



Small Conferences. BIG Ideas.

# Interfaces in Energy Materials

Presented by *APL Materials*

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**April 10-12, 2018**

Trinity College, University of Cambridge

# Interfaces in Energy Materials

April 10 – 12, 2018

Trinity College, University of Cambridge,  
Cambridge, UK

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**Interfaces in Energy Materials** is an AIP Publishing Horizons conference presented by *APL Materials*. Designed to facilitate conversation between innovative researchers at the forefront of materials science, this conference will help shape the future of the field.

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## PROGRAM

All scientific talks will take place in the Winstanley Lecture Theatre. Poster sessions will be held in the Old Combination Room. Dinner on April 10 will be in the Old Kitchen, and dinner on April 11 will be in the Great Hall. Breakfast and Lunch all days will be in the Great Hall.

### Tuesday, April 10

12:00PM – 6:00PM . . . . .	Registration	4:30PM – 6:00PM . . . . .	Poster Session I
2:00PM – 3:00PM . . . . .	College Tour	6:00PM – 8:00PM . . . . .	Dinner & Welcome Reception (Old Kitchen)
4:20PM – 4:30PM . . . . .	Welcome Remarks		

### Wednesday, April 11

8:00AM – 10:00AM . . . . .	Registration	8:15AM – 9:00AM . . . . .	Breakfast (Great Hall)
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#### SESSION I CHAIR: CHANG-BEOM EOM

9:00AM – 9:10AM . . . . .	Introductory Comments
9:10AM – 9:40AM . . . . .	Darrell Schlom (Cornell University) <i>Customizing Oxide Interfaces with Atomic Precision</i>
9:40AM – 10:10AM . . . . .	Nini Pryds (Technical University of Denmark)   <i>Role of Oxide Interfaces in Highly Confined Electronic and Ionic Conductors</i>
10:10AM – 10:40AM . . . . .	Ivan Božović (Brookhaven National Laboratory) <i>High-<math>T_c</math> Interface Superconductivity</i>
10:40AM – 10:50AM . . . . .	Contributed Talk: Hongguang Wang (Max Planck Institute for Solid State Research)   <i>Atomically-Resolved Investigations of Local Structure and Cationic Intermixing at SrMnO<sub>3</sub>-SrTiO<sub>3</sub> Heterointerfaces by Aberration-Corrected Analytical Transmission Electron Microscopy</i>
10:50AM – 11:00AM . . . . .	Contributed Talk: Jingoo Lee (St. Andrews University) <i>Ni-exsolved CaTiO<sub>3</sub> Catalysts for Oxygen-evolution Reactions in Alkaline Conditions</i>
11:00AM – 11:20AM . . . . .	Coffee/Tea Break

#### SESSION II CHAIR: G. JEFFREY SNYDER

11:20AM – 11:50AM . . . . .	David Cahill (University of Illinois, Urbana-Champaign) <i>Plasmonic Probes of Ultrafast Interfacial Heat Transfer and Liquid-Vapor Phase Transformations</i>
11:50AM – 12:20PM . . . . .	Gang Chen (Massachusetts Institute of Technology)   <i>Phonon Thermal Transport through Single and Multiple Interfaces</i>
12:20PM – 12:30PM . . . . .	Contributed Talk: Jimmy Kuo (Northwestern University)   <i>Grain boundary dominated charge transport in Mg<sub>3</sub>Sb<sub>2</sub>-based compounds</i>
12:30PM – 12:40PM . . . . .	Contributed Talk: Patrick Hopkins (University of Virginia) <i>Ultrahigh Thermal Boundary Conductances at Crystalline and Amorphous Interfaces</i>
12:40PM – 2:00PM . . . . .	Lunch (Great Hall)

#### SESSION III CHAIR: SIÂN DUTTON

2:00PM – 2:30PM . . . . .	Junichiro Shiomi (University of Tokyo)   <i>Designability of Nanostructure Interfaces of Phonon and Electron Transport</i>
2:30PM – 3:00PM . . . . .	Bilge Yildiz (Massachusetts Institute of Technology) <i>Chemical and Electrochemical Stability of Perovskite Oxide Surfaces in Energy Conversion: Mechanisms and Improvements</i>
3:00PM – 3:30PM . . . . .	Mogens Mogensen (Technical University of Denmark)   <i>Controlling the Composition of Surfaces and Interfaces in Solid Oxide Cells</i>
3:30PM – 4:00PM . . . . .	Ainara Aguadero (Imperial College London) <i>Local Chemical Degradation Processes and Ionic Transport in Garnet All-Solid-State Batteries</i>
4:00PM – 4:10PM . . . . .	Contributed Talk: Matias Acosta (Cambridge University)   <i>Epitaxial Mesoporous Thin Films for Solid Oxide Fuel Cells Cathodes</i>
4:10PM – 4:20PM . . . . .	Contributed Talk: Annalena R. Genreith-Schriever (RWTH Aachen University)   <i>Field-enhanced Ion Transport at Grain Boundaries</i>
4:20PM – 4:30PM . . . . .	Contributed Talk: Benjamin Morgan (University of Bath) <i>Combined Atomistic + Semi-Continuum Modelling of Nanoionic Space Charge Regions in CeO<sub>2</sub></i>
5:30PM – 7:00PM . . . . .	Poster Session II
7:00PM – 9:00PM . . . . .	Dinner (Great Hall)

## Thursday, April 12

8:15AM – 9:00AM ..... Breakfast (*Great Hall*)

## SESSION IV CHAIR: CLARE GREY

- 9:00AM – 9:30AM ..... Ryoji Kanno (Tokyo Institute of Technology) | *Lithium Superionic Conductor and All-Solid-State Battery—Materials and Electrode/Electrolyte Interface*
- 9:30AM – 10:00AM ..... Virginie Viallet (University de Picardie) | *Interfacial Issues and Challenges for Bulk-Type All-Solid-State Batteries*
- 10:00AM – 10:30AM ..... Taro Hitosugi (Tokyo Institute of Technology) | *A Very Low Resistance at Solid-Electrolyte and Electrode Interfaces: Introducing Oxide Epitaxial Thin-Film Technology to Battery Research*
- 10:30AM – 10:40AM ..... Contributed Talk: Steffen Emge (Cambridge University) | *Solid-State NMR as a Tool to Study Structure and Dynamics in Solid Electrolytes*
- 10:40AM – 10:50AM ..... Contributed Talk: James Dawson (University of Bath) | *Atomic-Scale Influence of Grain Boundaries on Li-Ion Conduction in Solid Electrolytes for All-Solid-State Batteries*
- 10:50AM – 11:00AM ..... Contributed Talk: Fumitake Kametani (Florida State University) | *Atomic Investigation of Localized Oxygen Variation Induced by Strain at the Interface and Grain Boundaries in Perovskite Oxide High Temperature Superconductors*
- 11:00AM – 11:30AM ..... Coffee/Tea Break
- 11:30AM – 12:15PM ..... Panel Discussion (Chair: Judith Driscoll)
- 12:15PM – 12:20PM ..... Closing Remarks
- 12:30PM – 1:30PM ..... Lunch (*Great Hall*)



