithium-enriched compounds, Li_2MeO_3 (Me = Mn^{4+}, Ru^{4+} etc.), have been extensively studied for high-capacity positive electrode materials of lithium batteries. Although the origin of high reversible capacities was a debatable subject for a long time, recently it has been evidenced that charge compensation is partly achieved by solid-state redox of non-metal anions, *i.e.*, oxide ions (anionic redox),[1] coupled with solid-state redox of transition metal ions (cationic redox), which is the basic theory used for classical lithium/sodium insertion materials. Competition between cationic and anionic redox reactions is often evidenced for the lithium-enriched materials because the energy level of oxygen 2p band is lowered by the presence of excess lithium ions with high ionic characters in the crystal lattice. Reversibility of anionic redox reactions is also influenced by ionic and covalent characters for chemical bonds of transition metal ions.[2, 3] In contrast, when the energy of metal 3d band is low enough than that of oxygen 2p, pure cationic redox is realized even for the lithium-excess system.[4, 5] Moreover, this concept is further extended to sodium battery applications.[6] From these findings, we discuss the stabilization and destabilization mechanisms and material design strategy with the concept of cationic and anionic redox reactions to develop new high-capacity lithium/sodium insertion materials for battery applications.

References

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[6] T. Sato *et al*., and N. Yabuuchi., *Journal of Materials Chemistry A*, **6**, 13943 (2018).

Biography:

Naoaki Yabuuchi is a professor at Yokohama National University. He completed his PhD at Osaka City University in 2006 and his postdoc at MIT, with research expertise in the development of new electrode materials and study on reaction mechanisms for high energy Li/Na batteries. He has over 90 publications in these areas. He is the recipient of the First International Award, “Science Award Electrochemistry” by Volkswagen and BASF, The 2nd ISSI Young Scientist Award, and ISE Prize for Applied Electrochemistry, The Young Scientists’ Prize from the Minister of Education, Culture, Sports, Science and Technology, Japan among other honors.

Keynote Lecture 5

In Operando Studies on Advanced Batteries

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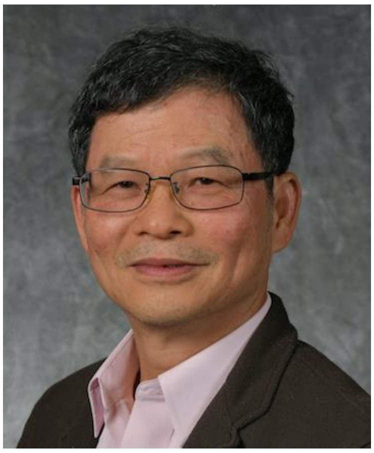
Abstract

Advanced materials play important roles in fundamental advances for energy storage systems, which are vital to meet the challenge of global warming and air pollutions due to the unlimited consumption of fossil fuels. In-situ/in operando investigating the morphology, structural evolutions together with electronic transitions of advanced materials during the course of their operation is of great interest for further designing new materials and improving the performance of either energy storage systems. A brief introduction of in-situ/in operando spectroscopic techniques will be given first and then the operational mechanisms of several advanced materials for energy storage reactions investigated by various in-situ/in operando spectroscopies will be presented in this talk. I will also report in-situ/in operando spectroscopic observations on the morphology evolution, structural transformation and electronic transitions of electrode materials and the formation mechanisms of solid-electrolyte-interphase (SEI) on electrode surface for energy storage reactions. The understanding of the charging-discharging and SEI formation mechanisms of electrode materials in a battery system gives a rational approach to advance the performance of energy storage systems.

Biography:



Bing-Joe Hwang is the Chair Professor Department of Chemical Engineering National Taiwan University of Science and Technology. He obtained his Ph.D. in Chemical Engineering from National Cheng Kung University in 1987. He is the Director, Sustainable Energy Development Center, Taiwan Tech (2012.2~present); Adjunct Researcher, National Synchrotron Radiation Research Center, Taiwan (2005~); Associate Editor, American Chemical Society Sustainable Chemistry & Engineering (ACS SCE) (2015~). He was the President, The Electrochemical Society of Taiwan (ECSTw) (2013.8~2017.12); Coordinator, Program of Chemical Engineering, Department of Applied Science and Engineering, MOST, Taiwan (2008.12~2011.12); Chairman, Department of Chemical Engineering, NTUST (2007.8~2010.7) ; President, Chinese Association for Chemical Sensors and Technology in Taiwan (2002.9~2004.8), and President, The Society of Hydrogen and Fuel Cells of Taiwan (2010.1~2013.12). He was awarded the National Chair Professorship in Engineering and Applied Science, Ministry of Education in 2018; elected Fellow, Taiwan Institute of Chemical Engineers (TwIChE) (2018); Academician of Asian Pacific Academy of Materials (APAM) (2017); Fellow of International Society of Electrochemistry (ISE) (2014); Outstanding Research Fellow of National Science Council, Taiwan (2011); Academician of the Academy of Sciences of Lisbon (2011). He is also the recipient of TECO award in Chem. Eng. and Materials Science, TECO Technology Foundation (2011); Academic Award in Engineering and Applied Science, Ministry of Education (2010) ; Outstanding research award from National Science Council of Taiwan (three times) He has published ~355 SCI papers and been granted ~24 patents. He received 12240 times SCI citation with an H index being ~60.

Invited lecture 1

Fiber-enabled Wearable Energy Storage Devices

Zijian Zheng[1]
[1] *Research Centre for Smart Wearable Technology, Institute of Textiles and Clothing, The Hong Kong Polytechnic University, Kowloon, Hong Kong SAR*
Email: tczzheng@polyu.edu.hk

Abstract

Wearable energy storage devices are indispensable corner stones for future wearable electronics. Current energy storage technologies are based on materials and devices that are rigid, bulky, and heavy, making them difficult to wear. On the other hand, fibers are flexible and lightweight materials that can be assembled into different textiles and have been worn by human beings thousands of years. Different from conventional two-dimensional thin films and foils, the three-dimensional fibre and textile structures not only provide superior wearing ability, but also much larger surface areas. This talk will introduce how our research group makes use of the attributes of fibres for high-performance wearable energy storage devices. We will demonstrate the strategies and discuss the perspectives to modify fibers and textiles for making wearable capacitators and batteries with excellent mechanical durability, electrochemical stability, and high energy/power density.

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[3] Y. Yu, C. Yan, Z. J. Zheng*, Adv. Mater. 2014, 26, 5508-5516.
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[5] J. Chang, Z.J.Zheng* et al., Nat. Commun. 2018, 2018, 9, 4480.

Biography:

Prof. Zijian Zheng is currently Full Professor at the Institute of Textile and Clothing (ITC) at The Hong Kong Polytechnic University. His research interests are surface science, self-assembly, nanolithography, polymer science, and bendable/stretchable/wearable/graphene materials and electronic devices. He received his B. Eng. in Chemical Engineering at Tsinghua University in 2003, and PhD in Chemistry at University of Cambridge in 2007. In 2008, he worked as postdoctoral researcher with Prof. Chad A. Mirkin at Northwestern University. He joined ITC as Assistant Professor in 2009, and was promoted to tenured Associate Professor in 2013 and Professor in 2017. He has published >90 papers in high-impact international scientific journals including *Science*, *Nature Commun.*, *Advanced Materials*, *Journal of the America Chemical Society*, *Angewandte Chemie*. He also files 18 international and China patents. He serves as Guest Editor for *Advanced Materials* and *Small*. He is recipient of more than 10 academic awards such as GENEVA Innovation Award, Future Leaders Programs and Early Career Awards. He is elected as Founding Member of The Young Academy of Sciences of Hong Kong.

