# Programme

## Faraday Discussion 151: Hydrogen Storage Materials
## 18 - 20 April 2011
## Rutherford Appleton Laboratory, Oxon, UK

**Monday 18 April**

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| | **Lunch Not Provided – Available to purchase in the restaurant** |
| 13:00 | **Welcome and Introductions – Stewart Parker** |
| **Session 1** | Session Chair: Alvaro Amierio-Fonseca |
| 13:15 | **Introductory Lecture**<br>Katsuhiko Hirose<br>*Toyota, Japan* |
| 14:15<br>**Paper 1** | **Pore with gate: modulating hydrogen storage in metal organic framework materials via cation exchange**<br>Sihai Yang, Samantha K Callear, Timmy A J Ramirez-Cuesta, William I F David, Junliang Sun, Alexander J Blake, Neil R Champness and Martin Schröder*<br>*University of Nottingham, UK* |
| **Paper 2** | **The effect of host relaxation and dynamics on guest molecule dynamics in $H_2$/tetrahydrofuran-hydrate**<br>Vanessa K Peterson*, Elvis Shoko and Gordon J. Kearley<br>*Australian Nuclear Science and Technology Organisation, Australia* |
| **Paper 3** | **The role of Ni in increasing the reversibility of the hydrogen release from nanoconfined $LiBH_4$**<br>Peter Ngene, Margriet H W Verkuijlen, Qiang Zheng, Joris Kragten, P Jan M van Bentum, Johannes H Bitter and Petra E de Jongh*<br>*Utrecht University, The Netherlands* |
| 15:45 | **Afternoon Tea** |
| 16:15<br>**Paper 4** | **Analysis of hydrogen storage in nanoporous materials for low carbon energy applications**<br>Nuno Bimbo, Valeska P Ting, Anna Hruzewicz-Kolodziejczyk and Timothy J Mays*<br>*University of Bath, UK* |
| **Paper 5** | **Characterisation of porous hydrogen storage materials: carbons, zeolites, MOFs and PIMs**<br>Steven Tedds*, Allan Walton, Darren P Broom and David Book<br>*University of Birmingham, UK* |
| 17:15 | **Close of Session** |
| 18:30 | **Dinner –** for all delegates in the Restaurant (R22) - tickets required |
| 19:30 – 21:00 | **Poster Session** in the Exhibition Centre (R18) |

**Tuesday 19 April**

| **Session 2** | Session Chair: Dag Noreus |
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| 09:00<br>**Paper 8** | **Synthesis of small metallic Mg-based nanoparticles confined in porous carbon materials for hydrogen sorption**<br>Claudia Zlotea, Clotaire Chevalier-César, Eric Léonel, Eric Leroy, Fermin Cuevas, Philippe Dibandjo, Cathie Vix-Guterl, Thierry Martens and Michel Latroche*<br>*ICMPE, France* |
| **Paper 9** | **The effect of complex halides and binary halides on hydrogen release for $2LiBH_4$:$MgH_2$ system**<br>Zhuxian Yang*, David M Grant, Ping Wang and Gavin S Walker<br>*University of Nottingham, UK* |
| **Paper 7** | **Incorporating magnesium and calcium cations in porous organic frameworks for high-capacity hydrogen storage**<br>Lin Wang, Yingxin Sun, and Huai Sun*<br>*Shanghai Jiao Tong University, China* |
| 10:30 | **Morning Coffee** |
| 11:00<br>**Paper 6** | **Control of hydrogen release and uptake in amine borane molecular complexes: thermodynamics of ammonia borane, ammonium borohydride, and the diammoniate of diborane**<br>Tom Autrey*, Mark Bowden and Abhi Karkamka<br>*Pacific Northwest National Laboratory, USA* |
| **Paper 22** | **Probing the binding and spatial arrangement of molecular hydrogen in porous hosts via neutron compton scattering**<br>Maciej Krzystyniak, Mark A Adams, Arthur Lovell, Neal T Skipper, Stephen M Bennington, Jerry Mayers and Felix Fernandez-Alonso*<br>*Rutherford Appleton Laboratory, UK* |
| 12:00 | **Close of Session and Lunch/Posters** |