## DARRELL SCHLOM

Cornell University

## Presentation Title

*Customizing Oxide Interfaces with Atomic Precision*

## ABSTRACT

Thin-film synthesis plays a crucial role in producing exquisite interfaces for today's semiconductor devices with the highest performance. Are these same techniques relevant for energy materials? With the desire to stimulate this discussion, this talk will be dedicated to showing examples of oxide interfaces customized at the atomic layer level using molecular-beam epitaxy. A broad range of systems will be shown—starting with perovskites, but including rutiles, pyrochlores, garnets, and more. Thin film tricks that are appropriate for engineering interfaces will be described. These include strain engineering, dimensional confinement, breaking symmetries to unleash symmetry forbidden properties, epitaxial stabilization of metastable phases, digital alloys as an alternative to solid solutions, and the ability to engineer the structure and chemistry of the surface independent from that of the subsurface just a monolayer away. The band structure is revealed by high-resolution angle-resolved photoemission (ARPES) on pristine as-grown surfaces of these complex oxides made possible by a direct ultra-high vacuum connection between the MBE and ARPES.

## BIOSKETCH

Darrell Schlom is the Herbert Fisk Johnson Professor of Industrial Chemistry in the Department of Materials Science and Engineering at Cornell University. After receiving a B.S. degree from Caltech, he did graduate work at Stanford University receiving an M.S. in Electrical Engineering and a Ph.D. in Materials Science and Engineering. He was then a post-doc at IBM's research lab in Zurich, Switzerland in the oxide superconductors and novel materials group managed by Nobel Prize winners J. Georg Bednorz and K. Alex Müller. He has received various awards including an Alexander von Humboldt Research Fellowship and the MRS Medal. He has published over 500 papers and 8 patents, is a Fellow of both the American Physical Society and the Materials Research Society, and is a member of the National Academy of Engineering of the U.S.A.

## FEATURED SPEAKERS



### NINI PRYDS

Technical University of Denmark

#### Presentation Title

*Role of Oxide Interfaces in Highly Confined Electronic and Ionic Conductors*

#### ABSTRACT

The conductance confined at the interface of complex oxide heterostructures provides new opportunities to explore nanoelectronic as well as nanoionic devices. When two oxides intimately contact each other, charge redistribution or mass transfer of ions may occur. I will show the possibility of stabilizing phases which are otherwise not stable using highly coherent interfaces of alternating layers. Remarkably, an exceptionally high chemical stability in reducing conditions and redox cycles at high temperature, usually unattainable for oxide materials, is achieved. I will further discuss and show that different scattering mechanisms at the 2D electron gas (2DEG) of SrTiO<sub>3</sub>-based interfaces can be controlled by defect engineering leading to enhanced mobility. Based on the enhanced mobility, in 2DEG samples of unprecedented structural perfection, we have recently studied the Quantum Hall Effect (QHE) which reveal the strength of enhancing the mobility. I will also show some results observed at these interfaces indicating a large positive magnetoresistance of 80,000% and the presence of a highly strain-tunable magnetic order. This collection of samples offers unique opportunities for a wide range of rich world and new functionality of oxide interfaces.

#### BIOSKETCH

Nini Pryds is a Professor and head the research section 'Electrofunctional Materials' at the Department of Energy Conversion and Storage, The Technical University of Denmark (DTU), where he leads a group of about 30 researchers working in the field of magnetic refrigeration, thermoelectricity and functional oxide thin films. During the last 10 years he has played a leading role in a new cross-disciplinary research fields in the area of functional materials for energy application. In Denmark he has started and matured an area now known as magnetic refrigeration, which is based on the magnetocaloric effect. His group is currently recognized internationally as one of the leading group worldwide in this area. At DTU he also started the work on high temperature thermoelectric materials and his group succeeded to develop the highest zT p-type oxide materials reported so far. His group has developed a thermoelectric oxide module, which currently holds the highest efficiency oxide module. He has also started the activity at DTU and in Denmark in the area of interfaces of complex oxides, which include materials physics of complex oxides. His current interests focus on the deposition and properties of complex metal oxide films and heterostructures. Current research lines include also the study of structure-properties relationship in new oxide functional materials with special charge, spin or electronic orders, and the study of novel oxides for technological applications.



### IVAN BOŽOVIĆ

Brookhaven National Laboratory

#### Presentation Title

*High-T<sub>c</sub> Interface Superconductivity*

#### ABSTRACT

Surface and interface superconductivity were envisioned by V. L. Ginzburg in early sixties. By early nineties, a group at Varian Research Center (Eckstein, Božović, Schlom) was already experimenting with interface superconductivity in heterostructures, multilayers, and superlattices that contained layers of high-T<sub>c</sub> superconducting (HTS) cuprates. The first HTS tunnel junctions were fabricated, and even several novel artificial (i.e., metastable) HTS compounds were synthesized. The enabling technique has been atomic layer-by-layer molecular beam epitaxy (ALL-MBE).

In the two decades that followed, the ALL-MBE technique has been further developed and improved, and interface superconductivity became a 'hot' (i.e., fashionable) topic. This provided an impetus to devise new techniques for unraveling the precise atomic structure of buried interface layers as well as for studying their physical properties. New physics has also emerged from studies of 2D quantum confinement (leading to giant thermal or quantum critical fluctuations), of broken symmetries (resulting e.g. in large Rashba spin-orbit coupling or in topological superconductivity), and of a variety of proximity effects (resulting in extreme susceptibility and colossal responses to small perturbations). These developments will be illustrated by a number of simple examples largely drawn from my own practice with ALL-MBE of HTS cuprates but intended to illustrate the more general concepts listed above.

We will conclude by comparing interface superconductivity in cuprates and in other classes of materials, especially Fe-based superconductors, and lay out some grand challenges for the field.

#### BIOSKETCH

Ivan Božović received his PhD in Solid State Physics from Belgrade University, Yugoslavia, where he was later elected a professor and the Physics Department Head. After moving to USA in 1985 he worked at Stanford University, the Varian Research Center, and in Oxxel, Bremen, Germany. Since 2003, he is the MBE Group Leader at Brookhaven National Laboratory, and since 2014 also an Adjunct Professor of Applied Physics at Yale University. He is a Member of European Academy of Sciences, Foreign Member of the Serbian Academy of Science and Arts, Fellow of APS, and Fellow of SPIE. He received the Bernd Matthias Prize for Superconducting Materials, SPIE Technology Award, the M. Jaric Prize, the BNL Science and Technology Prize, was Max Planck and Van der Waals Lecturer, and is a Gordon and Betty Moore Foundation Pl. Ivan's research interests include basic physics of condensed states of matter, novel electronic phenomena including unconventional superconductivity, innovative methods of thin film synthesis and characterization, and nano-scale physics. He has published 11 research monographs and over 280 research papers, including 25 in *Science* and *Nature* journals.

