



Zero Carbon Energy - The Future
Royal Society of Edinburgh
22 George St. EH2 Edinburgh, United Kingdom
27th May, 2015

Following a discussion of Climate Change (details below), leading chemists discuss possible ways in which energy can be provided with no greenhouse gas emissions.

- 14:00 The Energy Trilemma - Developing Energy Futures** – *Mercedes Maroto Valer, Mechanical, Process and Energy Engineering, Heriot Watt University, Edinburgh*
- 14:40 Molecular Engineering of Sensitizers and Redox Mediators for Dye Sensitized Solar Cells**, *Md. K. Nazeeruddin, Institute of Chemical Sciences and Engineering, École Polytechnique Fédérale de Lausanne*
- 15:20 Artificial Photosynthesis - Hydrogen from Solar Driven Water Splitting** - *James Durrant, Department of Chemistry, Imperial College, London*
- 16:00 Hydrogen Storage using Aromatic Hydrocarbons – The Solution for Mobile Applications?** - *Peter Wasserscheid, Lehrstuhl für Chemische Reaktionstechnik, Friedrich-Alexander-Universität Erlangen-Nürnberg*
- 16:40 Networking reception**

Registration: <http://bit.ly/1P5U8h9>

This meeting follows:

09:00-13:00 Climate Change - Science and Society (at the Royal Society of Edinburgh)

The Energy Trilemma - Developing Energy Futures

Mercedes Maroto-Valer

Robert Buchan Chair in Sustainable Energy Engineering; Head of Institute of Mechanical, Process and Energy Engineering (IMPEE); Director of Energy Academy; Heriot Watt University, Edinburgh, United Kingdom

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Global population will continue to rise and is expected to surpass 8 billion by 2030, and inescapably we can anticipate an associated global increase of around 50% more food and energy, together with 30% more fresh water. This presents us with a formidable triple challenge, known as the 'energy trilemma', to develop energy technologies that are secure, affordable and environmentally friendly. Here, we will describe the links between the energy-food-water nexus and the energy trilemma, highlighting options for achieving a balance. In this presentation we will also describe solar fuel technologies, as an option for addressing both the consumption of non-renewable fossil fuels and global warming, with CO₂ photoreduction as an attractive strategy to reduce emissions while offering sustainable, safe and useful carbon utilisation. Large-scale, economic conversion of CO₂ into solar fuels represents a formidable scientific and technical challenge. We will discuss recent progress on the development of novel catalysts through advances in nanotechnology, as well as the engineering challenge of optimal CO₂ photoreactor design that can achieve efficient hydrocarbon conversion and separation for solar fuel production. In summary, an integrated approach across disciplines is needed to provide energy futures that meet the energy trilemma.

Artificial Photosynthesis - Hydrogen from Solar Driven Water Splitting

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My talk will address the challenge of harnessing sunlight to synthesis molecular fuels. This strategy - storing solar energy in chemical bonds - could both address the intermittency limitation of sunlight, and provide a sustainable, scalable pathway to carbon-neutral transportation fuels. However

it also represents a substantial scientific and technical challenge. It is already possible to for example use sunlight to split water, generating molecular hydrogen as a renewable fuel and chemical feedstock. However current water splitting materials and devices are too expensive, too inefficient and / or too unstable (or all three). Rapid progress is now being made to address these challenges, particularly on new nanostructured materials for light harvesting and new redox catalysts for fuel synthesis. My talk will provide an overview of this field, discussing some of the challenges and opportunities and recent progress, drawing in particular from some of my group's own research on metal oxide photoelectrodes for solar driven water splitting.

