



20<sup>th</sup> International Conference on

## **Advanced Energy Materials and Research**

August 13-14, 2018 | Dublin, Ireland

# Keynote Forum

## Day 1

Advanced Energy Materials 2018

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## Xiaodong Li

*University of Virginia, USA*

### Biomass-derived activated carbon scaffolds for electrochemical energy storage

With increasing energy and environment concerns, how to efficiently convert and store energy has become a critical topic. Electrochemical energy storage devices, such as supercapacitors and batteries, have been proven to be the most effective energy conversion and storage technologies for practical application. Supercapacitors and lithium-based batteries are particularly promising because of their excellent power density and energy density. However, further development of these energy storage devices is hindered by their poor electrode performance. The carbon materials in supercapacitors and batteries, such as graphite, activated carbons and various nanostructured carbon materials (ordered porous carbon, CNT, graphene etc.), are often derived from nonrenewable resources under relatively harsh environments. Naturally abundant biomass with hierarchically porous architecture is a green, alternative carbon source with many desired properties for supercapacitors and lithium-based batteries. Recently, we converted cotton, banana peel, and recycled paper into highly porous, conductive activated carbon scaffolds for advanced energy storage applications via a low-cost and high throughput manufacturing process. The activated carbon scaffolds were further coated with active materials such as  $\text{NiCo}_2\text{O}_4$ ,  $\text{NiO}$ , Co-Al layered double hydroxides (Co-Al LDHs),  $\text{Ni}_2\text{S}$ , sulfur nanoparticles, and graphene to enhance their electrochemical properties. The biomass-derived activated carbon materials are effective in improving supercapacitor's energy density and in blocking the dissolution of reaction intermediates in lithium sulfur batteries. Especially, the biomass-derived carbons provide scaffolds for hosting sulfur in lithium sulfur batteries to manipulate the "shuttle effects" of polysulfides and improve the utilization of sulfur. In particular, the activated carbon textiles (derived from cotton textiles) are flexible and conductive, and an ideal substrate for constructing flexible supercapacitors, batteries, and self-powered flexible solar cell/supercapacitor (or battery) systems. Using biomasses is definitely the right track towards making renewable carbon materials for future energy storage devices.

### Recent Publications

1. Gao Z, Bumgardner C, Song N, Zhang Y, Li J, Li X (2016) Cotton-textile-enabled flexible self-sustaining power packs via roll-to-roll fabrication. *Nature communications* 7: 11586.
2. Gao Z, Song N, Zhang Y, Li X (2015) Cotton Textile enabled, flexible lithium-ion batteries with enhanced capacity and extended Lifespan. *Nano letters* 15: 8194–8203.
3. Bao L, Li X (2012) Towards textile energy-storage from cotton T-shirts. *Advanced materials* 24: 3246-3252.
4. Zhang Y, Gao Z, Li X (2017) Capillarity composited recycled paper/graphene scaffold for lithium-sulfur batteries with enhanced capacity and extended lifespan. *Small* 13: 1701927.
5. Zhang Y, Gao Z, Song N, Li X (2016) High-performance supercapacitors and batteries derived from activated banana-peel with porous structures. *Electrochimica acta* 222: 1257–1266.

### Biography

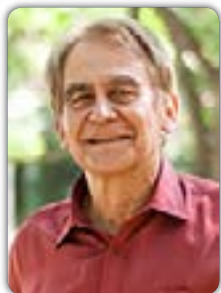
Xiaodong Li is a Rolls-Royce Commonwealth Professor at the University of Virginia with expertise and interests including nanomaterial-enabled energy systems, biological and bio-inspired materials and devices, additive manufacturing, smart manufacturing, biomechanics, micro/nanomechanics, surface engineering, and tribology. His stature in the field of his expertise includes over 230 peer-reviewed journal articles in prestigious journals such as *Science*, *Nature Communications*, *Advanced Materials*, and *Advanced Energy Materials*; over 12,000 citations with H-index of 54; TMS MPMD Distinguished Scientist/Engineer Award (2015), Professional Engineering Publisher's PE Prize (2008); over 80 invited plenary lectures/keynotes/talks at international conferences/workshops; Fellow of the American Society of Mechanical Engineers (ASME); and Fellow of the Society of Experimental Mechanics (SEM). His breakthrough work has been featured by over 1,000 media outlets worldwide including BBC, Discovery News, Science Daily, and MSNBC. His innovation on cotton textile based composites was recently selected by New York Times – Year in Ideas for Year 2010.