## FEATURED SPEAKERS



### DAVID CAHILL

University of Illinois, Urbana-Champaign

#### Presentation Title

*Plasmonic Probes of Ultrafast Interfacial Heat Transfer and Liquid-Vapor Phase Transformations*

#### ABSTRACT

We are using characteristics of the localized plasmon resonance of Au nanostructures as an ultrafast thermometer and ultrafast probe of interfacial heat transfer and liquid-vapor phase transformations:

1. The magnitude of the peak optical absorption has a relatively strong dependence on temperature and enables high dynamic-range, time-resolved measurements of the changes in temperature of a Au nanostructure following heating by a picosecond optical pulse. These data can be analysed to determine the heat capacity and thermal conductivity of surfactant layers.
2. The wavelength of the peak optical absorption shifts with a change in the index of refraction of the surrounding material. This physics can be used to measure changes in the temperature of liquids within ~10 nm of a nanostructure; the rise in the temperature of the liquid near a metal/liquid interface is a more sensitive probe of the interface thermal conductance than the decay of the temperature of the metallic nanostructure.
3. The wavelength of peak optical absorption shifts with a change in the thickness of an adsorbed molecular layer that forms at a solid/vapor interface. This approach enables the detection of transient changes in the thickness of an adsorbed layer with picosecond time resolution and a sensitivity

to thickness changes of ~10 pm. For vapor pressures near 1 atm, the response of the thickness to a small temperature excursion has a time constant of ~1 ns.

#### BIOSKETCH

David Cahill is the Willett Professor and Department Head of Materials Science and Engineering at the University of Illinois at Urbana-Champaign. He joined the faculty of the U. Illinois after earning his Ph.D. in condensed matter physics from Cornell University, and working as a postdoctoral research associate at the IBM Watson Research Center. His research program focuses on developing a microscopic understanding of thermal transport at the nanoscale; the discovery of materials with enhanced thermal function; the interactions between phonons, electrons, photons, and spin; and advancing fundamental understanding of interfaces between materials and water. He received the 2018 Innovation in Materials Characterization Award of the Materials Research Society (MRS); the 2015 Touloukian Award of the American Society of Mechanical Engineers; the Peter Mark Memorial Award of the American Vacuum Society (AVS); and is a fellow of the MRS, AVS, and APS (American Physical Society).



### GANG CHEN

Massachusetts Institute of Technology

#### Presentation Title

*Phonon Thermal Transport through Single and Multiple Interfaces*

#### ABSTRACT

Phonons are quantized lattice vibrations. At an interface, reflection of the phonon waves occurs. This reflection causes resistance to heat flow. Phonons contributing to heat conduction are broadband in both frequency and wavelength. Different transport processes can occur due to the presence of single and multiple interfaces and interface roughness. Sorting out the transport pictures require continuous improvements in experiments and simulations. In this talk, I will start from phonon transport across a single interface, to multiple interfaces especially superlattices with atomic mixing at interfaces and nanodot decorated interfaces. At a single interface, roughness can improve thermal transport while in superlattices, roughness leads to overall thermal conductivity reduction of the structure. In superlattice structures, long wavelength phonons transport across the entire thickness of the superlattices, implying phase coherence of these phonons; while atomic interface mixing destroys coherence of high frequency phonons. We observed this coherent transport in GaAs/AlAs superlattices by fixing the periodic thickness but varying the number of periods. We show further that phonon heat conduction localization happens in GaAs/AlAs superlattice by placing ErAs nanodots at interfaces. This heat-conduction localization phenomenon is confirmed by nonequilibrium atomic Green's function simulation. These ballistic and localization effects can be exploited to improve thermoelectric energy conversion materials via reducing their thermal

conductivity. This material is based upon work supported as part of the "Solid State Solar-Thermal Energy Conversion Center (S3TEC), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number: DE-SC0001299/DE-FG02-09ER46577.

#### BIOSKETCH

Gang Chen is currently the Head of the Department of Mechanical Engineering and Carl Richard Soderberg Professor of Power Engineering at Massachusetts Institute of Technology (MIT), and the director of the "Solid-State Solar-Thermal Energy Conversion Center (S3TEC Center)" — an Energy Frontier Research Center funded by the US Department of Energy. He obtained his PhD degree from the Mechanical Engineering Department, UC Berkeley. He was a faculty member at Duke University and UCLA, before joining MIT in 2001. He received an NSF Young Investigator Award, an R&D 100 award, an ASME Heat Transfer Memorial Award, a Nukiyama Memorial Award by the Japan Heat Transfer Society, a World Technology Network Award in Energy, an Eringen Medal from the Society of Engineering Science, and the Capers and Marion McDonald Award for Excellences in Mentoring and Advising from MIT. He is a fellow of the American Association for Advancement of Science, APS, ASME, and Guggenheim Foundation. He is an academician of Academia Sinica and a member of the US National Academy of Engineering.

## FEATURED SPEAKERS



### JUNICHIRO SHIOMI

University of Tokyo

#### Presentation Title

*Designability of Nanostructure Interfaces of Phonon and Electron Transport*

#### ABSTRACT

As nanostructuring has been successful to improve figure-of-merit of thermoelectric materials, understanding and controlling phonon and electron transport at nanostructure interfaces have increasingly become important. The correlation between single/multiple interfacial structures and the transport properties is complex, but this complexity gives rise to possibility to decouple heat and electrical conduction. While the challenge here is multifold and requires advances in transport theory, structure synthesis, and property measurements, a key challenge is to develop technologies that enhance the controllability and designability to utilize and overcome the complexity. In this talk, I will introduce some of the recent works done by the members of Thermal Energy Engineering Lab at The University of Tokyo together with the collaborators, for instance, in controllability gained by ultimate phonon scattering, thermoelectric strain engineering, and phonon coherence, and designability realized by materials informatics.

#### BIOSKETCH

Dr. Junichiro Shiomi is Professor in Department of Mechanical Engineering, School of Engineering, the University of Tokyo. He received B.E. (1999) from Tohoku University, and Ph.D. (2004) from Royal Institute of Technology (KTH), Sweden. Leading the Thermal Energy Engineering Lab, he has been pursuing research to advance thermal management, waste heat recovery, and energy harvesting technologies based on nano-to-macro innovation in materials, structures, and systems. He has been leading several projects including Core Research for Evolutional Science and Technology (JST-CREST), Precursory Research for Embryonic Science and Technology (JST-PRESTO), and New Energy and Industrial Technology Development Organization (NEDO) projects. He is Fellow of Japan Society of Mechanical Engineers and serves as associate editors of *Applied Physics Express*, *Japanese Journal of Applied Physics*, and *Transactions of the Japan Society of Mechanical Engineers*. He is a recipient of the Zeldovich Medal from the Committee on Space Research, the Young Scientists' Prize, the Commendation for Science and Technology by the Minister of Educational, Culture, Sports, Science and Technology, and the Academic award of Heat Transfer Society of Japan.