| **Session 3** | Session Chair: Klaus Yvon |
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| 13:30<br>**Paper 10** | **Mobility and dynamics in the complex hydrides $LiAlH_4$ and $LiBH_4$**<br>A Borgschulte*, A Jain, A J Ramirez-Cuesta, P Martelli, A Remhof, O Friedrichs, R Gremaud and A Züttel<br>*Empa, Swiss Federal Laboratories for Materials Testing and Research, Hydrogen & Energy, Switzerland* |
| **Paper 11** | **Novel sodium aluminium borohydride containing the complex anion $[Al(BH_4,Cl)_4]^-$**<br>Inge Lindemann*, Roger Domènech Ferrer, Lothar Dunsch, Radovan Černý, Hans Hagemann, Vincenza D'Anna, Yaroslav Filinchuk, Ludwig Schultz and Oliver Gutfleisch<br>*IFW Dresden, Germany* |
| **Paper 12** | **Theoretical study of the vibrational properties of $NaAlH_4$ with $AlH_3$ vacancies**<br>Feng Zhang, Yan Wang and M Y Chou*<br>*Georgia Institute of Technology, USA* |
| 15:00 | **Afternoon Tea** |
| 15:30<br>**Paper 13** | **Synthesis of $LiNH_2$ + LiH by reactive milling of $Li_3N$**<br>Christian Bonatto Minella*, Carine Rongeat, Roger Domènech-Ferrer, Inge Lindemann, Lothar Dunsch, Natalie Sorbie, Duncan H Gregory and Oliver Gutfleisch<br>*IFW Dresden, Germany* |
| **Paper 14** | ***In situ* powder neutron diffraction study of non-stoichiometric phase formation during the hydrogenation of $Li_3N$**<br>Daniel J Bull*, Natalie Sorbie, Gael Baldissin, David Moser, Mark T F Telling, Ronald I Smith, Duncan H Gregory and D Keith Ross<br>*University of Salford, UK* |
| **Paper 15** | **Hydrogen storage and ionic mobility in amide–halide systems**<br>Paul A Anderson*, Philip A Chater, David R Hewett and Peter R Slater<br>*University of Birmingham, UK* |
| 17:00 | **Close of Session** |
| 19:00 | **Pre-Dinner Drinks** in the Coffee Lounge (R22)<br>Sponsored by Cella Energy Ltd |
| 19.30 | **Conference Dinner** in the Restaurant (R22) |

**Wednesday 20 April**

| **Session 4** | Session Chair: Duncan Gregory |
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| 09:00<br>**Paper 16** | **Homogeneous dehydrogenation of liquid organic hydrogen carriers catalyzed by an iridium PCP complex**<br>Zhaohui Wang, Jack Belli and Craig M Jensen*<br>*University of Hawaii, USA* |
| **Paper 17** | **$YMn_2H_x$ and $RMn_{2-y}Fe_yH_6$ (R=Y, Er) studied by Raman, infrared and inelastic neutron scattering spectroscopies**<br>V Paul-Boncour*, S F Parker, H Hagemann, S M Filipek, R Wierzbicki and M Latroche<br>*ICMPE, France* |
| **Paper 18** | **Hydride formation in Mg-based systems processed by reactive milling**<br>Stefano Deledda* and Bjørn C Hauback<br>*Institute for Energy Technology, Norway* |
| 10:30 | **Morning Coffee** |
| 11:00<br>**Paper 19** | **Performance of a full-scale hydrogen-storage tank based on complex hydrides**<br>Terry A Johnson*, Scott W Jorgensen and Daniel E Dedrick<br>*Sandia National Laboratories, USA* |
| **Paper 20** | **Performance of a metal hydride store on the "Ross Barlow" hydrogen powered canal boat**<br>A I Bevan*, A Züttel, D Book and I R Harris<br>*University of Birmingham, UK* |
| **Paper 21** | **A multidisciplinary combinatorial approach for tuning promising hydrogen storage materials towards automotive applications**<br>A Amieiro-Fonseca, S R Ellis, C J Nuttall*, B E Hayden, S Guerin, G Purdy, J-Ph Soulié, S K Callear, S D Culligan, W I F David, P P Edwards, M O Jones, S R Johnson and A H Pohl<br>*Johnson Matthey Technology Centre, UK* |
| 12:30 | **Concluding Remarks**<br>Bill David<br>*STFC Rutherford Appleton Laboratory, UK* |
| 13:00 | **Acknowledgements – Stewart Parker** |
| 13:15 | **Close of Meeting** |