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## Jerzy. A. Szpunar

*University of Saskatchewan, Canada*

### Hydrogen generation in metal water reaction and strategies of storage

Hydrogen has been recognized as a clean and sustainable fuel. However still many problems have to be solved in area of generation, transport and storage of this fuel for future hydrogen based economy to be realized. Some of our research in this area will be presented. Reaction of water with activated aluminum powder is considered as one of the methods to generate hydrogen. The reaction produces also aluminum hydroxide ( $\text{Al}(\text{OH})_3$  or  $\text{AlOOH}$ ) as the byproduct; these compounds change to alumina ( $\text{Al}_2\text{O}_3$ ) after calcination process, and alumina can produce aluminum [1, 2]. Hydrogen production rate can be increased if effective surface area of aluminum exposed to oxidation is increased. We found that microstructural refinement can be used to promote the reaction and allow major increase of the production of hydrogen. The addition of water soluble salts (potash or salt) also allow to increase the oxidation rate and hydrogen generation. However, we established that presence of salt has smaller influence than microstructural modifications. The storage of hydrogen will also require structural modification of the storage system. One of storage system that was developed by our team will be discussed [3]. We designed a Pd-graphene composite for hydrogen storage with spherical shaped nanoparticles of 45 nm size homogeneously distributed over a graphene substrate. This new hydrogen storage system has attractive features like high gravimetric density, ambient conditions of hydrogen charge and low temperature of the hydrogen discharge. The palladium particles produce a low activation energy barrier to dissociate Plenary this helps delaying the formation of metallic clusters and can improve hydrogen storage in metal graphene systems.

### Recent Publications

1. Razavi-Tousi, J.A. Szpunar, Effect of addition of water-soluble salts on the hydrogen generation of aluminium in reaction with hot water, *Journal of Alloys and Compounds*, 679 (2016) 364-374.
2. Razavi-Tousi, J.A. Szpunar, Microstructural evolution and grain subdivision mechanisms during severe plastic deformation of aluminum particles by ball milling, *Philosophical Magazine*, 95 (2015) 1425-1447.
3. C.Y. Zhou, J.A. Szpunar, X.Y. Cui, Synthesis of Ni/graphene nanocomposite for hydrogen storage, *ACS Applied Materials & Interfaces*, 8 (2016) 15232-15241.
4. A. Choudhary, L. Malakkal, R.K. Siripurapu, B. Szpunar, J.A. Szpunar, First principles calculations of hydrogen storage on Cu and Pd-decorated graphene, *International Journal of Hydrogen Energy*, 41 (2016) 17652-17656.
5. O. Faye, U. Eduok, J. Szpunar, B. Szpunar, A. Samoura, A. Beye, Hydrogen Storage on bare Cu atom and Cu-functionalized boron-doped graphene: a first Principles study, *International Journal of Hydrogen Energy*, 42 (2017) 4233-4243.

### Biography

Jerzy. A. Szpunar, joined the Department of Mechanical Engineering at the University of Saskatchewan in August 2009, as Tier I Canada Research Chair. He came from McGill University where he was Professor of Materials Science and Birks Chair in Metallurgy. His research interests extend to various areas of materials related investigations. More recently his research has focused on environmentally friendly energy generation, in particular the extraction and purification of hydrogen, accident tolerant nuclear fuel and research on advanced materials for Generation IV nuclear reactors. His research supports also various clean energy programs and research on more safe and secure materials for oil and gas transportation. Dr Szpunar has a strong record of research productivity. 40 PhD students and 27 MSc. students graduated under his supervision. He is an author and co-author of more than 900 research papers.

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## Hyoyoung Lee

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### Controlling energy bandgap of semiconducting materials for energy and environment