Invited lecture 2

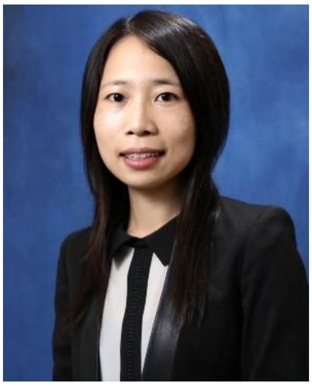
Toward High-Energy-Density Energy Storage: Redox Processes and Design Strategies

Yi-Chun Lu
The Chinese University of Hong Kong

Abstract

Energy storage system is a critical enabling factor for deploying unstable and intermittent renewable power sources such as solar and wind power sources. Energy storage devices including metal-oxygen, metal-sulfur, and redox flow batteries have received extraordinary attentions owing to their high energy density and flexible designs in power and energy. In this presentation, we will discuss fundamental redox processes and design strategies in these battery systems. We exploit various spectroscopic techniques coupled with single-cell electrochemical characterizations to probe the metal-S and metal-O_2 reactions. In addition, we will discuss new redox chemistries and synergistic interplay between solvent and redox-active materials at solid and liquid interfaces that commonly exist in these high-energy-density energy storage systems.

Biography:



Prof. Yi-Chun Lu received her Ph.D. degree in Materials Science & Engineering from the Massachusetts Institute of Technology in 2012. She is currently an Associate Professor in the Department of Mechanical and Automation Engineering at The Chinese University of Hong Kong (CUHK).

She is the Elected Member of Young Academy of Science of Hong Kong and was the recipient of the Hong Kong SAR Research Grants Council Early Career Award (2014), Young Researchers Award (2016), University Education Award, CUHK (2016), and Vice-Chancellor's Exemplary Teaching Award, CUHK (2014).

Dr. Lu's research interest centers on developing fundamental understandings and material design principles for clean energy storage and conversion. Specifically, her research group is studying: Electrode and electrolyte design for high-energy metal-air and metal sulfur batteries; Redox-active components and solution chemistry for redox-flow batteries. Electrocatalysts and electrode design for low-temperature fuel cells and electrolyzers; Mechanistic understanding of interfacial phenomena governing electrochemical energy conversion and storage processes.

Invited lecture 3

Development of stable Si anode for lithium-ion batteries

Denis Y.W. Yu
City University of Hong Kong

Abstract

Silicon has been the focus of many research studies as the next generation high-capacity anode material for lithium-ion batteries (LIB). However, the mechanical stability of the electrode is a major bottleneck to the commercialization of the material. Many studies were devoted to nanostructured silicon composites with voids to accommodate the volume expansion. Yet, few of these technologies have been successfully applied to full batteries, due to various reasons including manufacturing process and cost.

In this presentation, we will showcase a few strategies we have developed in the past few years, ranging from binder engineering, secondary particle formation to alloying to improve the stability of Si-based electrodes. Through the different studies, we hope to understand the critical factors that govern the various performances of the anode, and to propose practical solutions for next-generation LIBs.

Biography:

Dr Denis Yu is an associate professor at the School of Energy and Environment at City University of Hong Kong. He received his Ph. D. in Applied Physics from the School of Engineering and Applied Sciences at Harvard University in 2003. He then worked as an engineer at SANYO Electric Co. Ltd. in Japan for 8 years, developing cathode and anode materials for Li-ion batteries. Afterwards, he led the battery activities at the Energy Research Institute at Nanyang Technological University and TUM CREATE Centre for Electromobility in Singapore as a senior scientist for two years before joining City University of Hong Kong. His research interests include the development and characterization of novel materials and systems for energy storage applications.

Invited lecture 4

Defect Chemistry and Li Transport in Antiperovskite Materials

Francesco Ciucci
The Hong Kong University of Science and Technology

Abstract

Solid-state electrolytes with fast lithium conduction are the core of the all-solid-state Li battery technology. By substituting the organic electrolyte with a piece of non-flammable ceramic material, we can achieve better safety, a higher specific capacity and a higher energy density. To date, the major bottleneck for this technology is the slow bulk diffusion of solid-state electrolyte and the interfacial incompatibility between the electrolyte and electrodes. To resolve these issues, several families of fast ionic conductors have been developed. The understanding of Li diffusion in these materials is essential to the development of novel family fast ionic conductors. In this sense, atomistic modeling provides us with a unique tool to obtain comprehensive information on the atom motion, which is difficult to access with experimental techniques. In this work, we use density functional theory (DFT) calculations as well as large-scale classical molecular dynamics (MD) simulations to simulate the Li diffusion in a novel family of superionic conductors, lithium-rich anti-perovskites and provide an understanding of the Li diffusion behavior.

Lithium-rich anti-perovskites (LiRAPs) are a promising family of solid electrolytes, which exhibit ionic conductivities above 10^{-3} S cm^{-1} at room temperature, among the highest reported values to date. We investigate the defect chemistry and the associated lithium transport in Li_3OCl, a prototypical LiRAP, using DFT calculations and classical MD simulations. We studied three types of charge neutral defect pairs, namely the LiCl Schottky pair, the Li_2O Schottky pair, and the Li interstitial with a substitutional defect of O on the Cl site. Among them, the LiCl Schottky pair has the lowest binding energy and is the most energetically favorable for diffusion as computed by DFT. This is confirmed by classical MD simulations, where the computed Li-ion diffusion coefficients for LiCl Schottky systems are significantly higher than those for the other two defects considered, and the activation energy in LiCl deficient Li_3OCl is comparable to experimental values. The high conductivities and low activation energies of LiCl Schottky systems are explained by the low energy pathways of Li between the Cl vacancies. We propose that Li vacancy hopping is the main diffusion mechanism in highly conductive Li_3OCl.

Biography:

Francesco Ciucci is an associate professor at the Hong Kong University of Science and Technology. He graduated *cum laude* from Politecnico di Milano, Italy and Ecole Centrale de Paris, France with degrees in Aerospace Engineering and Applied Physics, respectively. He pursued his Ph.D. in Engineering and Applied Sciences from the California Institute of Technology, USA, where he was supported by the internationally renowned Rotary Ambassadorial Scholarship (he was one of the three Italian recipients receiving the award in 2002). Francesco did his postdoctoral work at the Heidelberg Graduate School of Mathematical and Computational Methods for the Sciences of the University of Heidelberg, Germany. There, he obtained a Marie Curie Fellowship and a Heidelberg Graduate School Fellowship. His research articles have been featured in major journals, including, Nature Chemistry, Advanced Energy Materials, Chemistry of Materials, Chemical Reviews and many more. Francesco's current research centers around solid-state energy materials, including those used in high-temperature fuel cells and solid-state batteries, with particular emphasis on the modeling of such systems and the development of new ceramic materials.

Invited lecture 5

Recent Development on Battery Research at GP

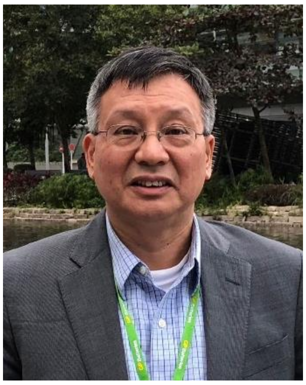
Mingde Wang

Head of Center of Excellence-RD (Acting)
Head of Strategic Business Unit-Lithium,
GP Batteries International.