### BILGE YILDIZ

Massachusetts Institute of Technology

#### Presentation Title

*Chemical and Electrochemical Stability of Perovskite Oxide Surfaces in Energy Conversion: Mechanisms and Improvements*

#### ABSTRACT

A broad range of highly active doped ternary oxides, including perovskites, are desirable materials in electrochemical energy conversion, catalysis and information processing applications. At elevated temperatures related to synthesis or operation, however, the structure and chemistry of their surfaces can deviate from the bulk. This can give rise to large variations in the kinetics of reactions taking place at their surfaces, including oxygen reduction, oxygen evolution, and splitting of H<sub>2</sub>O and CO<sub>2</sub>. In particular, aliovalent dopants introduced for improving the electronic and ionic conductivity enrich and phase separate at the surface perovskite oxides. This gives rise to detrimental effects on surface reaction kinetics in energy conversion devices such as fuel cells, electrolyzers and thermochemical H<sub>2</sub>O and CO<sub>2</sub> splitting. This talk will have three parts. First, the mechanisms behind such near-surface chemical evolution will be discussed. Second, the dependence of surface chemistry on environmental conditions, including temperature, gas composition, electrochemical potential and crystal orientation will be described. Third, modifications of the surface chemistry that improve electrochemical stability and activity, designed based on the governing mechanisms, will be presented. Guidelines for enabling high performance perovskite oxides in energy conversion technologies will be presented.

#### BIOSKETCH

Bilge Yildiz is a professor in the Nuclear Science and Engineering and the Materials Science and Engineering Departments at Massachusetts Institute

of Technology (MIT), where she leads the Laboratory for Electrochemical Interfaces. She received her PhD degree at MIT in 2003 and her BSc degree from Hacettepe University in Turkey in 1999. After working at Argonne National Laboratory as research staff, she returned to MIT as an assistant professor in 2007. Her leadership responsibilities at MIT include the Low Carbon Energy Center on Materials in Energy and Extreme Environments, and one of the Integrated Research Groups of MIT's NSF sponsored Materials Research Science and Engineering Center. Her research focuses on laying the scientific groundwork and proof-of-principle material systems for the next generation of high-efficiency devices for energy conversion and information processing, based on solid state mixed ionic-electronic conducting (MIEC) material, by combining in situ surface sensitive experiments with first-principles calculations and novel atomistic simulations. Her work has made significant contributions to advancing the molecular-level understanding of oxygen reduction and oxidation kinetics on MIEC solid surfaces, and of ion and electron transport, under electro-chemo-mechanical conditions. The scientific insights derived from her research guide the design of novel surface chemistries for efficient and durable solid oxide fuel cells, thermo-/electro-chemical splitting of H<sub>2</sub>O and CO<sub>2</sub>, corrosion resistant films, high energy density solid state batteries, and red-ox based memristive information storage. Her teaching and research efforts have been recognized by the Argonne Pace Setter (2016), ANS Outstanding Teaching (2008), NSF CAREER (2011), IU-MRS Somiya (2012) and the ECS Charles Tobias Young Investigator (2012) Awards.

## FEATURED SPEAKERS



### MOGENS MOGENSEN

Technical University of Denmark

#### Presentation Title

*Controlling the Composition of Surfaces and Interfaces in Solid Oxide Cells*

#### ABSTRACT

It is well-known that surfaces and interfaces have chemical compositions different from the bulk of the materials, but it is usually not easy to control the surface or interface chemistry. The detailed interface chemistry is generally not known and is very difficult to characterise. This is a main reason why it is so difficult to control the composition of the interface.

The presentation will very briefly review surface analysis techniques suitable for analysis of solid oxide cell (SOC) surfaces; in particular techniques that may be applied in operando will be emphasized. Results from these techniques will be used to illustrate how surfaces may change composition away from bulk composition due to segregation of components that do not fit well into the SOC materials. An example is migration of SrO to the surface of  $(La_{1-x}Sr_x)SFeO_{3-\delta}$  due to  $Sr^{2+}$ -ions being bigger than the  $La^{3+}$ -ions.

Furthermore, it will be reported how trace impurities tend to accumulate and block SOC surfaces, and how composition and structure of surfaces may change with variation in temperature and oxygen partial pressure, and with small variation in gas composition like change in moisture level.

Finally, it will be illustrated how the surface composition may be controlled by controlling the composition of the bulk, e.g. by the value of  $s$  in  $(La_{1-x}Sr_x)SFeO_{3-\delta}$ , i.e. by controlling the ratio of big to small cations in such perovskite structured oxides. Also, the possible use of

scavengers to protect the surface from being blocked by trace impurities will be outlined.

#### BIOSKETCH

Mogens B. Mogensen is Research Professor at Department of Energy, Technical University of Denmark. He received his M.Sc. in Chemical Engineering, 1973, and Ph.D. in Corrosion 1976, both from the Technical University of Denmark (DTU). 45 years in electrochemistry; 30 years in SOC R&D; 9 years in 200 - 250 °C alkaline, and 4 years in PEM electrolysis. Contributed to the understanding of electrode reaction and degradation mechanisms in SOCs, alkaline cells, and Li-SOCl<sub>2</sub> batteries. New strategies in application of electrochemical impedance spectroscopy. h-index 60; 282 papers on Web of Science cited > 13,250 citations and > 12,150 without self-citations. 2 paper cited > 1,000, and 34 > 100 times. He has 23 published patents/applications, 9 book chapters and ca. 170 other research publications. Active in the Executive Committee of the High Temperature Materials Division of ECS for 20 years, and associated editor of SSI during a decade. He is an experienced manager, previously Head of Program (2 y), coordinator of EU projects, leader of Strategic Electrochemical Research Center (6 y), and manager of many Danish and international R&D projects. Received Christian Friedrich Schönbein Medal of Honour, 8th European Fuel Cell Forum, 2008; Science of Hydrogen & Energy Award, 6th Hydrogen & Energy Symposium, 2012; Fellow of the Electrochemical Society since 2015.



### AINARA AGUADERO

Imperial College London

#### Presentation Title

*Local Chemical Degradation Processes and Ionic Transport in Garnet All-Solid-State Batteries*

#### ABSTRACT

Lithium all-solid-state batteries are considered as the most promising and safe alternative for the development of the next generation of Li-metal batteries with high energy density. The garnet-type electrolytes based on  $Li_7La_3Zr_2O_{12}$  (LLZO) structures are of great interest as electrolytes with reported conductivities greater than  $1 \text{ mS cm}^{-1}$  at room temperature. However, problems with moisture reactivity during processing, high polarisation resistance with Li metal electrodes and dendritic-driven cell failure are limiting their performance and their potential commercial application.