A control of the energy bandgap of semiconducting materials including transition metal chalcogenides (TMCs) including  $\text{TiO}_2$ ,  $\text{MoS}_2$  and  $\text{CoS}_2$  have been paid attention for energy conversion and environmental issues. Herein, we like to introduce new findings about the visible-light driven blue  $\text{TiO}_2$  materials for photo-catalytic hydrogen evolving reaction (HER) and for an application to remove algae from water.<sup>1,2</sup> In addition, we like to report new layered ternary transition metal chalcogenides (TTMCs) material to overcome to the limitation of active sites which is challenging in binary transition metal chalcogenides (BTMC) such as  $\text{MoS}_2$  towards electrochemical hydrogen production. The TTMC,  $\text{Cu}_2\text{MoS}_4$  has been successfully synthesized by a facile solution-processed method. Moreover, by anion doping such as Se in as the synthesized  $\text{Cu}_2\text{MoS}_4$ , it has been found that TTMC can be exfoliated into single layer nanosheets and the single layered TTMC exhibits the highest electrocatalytic activity towards HER.<sup>3</sup> We also report an advanced bi-functional hybrid electrocatalyst for both oxygen reduction reaction (ORR) and oxygen evolution reaction (OER), which is composed of WS<sub>2</sub> and CNT connected via tungsten carbide (WC) bonding. WS<sub>2</sub> sheets on the surface of CNTs provide catalytic active sites for electrocatalytic activity while the CNTs act as conduction channels and provide a large surface area. We found that four to five layers of WS<sub>2</sub> sheets on the surface of CNTs produces excellent catalytic activity towards both ORR and OER, which is comparable to noble metals (Pt,  $\text{RuO}_2$ , etc.). Our findings show the many advantages enabled by designing highly-active, durable, and cost-effective ORR and OER electrocatalysts.<sup>4</sup> Finally, we like to demonstrate new strategy to satisfy all requirements for the development of a highly active and remarkably durable HER electrocatalyst in both acidic and alkaline media via anion-cation double substitution into a  $\text{CoS}_2$  moiety for preparing 3D mesoporous pyrite-metal vanadium-cobalt phosphorsulphide ( $\text{Co}_{1-x}\text{V}_x\text{SP}$ ).<sup>5</sup>

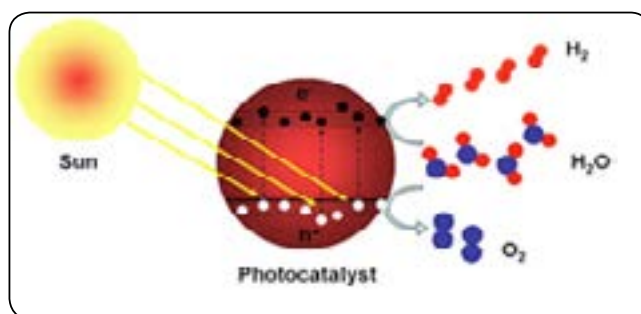


Figure 1: Schematic of solar photo-catalyst.

### Recent Publications

1. Kan Zhang, et al. (2016) An order/disorder/water junction system for highly efficient co-catalyst-free photocatalytic hydrogen generation. *Energy & Environmental Science*, 9, 499-503.
2. Youngmin Kim, Hee Min Hwang, Luyang Wang, Ikjoon Kim, Yeoheung Yoon and Hyoyoung Lee\* (2016) Solar-light photocatalytic disinfection using crystalline/amorphous low energy bandgap reduced  $\text{TiO}_2$ . *Scientific Reports*, 6, 25212; doi: 10.1038/srep25212.

3. Anand P. Tiwari, Doyoung Kim, Yongshin Kim, Om Prakash, and Hyoyoung Lee\* (2016) Highly Active and Stable Layered Ternary Transition Metal Chalcogenide for Hydrogen Evolution Reaction. *Nano Energy*, 28, 366–372.
4. Anand P. Tiwari, Doyoung Kim, Yongshin Kim, and Hyoyoung Lee\* (2017) Bi-functional oxygen electrocatalysis through chemical bonding of transition metal chalcogenides on conductive carbons. *Advanced Energy Materials*, 1602217.
5. Ngoc Quang Tran, Quoc Viet Bui, Minh Hung Le, Yoshiyuki Kawazoe and Hyoyoung Lee\* (2017) Anion-Cation Double Substitution in Transition Metal Dichalcogenide to Accelerate Water Dissociation Kinetic for Electrocatalysis. *Advanced Energy Materials*, In-revision.

## Biography

Hyoyoung Lee has completed his PhD at Department of Chemistry, University of Mississippi, USA in 1997. He did his Postdoctoral studies at North Carolina State University. He worked at Electronics and Telecommunications Research Institute and then moved to Department of Chemistry, Sungkyunkwan University as a full Professor. He served as a Director of National Creative Research Initiatives. Currently, he has served as an Associate Director of Centre for Integrated Nanostructure Physics, Institute of Basic Science. His current research area is 0-2D semiconducting materials and their devices. He has written more than 140 journal articles in top-tier journals and has been serving as an Editorial Board Member of *Scientific Reports*.