Abstract:

Research and development at GPI is conducted at two fronts, one in Lithium Ion batteries and the other in NiMH. In Lithium Ion RD, recent work has been on the fast charging capacity of Li Ion cells with graphite + SiO, which was synthesized using a unique process in order to achieve high energy density. In NiMH RD, we have focused on the low temperature performance of the battery by utilizing the superlattice alloy as anode and unique processing techniques. Coupled with the anode development, cathode material is also modified to achieve the desired performance at low temperatures.

Biography:



Dr. Mingde Wang is the acting director of research and development for rechargeable batteries at GP batteries International (GPBI) while being the head of the Strategic Business Unit-Lithium. Dr. Wang leads the research and development teams for both Lithium Ion batteries as well as NiMH in order to fulfil the needs for business development and growth in the rechargeable batteries at GPBI. Prior to joining GPBI, Dr Wang has served in both senior business positions and RD positions in Battery companies such as A123 and Leyden Energy and Solar energy companies as such as Rena Solar and Green Crystal Energy. Dr. Wang obtained his Ph.D in Materials Science and Engineering at University of Pennsylvania, his Master and Bachelor degrees from Zhejiang University.

Invited lecture 6

Core-shell electrocatalysts for fuel cells: design, synthesis and fuel cell performance

Minhua Shao*
Department of Chemical and Biological Engineering, HKUST Energy Institute, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, P.R. China, kemshao@ust.hk

Abstract

Low temperature fuel cells are electrochemical devices that convert chemical energy directly to electricity. They have great potential for both stationary and transportation applications and are expected to help address the energy and environmental problems that have become prevalent in our society. Despite their great promise, commercialization has been hindered by lower than predicted efficiencies and high loading of Pt-based electrocatalysts in the electrodes. For more than five decades, extensive work has being focused on the development of novel electrocatalysts for fuel cell reactions. In this talk, I will present recent progress in developing advanced electrocatalysts mainly for oxygen reduction reaction in my group, with an emphasis on core-shell and shape controlled nanocrystals. Fuel cell testing results on these advanced catalysts will be shared. The mechanisms for activity enhancement will also be discussed based on the results of density functional theory calculations.

Biography:

Minhua Shao is an Associate Professor in the Department of Chemical and Biological Engineering at the Hong Kong University of Science and Technology (HKUST). He is also the Associate Director of the HKUST Energy Institute, Director of the Sustainable Energy Engineering Program, and Director of the Master of Science Program of Chemical and Biomolecular Engineering Program. He earned BS and MS degrees in chemistry from Xiamen University, and a PhD degree in materials science and engineering from the State University of New York at Stony Brook in 2006. Dr. Shao joined UTC Power in 2007 to lead the development of advanced catalysts and supports for fuel cells by collaborating with Toyota. He was promoted to UTC Technical Fellow in 2012. In 2013, he joined Ford Motor Company to conduct research on lithium-ion batteries. He then joined HKUST in 2014. He is an Associate Editor of *Journal of the Electrochemical Society* and Editorial Advisory Board Member for *Journal of Applied Electrochemistry, Catalysts, Materials Technologies, Journal of Physics D: Applied Physics,* and *Journal of Electrochemistry*. He has published over 100 peer-reviewed articles. He has also received a number of awards, including the Supramaniam Srinivasan Young Investigator Award from the ECS Energy Technology Division (2014), and Student Achievement Award from the ECS Industrial Electrochemistry and Electrochemical Engineering Division (2007).

Invited Lecture 7

Nanostructured Materials as Anodes for Energy Storages

Limin Zhou,
Mechanical Engineering Department
The Hong Kong Polytechnic University

Abstract
Considerable attention has been paid to rechargeable lithium ion batteries (LIBs) because of their high energy density and long cycle lifetime. However, exploring and developing novel electrode materials with sufficiently high energy and power density to meet the requirements imposed on application of LIBs in high-power devices such as electric vehicles (EV) and hybrid electric vehicles (HEV) remains a challenge. In this study, we have successfully prepared amorphous carbon nanofibers and carbon nanotubes decorated with hollow graphitic carbon nanospheres by electrospinning method. A hollow-tunnel structure in electrospun carbon/Ni nanofibres was also produced by diffusing Ni nanoparticles from the graphitic carbon spheres into amorphous carbon nanofibres, which turns amorphous carbon into graphitic carbon. The resultant materials were further treated by chemical activation and acid treatment to develop activated N-doped hollow-tunneled graphitic carbon nanofibers (ANHTGCNs). In a typical application, we demonstrated that the prepared ANHTGCNs are excellent anode materials for LIBs, displaying a super high reversible specific capacity of over ~1560 mAh g^{-1} and a remarkable volumetric capacity of ~1.8 Ah cm^{-3} at a current density of 0.1 A g^{-1} with outstanding rate capability and good cycling stability. The other material is a novel porous TiO_2-carbon (TiO_2-C) composite nanofibers in which Sn nanoparticles is encapsulated. *In situ* TEM was used to study the structural changes and charging/discharging processes of TiO_2-C-Sn composite nanofibers. It was found that the porous TiO_2-C can accommodate volumetric change of Sn nanoparticles. As an anode, this material shows a high capacity (875 mAh/g after 50 cycles when the current density is 0.1 A/g), long cycle life (over 10000 cycles at rate of 3 A/g with maintained capacity of 160 mAh/g), and good rate capability.

Biography:

Prof. Limin Zhou received his BEng and MEng from Harbin Institute of Shipbuilding Engineering (current name: Harbin Engineering University) in 1982 and 1988 respectively, and his PhD from The University of Sydney in 1994. He was appointed as an Assistant Professor in 1996 and became a Professor in 2005 in the Department of Mechanical Engineering, The Hong Kong Polytechnic University. Prof. Zhou's major research interests include fibre-reinforced polymer composites, smart materials and structures; nanomaterials and nanotechnology for energy storages and conversions, and guided-wave based structural health monitoring techniques. He has published more than 280 technical articles including over 180 SCI refereed journal papers. After assuming the current appointment with the Hong Kong Polytechnic University, he received an Engineering Faculty Best Research Award in 1999 and the President's Award for Outstanding Achievements in Research in 2000. Prof. Zhou currently is a Vice President of Chinese Society for Composite Materials and a member of Engineering Panel, Hong Kong Research Grants Council. He serves currently as an Associate Dean, Faculty of Engineering, The Hong Kong Polytechnic University.

Invited Lecture 8

Shuttling-free lithium sulfur batteries using black phosphorus quantum dots as electrocatalysts

Shu Ping Lau
Department of Applied Physics, The Hong Kong Polytechnic University

Abstract

Black phosphorus (BP), has recently attracted world-wide attention owing to its great potential in novel nanoelectronics, optoelectronics and electrochemical devices. Solution exfoliation of BP reveals superior advances when compared with mechanical exfoliation. Remarkably, liquid-phase exfoliated BP flakes and quantum dots exhibit exciting properties in lithium sulfur batteries (LSBs). We demonstrated that the effectiveness of metal-free BP quantum dots (BPQDs) for lithium polysulfides immobilization and conversion in LSBs. The activity is attributed to the numerous catalytically active sites on the edges of the quantum dots. In the presence of a small amount of BPQDs (~2 wt% of the cathode weight) with a sulfur/porous carbon fiber cathode, the LSBs exhibit no diffusion of LPSs as well as excellent battery performance, including high rate capability (784 mA h g^{-1} at 4C) and exceptional cyclic stability (0.027% capacity fade per cycle for 1000 cycles).

