

## Report on TYC 5<sup>th</sup> Energy Workshop: From Atoms to Applications

The Thomas Young Centre (TYC) held their 5<sup>th</sup> Energy workshop, entitled “From Atoms to Applications” from the 25<sup>th</sup> to the 27<sup>th</sup> of July 2018 at the Department of Chemistry in University College London. The meeting was focussed on the evolution of computational materials design, specifically for Energy Materials. The aim of the workshop was to showcase the latest advances in computational materials design and to promote discussion and debate on bridging theory and experiment. We had a range of excellent speakers on the side of theory and of experiment, and it was clear from the discussions after talks and at the coffee breaks and lunches that the combination of theory and experiment is alive and thriving. The programme featured invited talks from established leaders in the field and from emerging early career researchers in the area. We scheduled 15 minutes for questions after every presentation, and this prompted lively discussion and debate. We had 99 attendees ranging from established academics, to PDRAs, PhD students and even Undergraduate students, with representation by Senior Editors from Nature and Nature Materials. The workshop featured diverse energy applications such as oxide and proton conducting fuel cells, photocatalysis, photovoltaics, LEDs, catalysis, solid state batteries, organic electronics and amorphous oxides semiconductors.

### **Programme:**

ALL LECTURES HELD IN THE CHEMISTRY AUDITORIUM, DEPARTMENT OF CHEMISTRY, 20 GORDON STREET, LONDON WC1H 0AJ, UK

### **Wednesday 25th July**

13:00 - 13:45 Registration, tea, coffee and juice in the Nyholm room

13:45 - 14:00 Opening remarks

Session 1 (Chair: Aron Walsh)

14:00 - 14:45 Alex Zunger - Discovery of energy materials with target properties as a design problem

14:45 - 15:30 Rachel Oliver - New opportunities for energy efficient devices using porous GaN

15:30 - 16:15 Chris van de Walle - Ion-transport engineering of hydrogen-conducting electrolytes

16:15 - 16:45 Chol-Jun Yu - Defect engineering in perovskite solar cells

17:00 - 20:00 POSTER SESSION with drinks and nibbles - NYHOLM ROOM - DEPARTMENT OF CHEMISTRY.

### **Thursday 26th July**

08:45 - 09:15 Arrival with tea, coffee and pastries in the Nyholm Room

Session 2 (Chair: David Scanlon)

09:15 - 10:00 Matthew Rosseinsky - New approaches to the discovery of inorganic materials and interfaces

10:00 - 10:45 Janet Tate - Metastable materials: heterostructural alloys and polymorphs

10:45 - 11:15 Tea and coffee in the Nyholm Room

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11:15 - 12:00 Ben Morgan - Composition-structure-conductivity relationships in argyrodite solid lithium-ion electrolytes

12:00 - 12:30 Yu Kumagai - Automation of first-principles point-defect calculations in non-metallic systems and its application

12:30 - 14:00 Lunch and posters in the Nyholm Room

Session 3 (Chair: Rachel Crespo-Otero)

14:00 - 14:45 Kim Jelfs - Exploring the crystal energy and charge carrier mobility landscapes of chiral helicenes

14:45 - 15:30 Volker Blum - Affordable all-electron theory of materials for light harvesting and light emission

15:30 - 16:15 Serena Corr - High Voltage: Designing materials for all solid-state batteries

16:15 - 16:45 Bartomeu Monserrat - Optoelectronic properties of materials at room temperature from first principles

### **Friday 27th July**

08:45 - 09:15 Arrival with tea, coffee and pastries in the Nyholm Room

Session 4 (Chair: Mark van Schilfgaarde)

09:15 - 10:00 Hideo Hosono - Catalysts for ammonia synthesis at mild conditions

10:00 - 10:30 Kenji Kojima - Shallow hydrogen site symmetry in ZnO as determined by muon spectroscopy

10:30 - 11:00 Tea and coffee in the Nyholm Room

11:00 - 11:45 Jon Major - Antimony selenide solar cells: A tale of device development

11:45 - 12:30 Alex Shluger - Charge trapping and degradation in amorphous oxide films

12:30 - 12:45 Closing remarks

### **Organisers:**

Dr David O Scanlon, University College London

Prof Aron Walsh, Imperial College London

Dr Rachel Crespo-Otero, Queen Mary University London

Prof Mark van Schilfgaarde, Kings College London

Karen Stoneham, University College London

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### List of Attendees:

Assoc. Prof Volker Blum	Duke University
Prof Janet Tate	Oregon State University
Prof Chris Van de Walle	University of California
Prof Alex Zunger	University of Colorado
Prof Hideo Hosono	Tokyo Institute of Technology
Dr Jon Major	University of Liverpool
Dr Kim Jelfs	Imperial College London
Dr Benjamin Morgan	University of Bath
Prof Matt Rosseinsky	University of Liverpool
Dr David Scanlon	University College London
Prof Aron Walsh	Imperial College London
Prof Alex Shluger	University College London
Dr Rachel Oliver	University of Cambridge
Dr Serena Corr	University of Glasgow
Dr Rachel Crespo-Otero	Queen Mary University
Prof Mark van Schilfgaarde	King's College London
Chol-Jun Yu	DPRK
Kum-Chol Ri	DPRK
Samantha Hood	Imperial College London
Ruoxi Yang	Imperial College London
Lucy Whalley	Imperial College London
Jacob Wilson	Imperial College London
Jisang Park	Imperial College London
Sunghyun Kim	Imperial College London
Youngkwang Jing	Imperial College London
Hui Yang	Imperial College London
Dr Bartomeu Monserrat	Cambridge
Dr Zdenek Futera	University College London
Dr Claire Hansell	Nature
Mr Thomas Durrant	University College London
Mr Lars Blumenthal	Imperial College London
Miss Xiuyun Jiang	University College London
Prof Matthew Foulkes	Imperial College London
Dr Joseph Prentice	Cambridge
Dr Adam Jackson	University College London
Dr Katherine Inzani	NTNU
Mr Patrick Rowe	University College London
Mr Zongda Xing	University College London
Dr Alex Aziz	University of Bath
Dr Martin Friak	Institute of Physics of Materials
Dr Benjamin Williamson	University College London
Mr Christopher Savory	University College London
Mr Ethan Rubinstein	University College London
Mr Alex Ganose	University College London
Mr Alex Squires	University of Bath
Dr Anna Regoutz	Imperial College London

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Mr Matthew Evans	Cambridge
Mr Elad Segev	Tel Aviv University
Dr Johannes Lischner	Imperial College London
Mr Suhas Mahesh	University of Oxford
Dr Kent Griffith	Cambridge
Dr Joaquin Calbo Roig	Imperial College London
Miss Suzanne Wallace	University of Bath
Mx Matt Ellis	University College London
Dr David Mora-Fonz	University College London
Dr John Buckeridge	University College London
Dr Kenji Kojima	TRIUMF, Canada
Mr Kou Harada	Titech
Prof Eduardo Menendez Proupin	Universidad de Chile
Miss Winnie Leung	University College London
Dr Pooja Panchmatia	Loughborough University
Dr Stephen Yeandel	Loughborough University
Dr Ryan Sharpe	Loughborough University
Mr Michael Watts	Loughborough University
Dr Dibyajyoti Ghosh	Bath
Prof Hiroki Taniguchi	Nagoya University
Prof Arash Mostofi	Imperial College London
Ms Maud Einhorn	University College London
Prof Dave Bowler	University College London
Dr Soumya Ghosh	University College London
Jack Poulton	University College London
Jack Strand	University College London
Dr Joachim Breternitz	Helmholtz Zentrum Berlin
Dr Éamonn Murray	Imperial College London
Miss Yiyuan Wang	Imperial College London
Dr Christopher Penschke	University College London
Dr Liam Wilbraham	University College London
Dr Paul Fossati	University College London
Dr Orestis Ziogos	University College London
Mr Rasmus Jakobsen	University College London
Dr Jonathon Cottom	University College London
Miss Fangyuan GU	Imperial College London
Dr Oksana Volnianska	Polish Academy of Sciences
Mr Manesh Mistry	University College London
Dr Daniel Fritsch	Helmholtz
Dr Anne Guilbert	Imperial College London
Mr Julian Gaberle	University College London
Dr Sanjay Sathasivam	University College London
Mr Chris Ablitt	Imperial College London
Mr Vinul Winalaweera	Imperial College London
Mr Jacob Robertson	Imperial College London
Mr Adrien Richard	University College London
Mr Neal Bhavsar	University College London
Dr Asim Mumtaz	University of Liverpool

## Report on TYC 5<sup>th</sup> Energy Workshop: From Atoms to Applications

Dr Josh Makepeace	University of Oxford
Dr Stephen Shevlin	Nature Materials
Mr Phillip Marks	University of Oxford
Dr Raul Quesada Cabrera	University College London
Dr Vincent Dusastre	Nature Materials