In this work, we have used a combination of surface sensitive chemical analysis techniques and the interface with garnet electrolytes. On the one hand, the local chemical inhomogeneities present in the polycrystalline garnets will be correlated to dendrites composition and the critical current density for the short-circuiting of the cells. On the other hand, we will reveal the effects of Li-H exchange on the Li ion dynamics with Li metal and within the garnet structure, showing the depth of the reactive regions in the pellets and the potential impact in the cell performance.

#### BIOSKETCH

Ainara Aguadero is a Lecturer in Materials at Imperial College London. Her research focuses on the understanding and optimisation of ion transport properties and redox processes taking place in bulk, surfaces and interfaces of ceramic oxides. The long-term goal of these efforts is to improve the life and performance of the next generation solid electrochemical devices such as solid oxide fuel cells, electrolysers and batteries.



## FEATURED SPEAKERS



### RYOJI KANNO

Tokyo Institute of Technology

#### Presentation Title

*Lithium Superionic Conductor and All-Solid-State Battery—Materials and Electrode/Electrolyte Interface*

#### ABSTRACT

All-solid-state is an ideal form of batteries. The solidification of the electrolyte provides an additional advantage for use in battery applications. However, despite the expected advantages of all-solid-state batteries, their power characteristics and energy densities must be improved to allow application in technologies such as long-range electric vehicles. All-solid-state batteries are based on the combination of cathodic, anodic, and electrolyte materials, with properties that depend mostly on the electrolyte characteristics. Recently, the ionic conducting materials LGPS ( $\text{Li}_{10}\text{GeP}_2\text{S}_{12}$ ) were discovered to show higher ionic conductivity than liquid electrolytes. Moreover, many types of materials have been found, which provided suitable combinations of the electrodes and the electrolyte. The all-solid-state cells using new LGPS-type materials provided high power and high energy density. These battery characteristics are derived from the intrinsic nature of the solid electrolytes (high ionic conductivity), and the reversible reaction at the electrode/electrolyte interface (high electrochemical stability at the interface), which indicate the advantages of the all-solid-state devices over the conventional electrochemical devices. The present study shows the materials varieties of the solid electrolytes and the effects of conductivities and electrochemical reaction at the electrode/electrolyte interface on the battery characteristics will be discussed.

#### BIOSKETCH

Ryoji Kanno is a professor at Institute of Innovative Research, Tokyo Institute of Technology. He received his PhD in science from Osaka University in 1985. Since 1980, Ryoji Kanno has been investigating materials for electrochemical energy conversion devices. His challenge is for the development of new materials is finding superionic conducting materials for lithium battery electrodes, electrolytes for all solid-state battery, and for solid oxide fuel cells. He was awarded from Chemical Society of Japan (Award for Young Chemists, 1989), Kato foundation for Promotion of Science (Kato memorial award 2016), and Battery Division Research Award (The Electrochemical Society 2017).



### VIRGINIE VIALLET

University de Picardie

#### Presentation Title

*Interfacial Issues and Challenges for Bulk-Type All-Solid-State Batteries*

#### ABSTRACT

Li-ion batteries that use a liquid electrolyte have been on the market for a few years; this technology's basic design creates problems in terms of packaging format, size, cost, and safety and as a result, much research has been devoted to developing a Li-ion polymer battery technology based on a solid polymer electrolyte. Such batteries have proven to be cost effective; moreover, this technology is now starting to make an impact in the marketplace, even though it offers lower energy densities.

A more important impact on the marketplace is expected for the all-solid-state technology, based on an inorganic solid electrolyte and which offers more possibilities in terms of gravimetric energy densities. The conventional battery shown in the center and denoted LIB consists of a porous negative electrode, typically graphite (gray spheres) and a positive electrode, typically a transition metal oxide (violet sphere), 100  $\mu\text{m}$  thick between which is placed a separator approximately 10  $\mu\text{m}$  thick (gray band). The liquid electrolyte impregnates the electrodes and the separator, ensuring the rapid transfer of ions. In an all-solid-state Li-ion battery, represented on the right and denoted Li-SSB, the liquid electrolyte is completely replaced by a solid electrolyte (\*orange spheres) within the electrodes and the separator impregnated with the liquid electrolyte is replaced too. The diagram on the left represents an all-solid-state battery with

lithium metal as the negative electrode, with which it is possible to significantly increase the energy density.

The development of the all-solid-state technology will also help to solve safety and environmental issues raised by most current batteries, which contain toxic materials, the liquid/gel electrolyte being one of the major considerations due to the possibility of leakages on disposal, as the all-solid-state cells should not require any special handling.

Two major technological challenges, common to any type of "all-solid" design, hinder the development of such batteries: the low intrinsic ionic conductivity of solid electrolytes and the difficulty of obtaining good solid/solid interfaces within the composite electrodes and the complete system.

Several sulphide and oxide glasses, glass-ceramics or ceramics, such as  $\text{Li}_7\text{P}_3\text{S}_{11}$  [2],  $\text{Li}_{10}\text{GeP}_2\text{S}_{12}$  [3],  $\text{Li}_{9.54}\text{Si}_{1.74}\text{P}_{1.44}\text{S}_{11.7}\text{Cl}_{0.3}$  [4] and  $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$  [5,6], have been developed as promising electrolytes for all solid state Li-ion batteries. Ionic conductivity values ranging, at 298 K, from  $10^{-4}$  to  $10^{-2}$  S/cm (i.e. close and even higher than organic electrolytes) have been reported that might possess electrochemical stability windows up to 10 V (vs Li/Li<sup>+</sup>). These inorganic solid electrolytes have been demonstrated as suitable to fabricate all-solid-state batteries with different electrode materials. In order to obtain good solid/solid interfaces, it is essential to adapt the shaping technique

## FEATURED SPEAKERS

to the specific characteristics of the chosen materials. Sulphur-based electrolytes can be easily deformed and allow the possibility of forming compact stacks by simple cold pressing, whereas oxides generally require densification at high temperatures such as assembly by spark plasma sintering (SPS), hot pressing (HP) or pulsed laser deposition (PLD).

The sensitivity to oxygen and moisture of sulphur-based solid electrolytes, the scale-up of the solid electrolyte synthesis, the reactivity towards positive electrode materials or negative electrode materials (in particular lithium), the conductivity through the electrodes, the chemical and mechanical stability of the solid-solid interfaces are still remaining issues for the development of Bulk-Type All-Solid-State Batteries.

This presentation will show challenges for development of solid cells and focus on interfacial issues.

### BIOSKETCH

Dr Virginie Viallet is currently an Associate Professor of inorganic chemistry and Solid State Chemistry at Laboratoire de Réactivité et Chimie des Solides, Université Picardie Jules Verne, France. She received her B.S., M.S. and Ph.D. in Inorganic Chemistry from Université Paris XI (Orsay) in 1993, 1995 and 1998, respectively. She started to work as Associate Professor in 1998 at Université Paris XI in Orsay and in 2007 at Université Picardie Jules Verne in Amiens. Her research is focused on the development of crystalline, glass and glass-ceramic solid electrolytes for lithium-ion or lithium-sulfur All-Solid-State batteries.