Biography:

Daniel Shu Ping Lau obtained his Ph.D., Materials Engineering, University of Wales Swansea, U.K. in 1995, BSc (Hons), First Class, Physics and Computer Electronics, The University of North London, U.K., in 1991. He is the Head and Professor, Department of Applied Physics, The Hong Kong Polytechnic University. He also serves as the Director, University Research Facility in Materials Characterization and Device Fabrication (UMF). Before joining HK PolyU, he was Assistant Head, Division of Microelectronics, School of Electrical and Electronic Engineering, Nanyang Technological University where he was also an Associate Professor. He is the recipient of Royal Society Grant for International Incoming Short Visit in 2008; Nanyang Award for Research and Innovation in 2006 (The highest recognition to individuals and teams who have made outstanding contributions in scientific knowledge through research breakthroughs, and significant technological innovations on the world stage.); R.F. Bunshah Award for the best published paper presented at the International Conference on Metallurgical Coatings and Thin Films (ICMCTF 2003) in 2004; Japan Society Promotion for Science (JSPS) Fellowship in 2001; Overseas Attachment Programme Fellowship (A*STAR Singapore) as a scientist at School of Physics, University of Melbourne, in 2001; Overseas Research Students Awards, UK Government, during 1992 -1995. He has published more than 220 papers with total number of Scopus citations over 3300 and an h-index being over 30.

Invited Lecture 9

Lithiophilic Cu-CuO-Ni Hybrid Structure: Advanced Current Collectors towards Stable Lithium Metal Anodes

Kaili Zhang
Mechanical Engineering, City University of Hong Kong

Abstract

Metallic lithium (Li) is a promising anode material for next generation rechargeable batteries. However, the dendrite growth of Li and repeated formation of solid electrolyte interface (SEI) during Li plating and stripping result in low Coulombic efficiency, internal short circuit, and capacity decay, hampering its practical application. In the development of stable Li metal anode, the current collector has been recognized as a critical component to regulate Li plating. In this talk, a lithiophilic Cu-CuO hybrid structure will be introduced as a current collector for Li metal anodes. The low over-potential of CuO for Li nucleation and the uniform Li+ ion flux induced by the formation of Cu nanowire arrays enable effective suppression of the growth of Li dendrites. Moreover, the surface Cu layer can act as a protective layer to enhance structural durability of the hybrid structure in long-term running. As a result, the Cu-CuO-Ni achieves a Coulombic efficiency above 95% for more than 250 cycles at a current density of 1 mA cm^{-2} and 580 h (290 cycles) stable repeated Li plating and stripping in a symmetric cell.

Biography:

Kaili Zhang received his PhD degree from National University of Singapore in 2006. He then worked as postdoctoral researchers at French National Center for Scientific Research (LAAS-CNRS) and Swiss Federal Institute of Technology Zurich (ETH Zurich). He joined in City University of Hong Kong as an assistant professor in 2009. He is now an associate professor at Department of Mechanical Engineering, City University of Hong Kong. His research interests include energetics-on-a-chip and nanomaterials for energy storage applications.

Invited Lecture 10

Probing oxide-ion conduction in low-temperature SOFCs

Bolong Huang
Department of Applied Biology and Chemical Technology
The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong SAR
Email: bhuang@polyu.edu.hk

Abstract

Driven by the fierce power issues, by no means fortuitous, Solid Oxide Fuel Cells (SOFCs) has arisen to be a competitive candidate because it no needs charging to initiate operation and exhibits environmental benignity and high energy efficiency (easily levels up to 40~60% or even 70%.). They do not necessarily follow Carnot-Cycle thermodynamic Law, and only rely on a fast redox reaction predominantly fed by O_2 or oxidizing agent. The in-system bio-circulating regenerative SOFCs have gradually aroused our attention, as it indeed serves as the embedded inclusion type renewable electrical generations. It has been recently applied in the deep-space exploration aircraft of China called “Lunar-Palace-One-Project”. This project results from their ability to optimally support the biologic internal recycle system and supply enough energy for living needs of astronauts at environment of moon, which can be attributed to recent outstanding progress on oxygen storage materials for electrodes, catalysts with high efficiency for oxygen/hydrogen generation and fast ion conductors.

As a challenge, fast ion transportation with electronically insulated will decrease the voltage loss and further determine the electrical performance, which usually could only be ensured in high working temperature. Moreover, most ordinary SOFCs have rather high working temperature at least above 800°C. Screening and characterizing the candidate electrolyte onsets in lower temperature without sacrificing electrical performance, become urgent. It is worthy considering that this demanding in-situ screening and characterization under such high dynamic temperature cannot be fulfilled by current technique.

Herein we report an in-situ and non-contact method to monitor the working condition of solid oxide fuel cells (SOFCs). With the combination of density functional theory calculation and upconversion (UC) luminescence, we give distinct and complementary perspective on the entangled interaction between thermal-driven formed O-ion Frenkel pair (native solubilizer) and Bi3+ dopant (competitive inhibitor) in $La_2Mo_2O_9$ derivatives, especially at a lower temperature required by a SOFCs device. As we know, innovating higher electrical performance at lower temperature mainly depends on the screening of the candidate electrolytes. The thermally driven formation of a-Fr pairs has been believed to be the initiation of ion conduction, which has rarely been investigated. Generally, only with certain amount of a-Fr pairs formed in lattice, ion conduction could be probed by equipment. However, this in-situ non-contact luminescence method supply a new reliable way of monitoring the complete process of a-Fr pairs formation and ion conduction with corporation of DFT calculations. This is important for thoroughly understanding the ion conduction mechanism and will further benefit controlling properties of materials to realize high conductivity in low temperature.

Biography:

Dr. Bolong Huang received PhD in 2012 from University of Cambridge, and obtained BSc in from Department of Physics, Peking University 2007. Following a systematic training period as research assistant in Chemistry Department in Peking University, and in Hong Kong, he started-up independent researches as PI in the Hong Kong Polytechnic University 2015. His main research fields are rare earth functional nanomaterials, defect theory of solid functional nanomaterials, renewable energy materials, DFT calculation development based on ab-initio electronic self-energy corrections, as an implement in the time-dependent DFT theory.

Invited Lecture 11

Porous Electrodes for Batteries and Fuel Cells

Kwong-Yu Chan, Ming Zhou, Chi-Ying Vanessa Li, Ching-Kit Ho, and Albert A. Voskanyan
Department of Chemistry, The University of Hong Kong, hrsccky@hku.hk

Abstract

Challenges in designing porous materials for electrodes of various electrochemical devices are discussed. Investigations are made with carbon electrodes template-synthesized with porosity controlled at different length scales. The oxygen electrode in a reversible lithium-oxygen battery faces difficulties with sluggish kinetics in aprotic solvents, irreversible lithium oxides deposition/dissolution, and components degradation. We report a Fe-N-doped carbon with hierarchical porosity for application as a Li-O_2 cathode [1] using a hollow-core mesoporous-shell (HCMS) carbon introduced for investigating structure-performance relationship [2, 3]. Results observed for Li-O_2 has capacity reaching 1/3 the theoretical energy density. The excellent performance of Fe-N-HCMS electrode loaded with RuO_2 can be attributed to: i) A well-defined core-shell mesoporous structure provides excellent mass transport and limits the Li_2O deposition to be dispersed in nanoscale; ii) The Fe-N doping of carbon provides the corrosion resistance, high conductivity, and active sites for favorable interaction with RuO_2; and iii) Small and amorphous RuO_2 provides highly catalytic activity for decomposition of Li_2O. Discharge capacity of 10,000 mAh/g is demonstrated with discharge potential of 2.4 V and recharge potential of 3.6 V maintained at 2 A/g based on total mass of catalyst and carbon support and maintained at 2.5 V and 3.5 V at 1 A/g over 50 cycles. The challenges for developing porous cathodes for sodium-oxygen batteries are different with the more reversible species sodium superoxide stored in both the solvent and the porous electrode. We also introduce a recently developed method of colloidal combustion for scalable synthesis of porous metal oxides.[4]

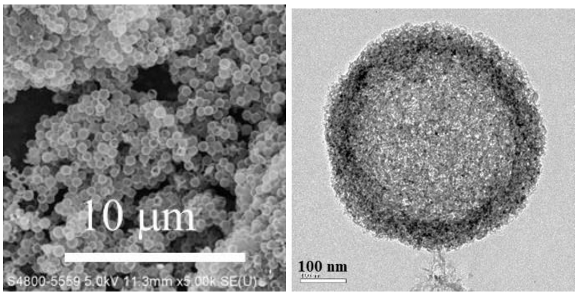


Fig. 1 (a) SEM image of the Fe-N-HCMS Carbon. (b) TEM image of Fe-N-HCMS carbon loaded with RuO_2.