Molecular Engineering of Sensitizers and Redox Mediators for Dye Sensitized Solar Cells

Md. K. Nazeeruddin

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The dye-sensitized Solar Cells (DSC) are promising alternative to traditional inorganic semiconductor-based solar cells due to favourable ecological and economical features.[1]

In these cells, sunlight is absorbed by a dye located at the junction between a nanostructured electron transporting (n-type) and hole transporting redox mediator. The former is a wide band gap semiconductor oxide based on mesoscopic TiO₂ nanoparticles and the latter is typically the triiodide/iodide (I₃⁻/I⁻) redox

electrolyte. Upon photo-excitation, the anchored dye injects an electron into the TiO_2 and I^- reduce the oxidized sensitizer. The electrons then travel through the nanostructure to be collected as current at the external contact, while the holes are transported to the cathode by the redox shuttle. An optimal sensitizer for DSC should absorb all photons below a threshold wavelength of about 920 nm. This limit is derived from thermodynamic considerations showing that the conversion efficiency of any single-junction photovoltaic solar converter peaks at approximately 33 percent near a threshold energy of 1.4 eV. In this respect the dye-sensitized solar cells are however not ideal, which under optimized conditions yields only 11.5% efficiency. The general losses in the dye-sensitized solar cells are due to lack of sensitizer absorption in the near IR region, and the loss-in-potential from the optical band gap to the open-circuit voltage. Therefore the development of novel sensitizers with reduced mismatch between sensitizer absorption and the solar emission spectra, and between the oxidation potential of the redox electrolyte and the sensitizer oxidation potential is paramount to enhancing photocurrent and open circuit potential, respectively. In this talk I will discuss strategies for design and development of new sensitizers and redox mediators that yield a very high short circuit current and open-circuit voltage, ~1000 mV resulting power conversion efficiency of above 15% and their commercial prospects.[2]

[1] M. Grätzel, R. A. Janssen, D. Mitzi and E. H. Sargent, *Nature*, 2012, 488, 304.

[2] Aswani Yella, Hsuan-Wei Lee, Hoi Nok Tsao, Chenyi Yi, Aravind Kumar Chandiran, Md.Khaja Nazeeruddin, Eric Wei-Guang Diau, Chen-Yu Yeh, Shaik M Zakeeruddin, Michael Grätzel, *Science*, 2011, 334, 629.

Hydrogen Storage Using Aromatic Hydrocarbons – The Solution for Mobile Applications ?

Peter Wasserscheid

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Hydrogen is often considered a very capable future energy vector. It can be produced from renewable wind or solar power via water electrolysis and has a wide range of potential applications in all important fields of energy supply. The gravimetric storage density of hydrogen is excellent. One kilogram H_2 carries 33,3 kWh (LHV) of energy. However, being the chemical element with the lowest density, the volumetric storage density of hydrogen is only 3 Wh/liter at ambient pressure. In existing technical applications hydrogen is therefore either stored as gas under very high pressures (up to 700 bar, called “Compressed Gaseous Hydrogen” or CGH₂) or in its liquid state at 253 °C (called “Liquid Hydrogen” or LH₂).

A very attractive way to store and release hydrogen is in form of “Liquid Organic Hydrogen Carriers” (LOHC) systems. Aromatic molecules, such as e.g. N-ethylcarbazole (NEC) [1] or dibenzyltoluenes [2] can be reversibly hydrogenated and dehydrogenated in order to store and transport hydrogen in form of diesel-like liquids. The presentation introduces shortly the LOHC concept for energy storage and future hydrogen logistics. Afterwards it concentrates on material and process aspects of LOHC hydrogenation and dehydrogenation catalysis covering the full range from studies on the molecular level (XPS-, IR-studies) [3] to demonstrator units [4]. Challenges and optimization potentials will be discussed; novel options (LOHC transfer hydrogenation, hydrogen purification through LOHC hydrogenation/dehydrogenation) will be presented. A focus will be given to mobile applications and related infrastructures.

[1] D. Teichmann, W. Arlt, P. Wasserscheid, R. Freymann, *Energy & Environmental Science* 2011, 4(8), 2767-2773.

[2] N. Brückner, K. Obesser, A. Bösmann, D. Teichmann, W. Arlt, J. Dungs, P. Wasserscheid, *ChemSusChem* 2014, 7(1), 229-235.

[3] C. Papp, P. Wasserscheid, J. Libuda, H.-P. Steinrück, *Chemical Record* 2014, 14(5), 879-896.

[4] W.Peters, M.Eypasch, T.Frank, J.Schwerdtfeger, C.Körner, A.Bösmann, P.Wasserscheid, *Energy & Environmental Science*, 2015, 8, 641–649.