### TARO HITOSUGI

Tokyo Institute of Technology

#### Presentation Title

*A Very Low Resistance at Solid-Electrolyte and Electrode Interfaces: Introducing Oxide Epitaxial Thin-Film Technology to Battery Research*

### ABSTRACT

Solid-state Li batteries are promising energy-storage devices owing to their high-energy densities with improved safety. However, the large interface resistance at the interface of solid-electrolytes and electrodes hinders the development of the solid-state Li batteries.

Our group has been investigating surfaces and interfaces of transition-metal oxides, such as SrTiO<sub>3</sub>, LaAlO<sub>3</sub>/SrTiO<sub>3</sub>, SrVO<sub>3</sub>, La<sub>0.7</sub>Ca<sub>0.3</sub>MnO<sub>3</sub>, and LiTi<sub>2</sub>O<sub>4</sub>, using epitaxial thin film deposition technology and scanning tunnelling microscopy.

Accordingly, we introduced the above knowledge of the atomic-scale investigation of oxide surfaces into battery research. We succeeded in fabricating the interface resistance below ~ 5 Ωcm<sup>2</sup> (Li<sub>3</sub>PO<sub>4</sub>/LiCoO<sub>2</sub> interface); the value is smaller than that of liquid-electrolyte-based Li-ion batteries. These studies strongly encourage solid-state Li battery research, by demonstrating a very low interface resistance leading to the fast charging and discharging.

### BIOSKETCH

Dr. Taro Hitosugi is currently a Professor in the Department of Applied Chemistry at Tokyo Institute of Technology. He received his Doctor of Engineering from the University of Tokyo, and has held positions at Hitachi Labs, the Sony Corporation, the University of Tokyo, KAST, and Tohoku University. His research focus is to develop new functional materials and interfaces that will outperform existing materials, including superconductors, magnetic materials, photo functional materials, ion conductors, and dielectric materials. His group's approach combines atom-by-atom engineering with ensemble-measurement techniques.

## CONTRIBUTED TALK SPEAKERS

### Congratulations to the following poster abstract submissions that were selected to give Contributed Talks!

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**HONGGUANG WANG** (Max Planck Institute for Solid State Research)  
**Atomically-Resolved Investigations of Local Structure and Cationic Intermixing at SrMnO<sub>3</sub>-SrTiO<sub>3</sub> Heterointerfaces by Aberration-Corrected Analytical Transmission Electron Microscopy**

Heterointerfaces in transition metal oxides promotes emergent physical properties like colossal magnetoresistance, magneto-electric coupling, fractional quantum Hall Effect and high-T<sub>c</sub> superconductivity which are not found in their bulk constituents. These properties can be attributed to the reconstruction of charge, spin, and orbital ordering due to interfacial lattice reconstruction. Therefore, atomically-resolved explorations of oxide heterointerfaces are essential for interpretation of these phenomena. In this study, we performed atomic-scale investigations of microstructure and electronic structure at SrTiO<sub>3</sub> (STO) - SrMnO<sub>3</sub> (SMO) heterointerfaces by high-angle annular dark-field (HAADF) combined with annular bright-field (ABF) imaging and electron energy-loss spectroscopy (EELS) using an aberration-corrected scanning transmission

electron microscope (STEM). Here from, two-dimensional strain maps are obtained, revealing tensile in-plane strain within the SMO film and manifest out-of-plane lattice deformation at the interface. An asymmetric cationic intermixing at the interface between STO and SMO is observed from STEM-EELS line scans, exhibiting a larger diffusion depth of Ti than Mn. In order to estimate the influence of electron beam spreading, simulations of STEM-EELS spectrum images of the heterointerface are performed, verifying elemental intermixing and weak beam-spreading effects. The energy-loss near-edge structures (ELNES) of the Mn-L<sub>2,3</sub> edges at the heterointerface reveal a decrease of the Mn oxidation state within the first 3 unit cells in SMO, which coincidences with tensile-strain-induced oxygen deficiency.

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**JINGOO LEE** (St. Andrews University)  
**Ni-exsolved CaTiO<sub>3</sub> Catalysts for Oxygen-evolution Reactions in Alkaline Conditions**

Increasing in the rate of chemical and electrochemical reactions requires well-designed catalysts where metal nano-particles are dispersed on high-surface-area supports. In-situ growth Ni nano-particles on perovskites have been recently reported to enhance catalytic activities in high-temperature systems such as solid oxide cells (SOCs). However, the microscale

perovskites prepared by conventional solid-state reactions not only have low surface area but also scarcely maximize exsolution efficiency, which limit further applications of such exsolution process to low-temperature systems. Here, we demonstrate that size and morphology of perovskite scaffolds are important to improve both exsolution efficiency and perovskite active

sites via Ni-exsolved CaTiO<sub>3</sub> submicron particles. The catalysts show high activity and stability for oxygen-evolution reaction (OER) due to their large number of active sites and strong metal support interaction (SMSI) between Ni and CaTiO<sub>3</sub>. Furthermore, we assume that Ni ions can be incorporated not only into B sites but

also into A-sites in CaTiO<sub>3</sub> perovskite structures, which showed different exsolution features. The findings obtained here may serve in the design and development of heterogeneous catalysts in various low-temperature electrochemical systems e.g. alkaline fuel cells, metal-air batteries and so on.

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**JIMMY KUO** (Northwestern University)  
**Grain boundary dominated charge transport in Mg<sub>3</sub>Sb<sub>2</sub>-based compounds**

Experimental evidence shows that grain boundaries are responsible for the thermally-activated conductivity in some thermoelectric materials, such as Mg<sub>3</sub>Sb<sub>2</sub>. Existing grain-boundary models using the Matthiessen's rule on the carrier scattering rate fail to explain the thermally-activated conductivity in n-type Mg<sub>3</sub>Sb<sub>2</sub>-based materials. We establish a model describing the carrier conductivity ( $\sigma$ ) and Seebeck coefficient (S) of polycrystalline thermoelectric materials. The key factor is to

treat the depletion region induced by the grain boundary as a secondary phase, which takes into account the relatively larger depletion width in semiconductors, as compared with classical metals. The model is successfully applied to explain both the temperature dependency (i.e.  $\sigma$ -T) and energy dependency (i.e.  $\log|S|$ - $\log\sigma$ ) of Mg<sub>3</sub>Sb<sub>2</sub>-based compounds. We discuss how the model can be extended to other thermoelectric materials.