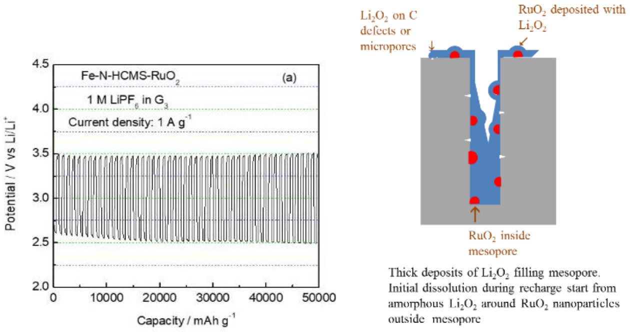


Fig. 2 (a) Fifty charge-discharge cycles of Fe-N-HCMS-RuO_2 at 1 A/g. (b) Possible morphologies of Li_2O in the hierarchical porous structure of Fe-N-HCMS carbon loaded with RuO_2.

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2. F. Li, M. Morris and K.Y. Chan, *J. Mater. Chem.* 21 (2011) 8880-8886.
3. Ming Zhou, Chunzhen Yang, Kwong-Yu Chan*, *Adv. Energy Mater.*, 4 (18), (2014) 1400840.
4. A.A. Voskanyan, K.Y. Chan, and C.Y.V. Li, *Chem. Mater. 28* (8), (2016) 2768-2775; A.A. Voskanyan and K.Y. Chan, *ACS Applied Nano Materials* 1(2) (2018) 556-563.

Biography:

Kwong-Yu Chan obtained his B.Sc. in Chemical Engineering, University of Alberta, in 1979, MS and PhD in Chemical Engineering from Cornell University respectively in 1984 and 1988. He is currently a Professor at Department of Chemistry, The University of Hong Kong. He is an Editorial Board Member of Molecular Simulation, Molecular Physics and Journal of Experimental Nanoscience, he served as Regional editor of Molecular Simulation and Journal of Experimental Nanoscience (2006-2014).

Previous Academic Positions Held

1995 - 2002	Senior Lecturer, Department of Chemistry, The University of Hong Kong
1988 - 1995	Lecturer, Department of Chemistry, The University of Hong Kong
1999	Senior Visiting Fellow, Tsinghua University, Beijing, China
1991	Visiting Research Associate, University of Utah, U.S.A.
1987 - 1988	Research Associate, Case Western Reserve University, Utah, U.S.A.
1979 - 1980	Assistant Lecturer, Hong Kong Polytechnic

Industrial Experience

1980 - 1981	Project Engineer, Hong Kong Oxygen and Acetylene Co.

Previous Relevant Research Work

Research interests in molecular simulation, fuel cells, batteries, water treatment, materials, and electrochemical applications. Published over 160 papers on various topics in electrochemistry, physical chemistry, chemical engineering, and materials science. Top 1% cited scientist, according to ISI Essential Science Indicators. Six inventions related to fuel cells, ozone generation, batteries, and catalysts. Web of Science: >4,400 citations, h-index 35.

Research Related Prizes and Awards

- Sino-British Fellowship Trust Visitorship (2017)
- HKU Outstanding Research Award (1998,2012)
- Croucher Foundation Senior Research Fellow (2010)
- Universitas 21 Fellow (2010)
- Salzburg Global Fellow (2008)

Poster Abstract 1

Na_2SeO_3: A Novel Na-Ion Battery Cathode Material with High Capacity

Bizhe Su, Jiaolong Zhang, Denis Y. W. Yu
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Sodium ion batteries (SIBs) is a potential alternative to LIBs for large-scale energy storage system because of the advantages of Na in terms of cost and abundance. However, one of the challenges of SIBs is that the capacity of typical sodium-ion battery cathodes is low. In the case of LIB, its capacity can be increased to more than 200 mAh g^{-1} by utilizing both the cationic and anionic redox processes in the material (i.e. Li-excess materials). Similar Na metal oxides such as Na_2RuO_3[1] and Na_2IrO_3[2] were also recently suggested to involve oxygen participation during charge and discharge. This raises hope that high-capacity Na-ion cathodes can be found. In this work, we study the possibility of using Na_2SeO_3 as cathode material for SIB. Na_2SeO_3 has a monoclinic (P 1 21/c 1) structure with 1D ion-channels for Na transport. Theoretical study has also shown that the O2p electrons predominate the vicinity of the Fermi level in the material, which makes it possible to provide anionic redox [3].

Experimentally, commercial Na_2SeO_3 is made into electrode and tested at 10 mA g^{-1}. When the electrode is first charged to 4.8 V, a voltage plateau near 4.5 V vs. Na/Na+ with a capacity of 98 mAh g^{-1} is observed (see Fig. 1a). When it is discharged to 1.5 V, a capacity of 52 mAh g^{-1} is obtained. This indicates that the material is electrochemically active. The capacity is found to depend on particle size. 1st discharge capacity is increased to 158 mAh g-1 after ball milling with 400 rpm for 4h. By substituting Ti into Na_2SeO_3, 1st discharge capacity is further improved to 171 mAh g^{-1}. Despite the high capacity that is achieved, reversibility is still poor. We are in the process of studying the effect of different parameters such as particle size, electrolyte, surface coating, and chemical composition etc. on the cycle performance of the material. In addition, characterizations such as XPS and XRD are being conducted to understand the charge-discharge mechanism of the material. These will be presented at the meeting.

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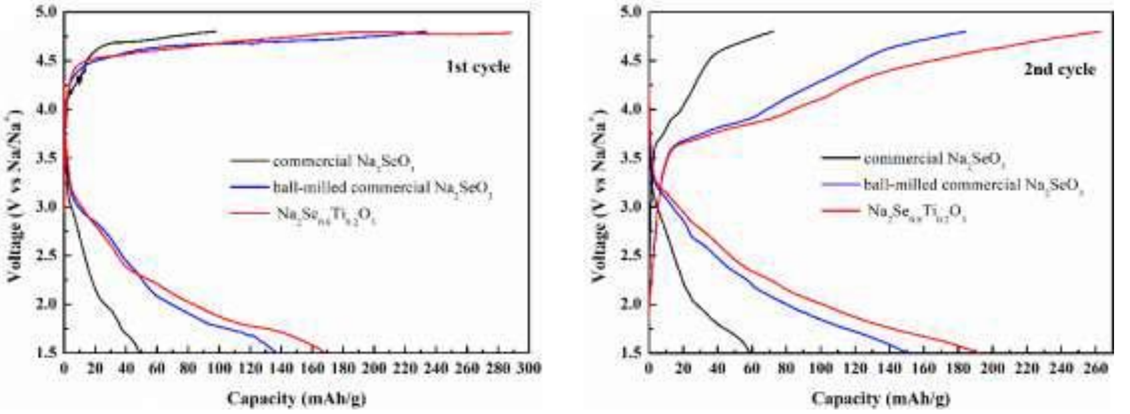

Fig. 1. First and second charge/discharge curves for commercial Na_2SeO_3, ball-milled commercial Na_2SeO_3, $Na_2Se_{0.8}Ti_{0.2}O_3$ samples in the voltage range of 1.5-4.8 V at 10 mA g^{-1}.