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# Keynote Forum

## Day 2

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## Olivier Joubert

*Jean Rouxel Institute of Materials in Nantes – CNRS, France*

### Promising oxy borates for solid-oxide fuel cell applications

The research on solid oxide fuel cell ( $H^+$  or  $O^{2-}$  SOFC) is based on both the synthesis of new materials and the design process of the cell. The main advantage of SOFC is that they can work under hydrocarbon fuel at temperature higher than  $\approx 700^\circ C$ . In the current SOFC systems, the most widely used electrolyte is yttria-stabilized zirconia (YSZ) which is inexpensive and shows an acceptable conductivity level. But YSZ is very refractory and its major drawback is its reactivity during the sintering process with lanthanum- and strontium-based cathode materials, which leads to the formation of an insulating layer such as  $SrZrO_3$  or  $La_2Zr_2O_7$ . There is also a great interest to find ceramic based fuel cells, for mobile application, working at low temperature ( $\approx 400^\circ C$ ). This can be achieved in  $H^+$ -SOFC with a ceramic membrane showing a good proton conductivity level. The state of the art perovskite type yttrium-doped  $BaCeO_3$  (called BCY) shows a proton conductivity level above 1 mS/cm at  $400^\circ C$ . But due to its high basicity, BCY tends to decompose, in this temperature domain, in air containing  $CO_2$ . Finding new electrolyte material is one of the issues. In this presentation, after a briefly state-of-the art concerning SOFC electrolyte, we will report on high-temperature proton and oxide ion conductivities in two new class of oxyborates,  $La_{26}O_{27}(BO_3)_8$  and doped  $Ba_3Ti_3O_6(BO_3)_2$  compounds. Both samples were prepared by solid-state reaction and characterized using x-ray diffraction and electrochemical impedance spectroscopy. Quite high conductivity level, about  $6.8 \times 10^{-4}$  and  $1.5 \times 10^{-4}$  S/cm at  $700^\circ C$  in air were observed respectively. The transport properties can be understood in terms of the presence in high concentrations of oxygen and barium vacancies as well as oxygen interstitials as observed in hybrid density-functional defect calculations.

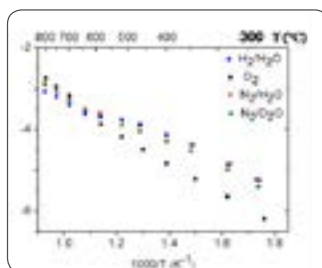


Figure 1: Conductivity vs. temperature of the oxyborate  $La_{26}O_{27}(BO_3)_8$  under different atmospheres

### Recent Publications

1. Lebreton M, Delanoue B, Baron E, Ricoul F, Kerihuel A, Subrenat A, Joubert O and Le Gal La Salle A (2015) Effects of carbon monoxide, carbon dioxide, and methane on nickel/yttria - stabilized zirconia-based solid oxide fuel cells performance for direct coupling with a gasifier. *International Journal of Hydrogen Energy* 40(32):10231-10241.
2. Jarry A, Joubert O, Suard E, Zanotti J M and Quarez E (2016) Location of deuterium sites at operating temperature from neutron diffraction of  $BaIn_{0.6}Ti_{0.2}Yb_{0.2}O_{2.6-n}(OH)_{2n}$ , an electrolyte for proton-solid oxide fuel cells. *Physical Chemistry Chemical Physics* 18:15751.
3. Quarez E, Noirault S, Caldes M T and Joubert O (2010) Water incorporation and proton conductivity in titanium substituted barium in date. *Journal of Power Sources* 195(4):1136-1141. Noirault S, Célérier S, Joubert O, Caldes M T and Piffard Y (2007).

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4. Noirault S, Célérier S, Joubert O, Caldes M T and Piffard Y (2007) Incorporation of water and fast proton conduction in the inherently oxygen deficient compound  $\text{La}_{26}\text{O}_{27}(\text{BO}_3)_8$ . *Advanced Materials* 19(6):867–870.
5. Doux J M, Hoang K, Joubert O and Quarez E (2017) Oxygen ion transport and effects of doping in  $\text{Ba}_3\text{Ti}_3\text{O}_6(\text{BO}_3)_2$ . *Chemistry of Materials* 29:6425–6433.

## Biography

Olivier Joubert is a Professor at Nantes University and Chairs the Fuel Cell group of Institut des Matériaux Jean Rouxel (CNRS-IMN). His major research interests concern new ceramic materials. He has participated to the development of novel ion and proton conductors as electrolyte for solid oxide fuel cell and electrolyser and also anode materials. He is co-author of 95 publications, 20 invited talks and 5 patents. He is chairing the HySPaC research grouping which assembles all French academic research groups in the field of production and storage of hydrogen and also fuel cell and electrolysers, about 108 laboratories mainly from the CNRS and CEA. He is the main organizer of the IDHEA meetings held in Nantes in 2014 and 2016. He is in charge of the expertise cell ERIMAT in Capacités SAS, a private subsidiary of the University of Nantes dedicated to the development of research, and provides assessment, advice to industries.