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**PATRICK HOPKINS** (University of Virginia)  
**Ultrahigh Thermal Boundary Conductances at Crystalline and Amorphous Interfaces**

The thermal boundary conductance (TBC) between two solids is often assumed to be related to the phonon densities of states in the materials comprising the interface. This picture ignores the potential unique vibrational energies that can occur at the interface between two solids. Thus, while efforts to decrease the TBC at interfaces have been realized from introducing defects and impurities at interfaces, efforts to increase the TBC to "ultrahigh" values have often been thought to be limited by the phonon energies comprised in the adjacent materials. In

this poster, we present a series of experimental measurements and atomistic simulations that demonstrate the ability to achieve "ultrahigh" thermal boundary conductances through mode conversion or unique vibrational modes that are confined to the interfacial region. We first study the TBC from 77-500 K across isolated heteroepitaxially grown ZnO films on GaN substrates. These data provide an assessment of the assumptions that drive the phonon gas model and atomistic Green's function formalisms for predicting TBC. Our

## CONTRIBUTED TALK SPEAKERS

measurements suggest that the TBC can be influenced by long wavelength, zone center modes in a material on one side of the interface as opposed to the often-assumed "vibrational mismatch" concept. At room temperature, we measure the ZnO/GaN TBC of 490[+150,-110] MW m<sup>-2</sup> K<sup>-1</sup>. In the second part of the study, we use crystalline disorder and interfacial defects as a mechanism to achieve ultrahigh TBCs. We

provide evidence that interfacial defects can enhance the TBC across interfaces through the emergence of unique high frequency vibrational modes that arise from atomic mass defects at the interface with relatively small masses. We demonstrate ultrahigh TBC at amorphous SiOC:H/SiC:H interfaces, approaching 1 GW m<sup>-2</sup> K<sup>-1</sup>, that is further increased through the introduction of nitrogen defects.

### MATIAS ACOSTA (Cambridge University)

#### Epitaxial Mesoporous Thin Films for Solid Oxide Fuel Cells Cathodes

Micro-solid oxide fuel cells (SOFC) can run with a broad variety of hydrocarbon fuels and feature low or even zero pollutant emissions, thus they can play a major role in the future portable power sources and can even act as sensors for the internet of things. Despite their potential, their applicability remains limited due to the high operating temperatures required for sufficiently high oxygen reduction and transport. In this work, we present a novel approach to synthesize epitaxial and mesoporous thin films. Using pulsed laser deposition, epitaxial vertically aligned nanocomposites based on (La,Sr)(Co,Fe)O<sub>3</sub> (LSCF) and MgO were grown. Deposition parameters were optimized to obtain a two-phase composite with nanopillars between

20 nm and 100 nm. Selective etching-out of the MgO rendered a mesoporous honeycomb-like nanostructures LSCF, with LSCF nanowalls of ~ 10-20 nm width. By modifying the density and size of nanopillars, it was shown that not only the nanostructure can be altered, but that it can be used as a strain engineering strategy to tune the LSCF conductivity. A thorough structural characterization of the mesoporous materials will be presented to reveal synthesis-nanostructure properties including electron microscopy and X-ray techniques. The results open a new route to develop nanostructured epitaxial mesoporous electrodes for micro-SOFC and to provide a model system to investigate electrochemical transport at the nanoscale.

### ANNALENA R. GENREITH-SCHRIEVER (RWTH Aachen University)

#### Field-enhanced Ion Transport at Grain Boundaries

The response of mobile oxygen ions in ceria CeO<sub>2</sub> to an external electric field was examined with classical Molecular Dynamics (MD) simulations. Simulation cells containing oxygen vacancies were subjected at temperatures 1000

≤ T / K ≤ 1600 to electric field strengths 10<sup>-3</sup> ≤ E / MV cm<sup>-1</sup> ≤ 10<sup>16</sup> to obtain the oxygen-ion mobility u<sub>i</sub> (E; T). In addition, static Nudged-Elastic-Band calculations were performed to obtain directly the forward and reverse barriers for oxygen-ion

migration, ΔH<sub>mig,f/r</sub>. Qualitatively, u<sub>i</sub> behaves as predicted by the standard Mott-Gurney model. Quantitatively, ΔH<sub>mig,f/r</sub> is underestimated at high E, resulting in an overestimation of u<sub>i</sub>. A new analytical expression for u<sub>i</sub> (E;T) was derived. The effects of a grain boundary, the Σ5(310)

[001] model grain boundary, on the oxygen-ion mobility were subsequently investigated. Excess grain-boundary quantities were determined as a function of the field strength and the orientation of the external field relative to the grain boundary.

### BENJAMIN MORGAN (University of Bath)

#### Combined Atomistic + Semi-Continuum Modelling of Nanoionic Space Charge Regions in CeO<sub>2</sub>

Increasing in the rate of chemical and electrochemical reactions requires well-designed catalysts where metal nano-particles are dispersed on high-surface-area supports. *In situ* growth Ni nano-particles on perovskites have been recently reported to enhance catalytic activities in high-temperature systems such as solid oxide cells (SOCs). However, the microscale perovskites prepared by conventional solid-state reactions not only have low surface area but also scarcely maximize exsolution efficiency, which limit further applications of such exsolution process to low-temperature systems. Here, we demonstrate that size and morphology of perovskite scaffolds are important to improve

both exsolution efficiency and perovskite active sites via Ni-exsolved CaTiO<sub>3</sub> submicron particles. The catalysts show high activity and stability for oxygen-evolution reaction (OER) due to their large number of active sites and strong metal support interaction (SMSI) between Ni and CaTiO<sub>3</sub>. Furthermore, we assume that Ni ions can be incorporated not only into B sites but also into A sites in CaTiO<sub>3</sub> perovskite structures, which showed different exsolution features. The findings obtained here may serve in the design and development of heterogeneous catalysts in various low-temperature electrochemical systems e.g. alkaline fuel cells, metal-air batteries and so on.

### STEFFEN EMGE (Cambridge University)

#### Solid-State NMR as a Tool to Study Structure and Dynamics in Solid Electrolytes

Conventional batteries that employ liquid electrolytes often risk spontaneous ignition upon malfunction. One possible solution to overcome these safety concerns is to replace the highly flammable, volatile organic electrolyte with a non-flammable solid electrolyte within an all-solid-state battery. However, before all-solid-state batteries can be realized as a safer alternative

to conventional batteries, several additional parameters of their performance must first be understood, controlled, and optimized to offer comparable power densities, capacities, and rates.

A more robust understanding of the ion conduction mechanism in solid electrolytes can help in developing electrolytes with

## CONTRIBUTED TALK SPEAKERS

higher conductivities. To better understand the conduction mechanism and the factors that lead to faster Li-ion diffusion in solid electrolytes, we used variable temperature <sup>7</sup>Li relaxometry to study the dynamics in the Li<sub>3</sub>PO<sub>4</sub>-Li<sub>4</sub>SiO<sub>4</sub> solid electrolyte system and compared it to results from diffraction, impedance, and molecular dynamics calculations. Here, we find that the 1:1 composition with the greatest disorder has the fastest jump rates, which is apparent by the minimum in the T1 data at the lowest temperature for all studied materials. This coincides with the highest conductivity, even

though the activation energy was relatively similar for all materials in the range of our study.

We have extended these relaxometry measurements to probe ion dynamics in Garnet type solid electrolytes, as well as explored PFG-NMR to understand the role of dopants on long range Li ion diffusion [2]. This can be combined with information about the local structure from high resolution MAS-NMR spectroscopy and calculations to gain deeper insights into the structure-property relationship for this class of solid electrolytes.

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### JAMES DAWSON (University of Bath)

#### Atomic-Scale Influence of Grain Boundaries on Li-Ion Conduction in Solid Electrolytes for All-Solid-State Batteries

Solid electrolytes are generating considerable interest for all-solid-state Li-ion batteries in attempts to improve safety and performance. Grain boundaries have a significant influence on solid electrolytes and are key hurdles that must be overcome for their successful application. However, grain boundary effects on ionic transport are not fully understood, especially at the atomic scale. The Li-rich anti-perovskite Li<sub>3</sub>OCl is a promising solid electrolyte, although there is debate concerning the precise Li-ion migration barriers and conductivity. Using Li<sub>3</sub>OCl as a model electrolyte, we apply large-scale molecular dynamics simulations to analyse the ionic transport at stable grain boundaries.

Our results predict high concentrations of grain boundaries and clearly show that Li-ion conductivity is severely hindered through the grain boundaries. The activation energies for Li-ion conduction traversing the grain boundaries are consistently higher than that of the perfect crystal, confirming the high grain boundary resistance in this material. Using our results, we propose a polycrystalline model to quantify the impact of grain boundaries on conductivity as a function of grain size. Such insights provide valuable fundamental understanding of the role of grain boundaries and how tailoring the microstructure can lead to the optimisation of new high-performance solid electrolytes.

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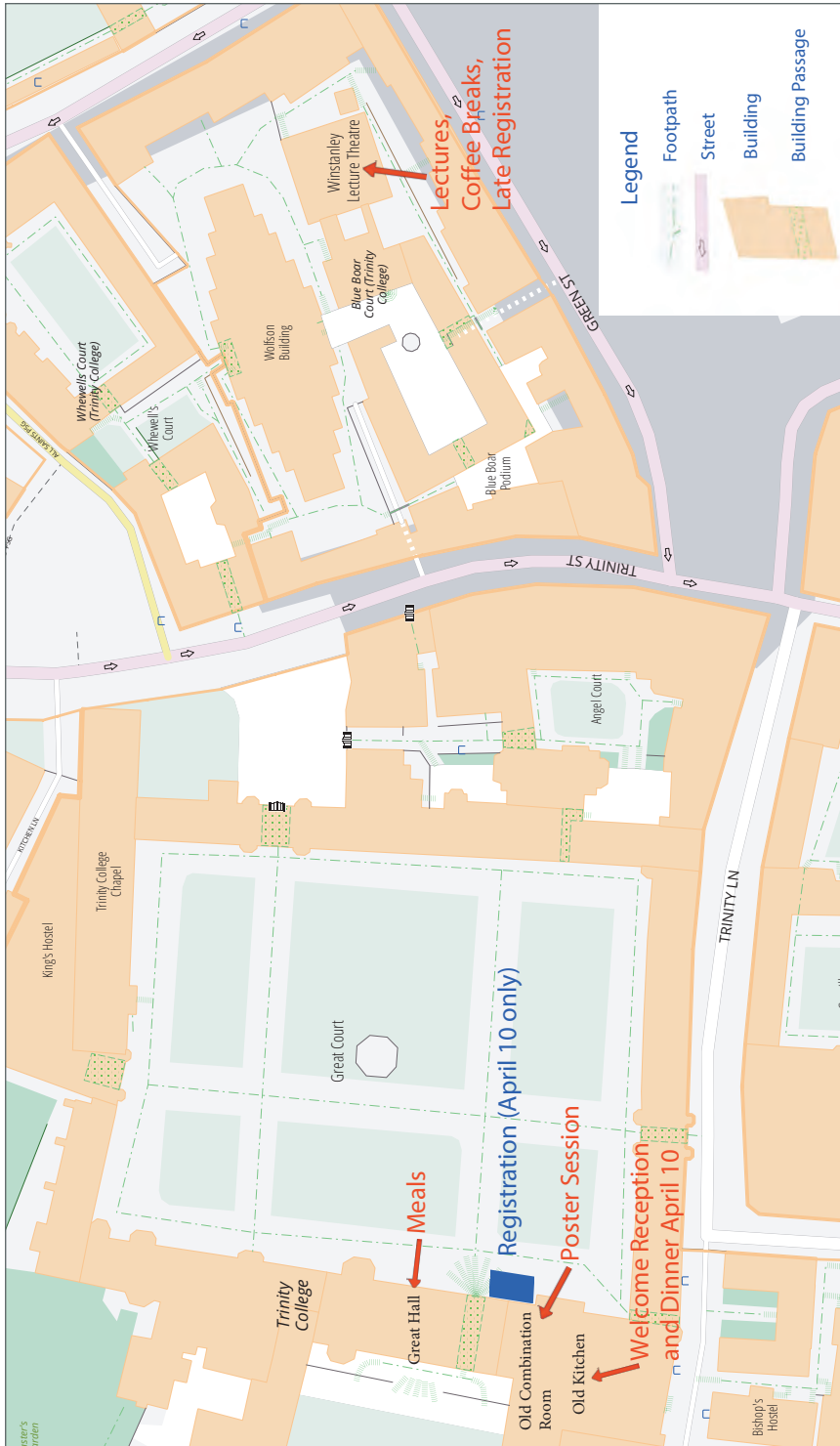
### FUMITAKE KAMETANI (Florida State University)

#### Atomic Investigation of Localized Oxygen Variation Induced by Strain at the Interface and Grain Boundaries in Perovskite Oxide High Temperature Superconductors

Perovskite oxide materials are complex multi-element composites, containing many different types of interfaces and/or boundaries of constituent material phases. Such interfaces and boundaries induce a variety of strain fields that can create local stoichiometry inhomogeneity which often dominates the overall properties. Perovskite copper oxide high temperature superconductors (HTS) are one of such materials. High temperature superconductivity is controlled by oxygen doping which is very sensitive to strain at and around the interface or boundaries. But their atomic structural correlations are still elusive. In this presentation, by using the atomic-resolution analytical scanning transmission electron microscopy (STEM) and first principle calculation (FPC), we show how strain creates

local variation of oxygen doping at the nano or atomic scale. Especially we will focus on the two types of interface/boundary which are the most influential for the performance of practical HTS conductors. The one is the interface between the flux pinning precipitates and REBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-δ</sub> (REBCO) matrix. And the other is the low angle grain boundary in REBCO. In both cases, the lattice mismatch, misfit dislocations, or threading dislocations create the complex tensile and compressive strain field at the atomic scale. The spectroscopy measurements such as electron energy loss spectroscopy or X-ray absorption near edge structure suggested that the tensile strain introduces oxygen deficiency which locally suppresses the superconductivity. Further details will be given at the presentation.

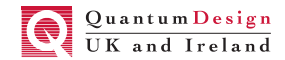
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