Poster Abstract 2

Effects of linear carbonate solvents on PF_6^- intercalation in graphite of dual-ion batteries

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Dual ion batteries (DIBs) based on the cations and anions as electroactive species have received tremendous attention due to their high energy density. Electrolytes play an important role in DIBs electrochemical performance. Here, the electrochemical intercalation of hexafluorophosphate (PF_6^-) anion into graphite electrodes were investigated using 3 M $LiPF_6$ dissolved in linear carbonate solvents of dimethyl carbonate (DMC), ethyl methyl carbonate (EMC) and diethyl carbonate (DEC). DEC solvent shows improved anodic stability towards Aluminum current collect while sevser electrolyte decomposition occur based on DMC. PF_6^- anion were more easily intercalated into graphite from EMC with a lower onset potential at around 4.39 V vs. Li/Li^+. In addition, DMC-based electrolyte shows a poor cycling stability while the highest capacity retention and columbic efficiency (CE) can be obtained with 3 M $LiPF_6$/EMC. Much better rate capability was also achieved in 3 M $LiPF_6$/EMC compared with that of the DEC electrolyte, although their CE were quite similar at all current densities. Thus EMC based electrolytes are very promising for their applications in DIBs with higher cycling and rate performance compared with DEC and DMC.

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Poster Abstract 3

Intercalation induced anomalous stability of microsized MoS_2 in K-ion batteries

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Potassium ion batteries (PIBs) have drawn intensive attention due to abundant reserves and low cost of potassium. A two-dimensional molybdenum disulfide (MoS_2) is studied as an anode in PIBs. It shows a stable capacity of over 400 mAh/g even with microsized particles. To unveil the underlying mechanism, the phase transitions of MoS_2 during K ion insertion/extraction are explored by in-situ x-ray diffraction combining with high-resolution transmission electron microscopy. An intercalation-dominant behaviour during K ion insertion has been unveiled, which differs from the conversion-governed reactions in Li and Na ion storage. The reason lies in the enlarged interlayer spacing from 6 Å to 8 Å during initial K ions uptake. The large volume expansion associated with conversion reactions is thus largely avoided, leading to the excellent capacity retention with neat MoS2 particles. It implies the requirement of prudent investigation when moving from Li- and Na- ion to K-ion systems. Our findings suggest the promising application of two-dimensional transitional metal dichalcogenides in PIBs, which represents a large family of compounds.

Poster Abstract 4

Interplay between the anion and cation storage in carbon cathode for advanced alkali-metal ion capacitors

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The wide application of Li-ion capacitors is limited by the relatively low energy densities. Efforts on increasing the energy density are put on two aspects. On the one hand, improve the operation voltage by shifting from acetonitrile- to carbonate-based electrolyte. On the other hand, boost the capacity of the electrode, particularly on the cathode by increasing the effective surface area of carbon materials. Porous carbon with high surface area (over 3000 $m^2 \cdot g^{-1}$) was fabricated from alkali lignin through a traditional KOH activation method assisted by self-activation. A wide voltage window of 1.0-4.8V is used where synergistic storage of anions and cations is achieved. It shows that deep discharging (< 2.5 V) triggers the adsorption of cations (Li^+), which facilitates the adsorption of anions (PF_6^-) upon the following cycling, resulting in the increased capacity. However, a compromise must be made on the energy efficiency (65%) due to the intensified battery polarization induced by the introduction of cations (Li^+) adsorption on the cathode side. In-situ Raman was conducted to investigate charge storage mechanism, which displays good agreement with the proposed ion migration scenario. Furthermore, to combat the concerns on the limited lithium reserves, the Na- and K-ion capacitors are also investigated using as-prepared carbon materials.

Poster Abstract 5

Achieving superior sodium storage properties of hard carbon by tailoring morphological structure and surface functional groups via ammonia post treatment

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Sodium-ion batteries (SIBs) are considered as one of the most promising next-generation energy storage technologies due to the abundance of sodium metal resources. Hard carbon, with its low cost and large reversible capacities in sodium storage, becomes the leading anode candidate for practical application of SIBs. Large sodium storage capacity of hard carbon is primarily contributed by the interlayer intercalation of sodium ions in the low voltage region below 0.1 V vs. (Na^+/Na), and subordinately contributed by surface reactions in the sloping voltage region above 0.1 V. However, interlayer intercalation of sodium ions in hard carbon, as the primary contributor of sodium storage, offers sluggish kinetics and structural degradation after long-term cycles, resulting in the poor rate capability and capacity loss of SIBs. Different from the mechanism of interlayer intercalation, sodium storage via surface reactions, in which sodium ions bind with surface defective sites and functional groups of hard carbon, presents much faster reaction kinetics without structural degradation, thereby enabling the excellent rate performance and cyclic stability of SIBs. Therefore, enhancing the surface reactions is an effective approach for enhancing sodium storage properties of hard carbon anodes. In this work, we propose a general route to enhance surface reactions of hard carbon, by tailoring morphological structure and surface functional groups via ammonia post treatment. Hard carbon sheets, obtained by carbonization of polyacrylonitrile (PAN) foam and ammonia post treatment, exhibits porous and directional lamellar structures with highly defective surface and active pyrrolic nitrogen dopants. Compared to hard carbon sheets without ammonia treatment, the storage capacity in the sloping voltage region is dramatically increased from 105 mAh g^{-1} to 238 mAh g^{-1} at a current density of 0.1 A g^{-1}. As a result, the hard carbon anodes show both excellent rate capability (111 mAh g^{-1} at 5 A g^{-1} and 40 mAh g^{-1} at 20 A g^{-1}) and superb cycling performance (112 mAh g^{-1} after 5000 cycles at 1 A g^{-1}). The sodium storage mechanisms of hard carbon anodes with and without ammonia treatment are also discussed. The realization of tailoring morphological structure and surface functional groups of hard carbon anodes via ammonia post treatment opens a window for breakthroughs in the development of SIBs.

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Poster Abstract 6

Performance of a passive direct ethylene glycol fuel cell using hydrogen peroxide as oxidant

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Fuel cells have attracted great research interest as a promising power source in the last decades, which is mainly attributed to their simple design, high efficiency, low emissions as well as quick refueling [1]. Recently, ethylene glycol (EG), which is regarded as an alternative choice for fuel, has attracted great attention on mobile, stationary, and portable applications due to its high theoretical energy capacity (4.8 Ah mL^{-1}), high boiling point (198oC), and high electron transfer rate (80%) [2]. In addition, extensive research has conducted on replacing air or pure oxygen with hydrogen peroxide as oxidant, which is attributed to three intrinsic superiorities by using hydrogen peroxide: (1) the theoretical voltage will experience a substantial increase; (2) activation loss of the reduction reaction will decrease dramatically because it will become a two-electron transfer process; and (3) the water flooding problem will be avoided [3]. Particularly in special situations such as outer space and underwater where the oxygen is not sufficient, the using of hydrogen peroxide is more favorable. However, the active fuel and oxidant delivery requires auxiliary equipment, making the system more complicated and heavier. A passive fuel cell with EG as fuel and hydrogen peroxide as oxidant is proposed in this work, which gets rid of the auxiliary devices such as external pumps and eliminates the parasitic power losses [4]. This passive direct ethylene glycol fuel cell (DEGFC) is composed of a palladium-based anode, a cation exchange membrane (CEM), and a gold-based cathode. This passive DEGFC exhibits a theoretical voltage of 2.47 V and a practical open circuit voltage (OCV) of 1.58 V. The performance of this fuel cell under the optimal operating conditions (1.58 V and 65.8 mW cm^{-2}) has an impressive improvement comparing to a passive DEGFC with oxygen as oxidant, which is more than 2 times in the OCV and more than 5 times in the peak power density.

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Poster Abstract 7

Developing phosphides for anode application of sodium ion batteries

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Tin phosphide (Sn_4P_3) has been proposed as a promising anode material for sodium ion batteries, owing to its high theoretical volumetric capacity of about 1292 A h/L, high gravimetric capacity of 1132 mA h/g and reasonable redox potentials (~0.3 V for Na–Sn alloying and ~0.65 V for the Na–P compound vs. Na/Na^+, respectively). In our work, we first develop a facile solution based method to synthesize the phase pure Sn_4P_3 nanotops, and investigate the performance of this phase pure Sn_4P_3 anode for sodium ion batteries[1]. With the discovery of the Sn segregation that lead to the performance decay of Sn_4P_3 during cycling, we then introduce the third element Sb or Cu to form the ternary phosphides (Sn_4P_3/SbSn nanocomposites[2]/Cu_4SnP_{10}[3]) anodes. Sn_4P_3/SbSn nanocomposites anode shows higher cycle stability than the phase pure Sn_4P_3. The intact interface between the Sn_4P_3 and SbSn in the nanocomposite and their synergetic effect play important roles in enhancing the electrochemical performance of the composite electrode. The introduction of Cu helps to stabilize a rather high P content in the compound (as compared to Sn_4P_3, for example), enabling a high capacity of 811 mA h g^{-1} at a current density of 25 mA g^{-1} for phase pure Cn_4SnP_{10} nanowire anode. However, possible volume expansion and instability of the solid electrolyte interface in the Cn_4SnP_{10} nanowire anode remain as problems causing cycle instability of the electrode. By forming composite with multiwall carbon nanotubes, we demonstrate significantly improved cycle performance of the Cu_4SnP_{10}/MWCNTs composites anode, which delivers a stable capacity of 512 mA h g^{-1} after 100th cycle at a current density of 100 mA g^{-1}. At higher current density of 1 A g^{-1}, the capacity of the composite electrode retains at 412 mA h g^{-1}, showing its good rate performance.

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Poster Abstract 8

Facile Fabrication of Porous Carbon Cloth Catalyzed by Metal Organic Framework as Sulfur Host for Lithium Sulfur Batteries

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We present a facile porosification method of carbon cloth through a simple two-step method and demonstrate for the first time the capability of metal organic framework (MOF) at catalyzing the activation of carbon cloth. The homogeneously grown polycrystalline ZIF-67 on carbon cloth can induce the even distribution of pores without the assistance of KOH[1] or CO_2[2], etc. Specifically, polycrystalline MOF grown on carbon cloth can be transformed to Co_3O_4 phase, which experiences a gradual transformation process to CoO due to the reaction with carbon fiber during the high temperature treatment, leading to the formation of porous carbon cloth. The as-obtained porous carbon cloth presents an interconnected hierarchical porous structure with the co-existence of macropores, mesopores and micropores. When utilized as the supports of sulfur for lithium sulfur battery, the free-standing sulfur-impregnated carbon cloth electrode demonstrates obvious advantages over carbon cloth supported sulfur melt or sulfur slurry electrode and it could deliver a specific capacity of 380 mAh/g after 500 cycles at a current density of 0.125 C (1 C=1672 mAh/g).

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Poster Abstract 9

Dual-phase TiO_2 nanowires for high-power and high-capacity sodium storage

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Sodium-ion batteries (SIBs) have attracted great attention in recent years, especially for large-scale energy storage, due to the natural abundance of sodium reserves relative to lithium. The development of superb anode materials has long been a big challenge in SIB research. TiO_2 is a promising candidate, but it faces critical issues of low initial coulombic efficiency and rapid capacity decay. In this study, we synthesized dual-phase TiO_2 nanowires consisting of a TiO_2–B phase and an anatase phase with a simple hydrothermal and heat treatment method to address the above issues. When applied as an SIB anode, the dual-phase TiO_2 nanowires (TiO_2 NWs) exhibited ultrahigh reversible capacities (290.1 mAh g^{-1} at 0.25C and 148.1 mAh g^{-1} at 20C), long and stable cyclabilities (184.0 mAh g^{-1} at 1C after 200 cycles and 93.6 mAh g^{-1} at 20C after 800 cycles), and high energy densities (330 Wh kg^{-1} at a power density of 93 W kg^{-1} and 167 Wh kg^{-1} at a power density of 7.5 kW kg^{-1}). Operando Raman spectroscopy shows that Na+ insertion decreased the crystallinity of the dual-phase TiO_2 NWs and that the sodiation–desodiation cycle is a single-phase intercalation process. Kinetic analysis with cyclic voltammetry (CV) and temperature-dependent electrochemical impedance spectroscopy (EIS) measurement demonstrated that the dual-phase nanowires possessed an ultralow diffusion energy barrier, thus enhancing the Na+ intercalation pseudo-capacitive process, which is in line with the single-phase transition mechanism. This work opens up new perspectives for the future design of electrode materials with high capacities and high power densities.

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Poster Abstract 10

Solvent-Mediated Li_2S Electrodeposition: A Critical Manipulator in Lithium-Sulfur Batteries

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Controlling electrochemical deposition of lithium sulfide (Li_2S) is a major challenge in lithium-sulfur batteries as premature Li_2S passivation leads to low sulfur utilization and low rate capability. In this work, we reveal solvent's roles in controlling solid Li_2S deposition and develop quantitative solvent-mediated Li_2S growth models as guides to solvent selection. We show that Li_2S electrodeposition is controlled by electrode kinetics, Li_2S solubility and the diffusion of polysulfide/Li_2S, which is dictated by solvent's donicity, polarity and viscosity, respectively. These solvent-controlled properties are essential factors pertaining to the sulfur-utilization, energy efficiency and reversibility of lithium-sulfur batteries. We further demonstrate that the solvent selection criteria developed in this study are effective in guiding the search for new and more effective electrolytes, providing effective screening and design criteria for computational and experimental electrolyte development for lithium-sulfur batteries.

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Poster Abstract 11

Artificial Solid Electrolyte Interface for High-Voltage Aqueous Batteries

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Aqueous Li ion battery is a promising candidate for safe and sustainable energy storage system, however, it is limited by the narrow thermodynamic stability window of water (1.23V). Recently a new type of LiTFSI-based “water-in-salt” electrolyte with wide operational window was developed by constructing a stable solid electrolyte interface (SEI) via salt anion decompositions.[1-3] However, it suffers from high cost and potential toxicity. In this study, we aim to develop an artificial SEI without highly concentrated salt to prevent water splitting for high-voltage aqueous batteries. Our experimental results show that the electrochemical stability window of water can be extended to about 3 V with SEI coating on stainless steel current collector. Various parameters and design consideration for constructing stable SEI will be discussed in the presentation. Our work suggests an important direction for environmentally friendly and cheap high-voltage aqueous lithium ion batteries.

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Poster Abstract 12

An ether-based electrolyte produces improved interfacial electrochemical characteristics for sodium-ion batteries

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The use of an ether-based electrolyte can increase the sodium-ion storage performance, but the underlying fundamentals are not fully understood. Here we studied TiO_2, Sn and two carbon material anodes to investigate this issue. By coupling them with an ether-based electrolyte, excellent rate and cyclic performance was achieved and much better than that with an ester-based electrolyte. The ether-based electrolyte facilitates the sodiation transition and increases the Na^+ intercalation pseudocapacitance. Insight into the cell dynamics shows that the charge transfer energy barrier at the electrolyte/electrode interface, being the factor governing the electrochemical performance, is significantly reduced compared to that with an ester-based electrolyte. The solid electrolyte interphase exhibits major differences in organic species and composition distribution along its depth, which accounts for the better sodiation dynamics in an ether-based electrolyte. Our approach offers unprecedented insight into the extraordinary performance and interfacial characteristics of SIBs anodes induced by an ether-based electrolyte.

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Poster Abstract 13

Investigation to NaLiFePO4F of High Voltage Cathode Material for Lithium-ion Battery

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The lithium-ion battery is one of the most promising electrochemical energy storage system having great potential for a wide range of applications. However, there are certain challenges which need to be addressed such as low practical energy density, reduced lifetime and low cost-effectiveness. Three-dimensional polyanion compounds $(XO_4)^{m-}$ (X=P, S) with impressing electrochemical performance and stability are considering as the cathode material for next generation lithium-ion battery[1, 2]. Meanwhile, combining high iconicity M-F bond with $(XO_4)^{m-}$ (X=P, S) is able to enhance the operating voltage, such as $LiVPO_4F$ has already been reported with good performance[3]. Comparing with other fluorophosphates, $NaLiFePO_4F$ has received particular interest due to its high operating voltage and the potential of more than one alkali ion can be activated[4, 5]. Meanwhile, several problems are associated with this material such as low electronic conductivity and limited knowledge about the mechanism of the second lithium-ion activation during the charging and discharging process[6]. In order to solve these problems, first principle simulation, which is based on density functional theory, is employed to investigate the mechanism of lithium-ion extraction of $NaLiFePO_4F$ (Li_2FePO_4F). It is found that not only the transition metal Fe^{2+} but also O^{2-} will lose electron during the delithiation process by electronic structure analysis. Operating voltages and structural evolution are obtained after the calculation of lithiated phases Li_xFePO_4F (x=2, 1.5, 1, 0.5, and 0). The oxidation potentials for different lithium ion concentrationin Li_xFePO_4F compounds are located at ~3.41V, 3.51V, 4.80, and 5.60V respectively.The lithium-ionactivation prefers in the form of a singlephase. The $NaLiFePO_4F$ is synthesized by annealing the mixture of $LiFePO_4$ and NaF with molar ratio 1:1 at 650ºC for 1.5h. The Li_2FePO_4F can be obtained by ion-exchange upon electrochemical testing. The electrochemical performance is characterized by galvanostatic charge-discharge test between 2~4.5V at rate 0.1C with an average potential~3.4V vs Li. A reversible specific capacity ~127mAh g^{-1} can be obtained.

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Poster Abstract 14

Optimal Design of yolk-shell carbon-coated silicon nanoparticle electrodes for lithium ion battery

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Yolk-shell carbon-coated silicon-nanoparticles(Si@void@CNPs) have been demonstrated to have a great promise in solving the problem of significant volume change of silicon-based anode materials during lithiation and delithiation cycling. And in order to obtain a long cycle life and high capacity for Si@void@CNPs anode materials, an optimal design guideline is proposed based on both experimental observation and theoretical modeling. It has been proved that the yolk-shell structures can remain integrity and achieve high capacity performance with proper void space and the thickness of carbon coating. According to the guideline, the optimally designed nanoparticle anode materials are synthesized and achieve a reversible capacity of 1666.9 mAh·g^{-1} after 80 cycles with 75.1% capacity retention. The results of the experiments certify that the design guideline should be of significant value to the yolk-shell structured anode materials for lithium ion battery.

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Poster Abstract 15

“Tungsten Disulfide (WS_2)” an Effective Polysulfide Shuttle Inhibitor for Lithium Sulfur Batteries

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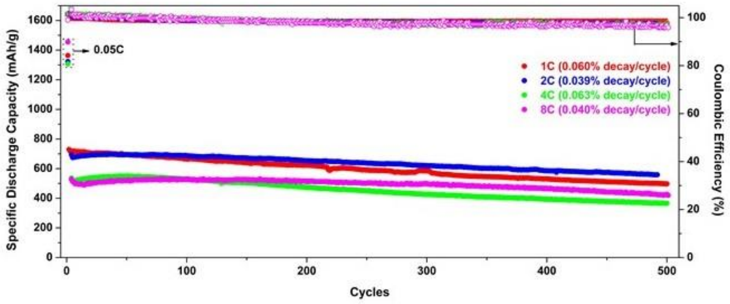
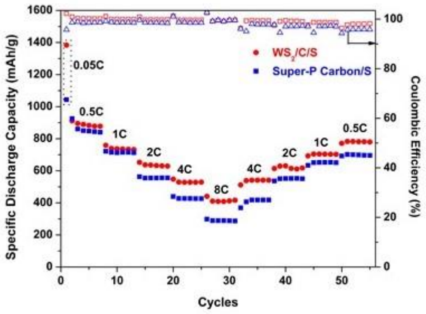
With the rapid advancement in portable electronic devices and electric vehicles, the demand for advanced research on next generation high energy density lithium ion batteries has gained significant importance. Among the different alternatives proposed to succeed lithium ion batteries, lithium sulfur batteries have drawn most attention because of the ultrahigh theoretical specific capacity(1675mAh/g) and specific energy density(2600Wh/kg) [1]. A dual function cathode consisting of tungsten disulfide and porous carbon nanosheets (WS_2/C) was synthesized to improve the performance of lithium sulfur batteries. The composite depicted very strong affinity towards lithium polysulfides. The cathode demonstrated excellent cycling stability and rate capability by delivering a reversible specific capacity of 419mAh g^{-1} at 8C after 500 cycles with low capacity fading at 0.04% per cycle. At high sulphur loading of 4.7mg cm^{-2} the batteries delivered 3.4mAh cm^{-2} areal capacity after 100 cycles at 0.5C. The synergistic effect of strong chemical interaction between lithium polysulfides and WS_2, and the superior electronic conductivity of carbon nanosheets are responsible for the enhanced performance.





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Poster Abstract 16

P-doped FeS_2 as High-Performance Anode for Lithium/Sodium ion Batteries

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For the development of high-performance lithium/sodium-ion batteries, building high capacity and long cycle life anode is appealing and challenging. Pyrite (FeS_2) is an attractive anode material with a high theoretical capacity of 894 mAh g^{-1} but the rapid capacity fading limits its application. Herein, by utilizing a simple one-step method, we have developed phosphorus-doped pyrite with different doping mass. This material exhibits excellent electrochemical performance for LIBs and SIBs. For LIBs, it delivers a high specific capacity of 650 mAh g^{-1} at 200 mA g^{-1} after 100 cycles. For SIBs, it gives a high specific capacity of 590 mAh g^{-1} at 100 mA g^{-1} after 50 cycles.