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## Marie Duquesne

Bordeaux INP - CNRS, France

### Organic biosourced phase change materials for seasonal thermal energy storage

Our work focused on thermal energy storage in a seasonal basis for heating and domestic hot water supply in buildings. The objective is to develop and study innovative organic bio sourced phase change materials (PCM) able to compete with water and surpass the performances of commonly used PCM today (low cost, high energy density, compactness, thermal losses reduction, environmentally friendly etc.). Sugar alcohols (SA) and their blends could provide high storage energy densities in the range of 120–190 kWh/m<sup>3</sup> at temperatures inferior to 100°C with limited thermal losses due to high undercooling. They are compatible with commonly used container materials and with cheap solar collectors. They present long-term stability (no separation, no segregation, controllable thermal degradation) and moderate-to-low volume changes. Their prices are acceptable. First, a screening of SA and SA-blends to select the ones with melting temperatures inferior to 100°C was done. Then, an experimental characterization of the selected SA and SA-blends was performed. This encompasses the measurements of their melting point, their latent heat of fusion and the experimental determination of all key physical properties (specific heat, thermal conductivity, thermal diffusivity, density, viscosity) as a function of the temperature. The activation of the energy discharge process (crystallization) is difficult and the subsequent crystallization rates (discharge powers) are very low. Therefore, it was important to find out an easy to implement and efficient solution to discharge the storage system at the required power when needed. When the energy is needed, the storage system is discharged by activating SA crystallization using the efficient method found out in previous step. The associated discharge power depends on the SA crystal growth kinetics. The final step aims at measuring and modeling crystal growth rates in undercooled melts of SA and SA blends according to the temperature and determining the involved crystal growth mechanisms.

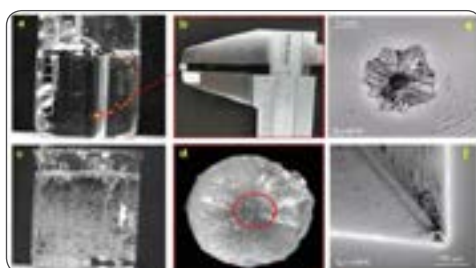


Figure 1: Activation of undercooled SA by bubbling (a-d) and optical and infrared images of one SA initiated crystallization (e & f)

#### Recent Publications

1. E Palomo Del Barrio, R Cadoret, J Daranlot and F Achchaq (2016) Infrared thermography method for fast estimation of phase diagrams. *Thermochimica Acta* 625:9-19.
2. E Palomo Del Barrio, R Cadoret, J Daranlot and F Achchaq (2016) New sugar alcohols mixtures for long-term thermal energy storage applications at temperatures between 70°C and 100°C. *Solar Energy Materials and Solar Cells* 155:454-468.
3. E Palomo del Barrio, A Godin, M Duquesne, J Daranlot, J Jolly, W Alshaer, T Kouadio and A Sommier (2017) Characterization of different sugar alcohols as phase change materials for thermal energy storage applications. *Solar Energy Materials and Solar Cells* 159:560-569.

4. H Zhang, M Duquesne, A Godin, S Niedermaier, E Palomo del Barrio, S V Nedeja and C C M Rindt (2017) Experimental and in silico characterization of xylitol as seasonal heat storage material. *Fluid Phase Equilibria* 436:55-68.
5. A Godin, M Duquesne, E Palomo del Barrio, F Achchaq and P Monneyron (2017) Bubble agitation as a new low intrusive method to crystallize glass-forming materials. *Energy Procedia* 139:352-357.

## Biography

Marie Duquesne defended her PhD: Resolution and reduction of a non-linear energy storage model by adsorption on zeolites in 2013. She is an Associated Professor at the National Polytechnic Institute of Bordeaux since 2015 and Researcher at Trefle Department (Fluids & Transfers) of the I2M and a member of TESLab (Thermal Energy Storage Laboratory), I2M/Abengoa Joint Research Unit. She has expertise in thermal energy storage at low-to-medium temperatures and contributes to an ANR Project SIMINTEC (National Project, 2008-2011) and to the European FP7 SAM.SSA Project (Sugar alcohol based material for seasonal storage applications, 2012-2015).

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## Notes: