

# THEO MURPHY INTERNATIONAL SCIENTIFIC MEETING

## Frontiers of computer simulation in chemistry and materials science

Thursday 6 – Friday 7 February 2014

Organised by Professor David Manolopoulos FRS, Professor David Logan, Dr Mark Wilson and Professor David Chandler ForMemRS

DAY 1				DAY 2			
SESSION 1 Chair: Michael Klein FRS		SESSION 2 Chair: David Chandler ForMemRS		SESSION 3 Chair: Ruth Lynden-Bell FRS		SESSION 4 Chair: Paul Madden FRS	
09.00	Welcome by Royal Society & lead organiser						
09.05	<b>Daan Frenkel ForMemRS</b> Granular packing and the Gibbs Paradox	13.30	<b>Michele Parrinello ForMemRS</b> From metadynamics to dynamics	09.00	<b>Roberto Car</b> First principles simulations of ice and water	13.30	<b>Emily Carter</b> At last: orbital-free DFT simulations of semiconductors and transition metals
09.30	Discussion	14.00	Discussion	09.30	Discussion	14.00	Discussion
09.45	<b>Gerhard Hummer</b> How biomolecules use hydrophobicity to function	14.15	<b>Sharon Glotzer</b> Assembly and packing on GPUs	09.45	<b>Mark Wilson</b> Network-forming materials in variable dimensions	14.15	<b>Mathieu Salanne</b> Modelling ion adsorption and dynamics in nanoporous carbon electrodes
10.15	Discussion	14.45	Discussion	10.15	Discussion	14.45	Discussion
10.30	<b>Coffee</b>	15.00	<b>Tea</b>	10.30	<b>Coffee</b>	15.00	<b>Tea</b>
11.00	<b>Peter Rossky</b> Quantum simulation of exciton dynamics in conjugated systems	15.30	<b>Peter Harrowell</b> How liquids become rigid: stress fluctuations in supercooled liquids	11.00	<b>David Limmer and Adam Willard</b> Collective behavior at the water platinum interface	15.30	<b>Annabella Selloni</b> First principles simulations of metal oxide electrodes for water oxidation
11.30	Discussion	16.00	Discussion	11.30	Discussion	16.00	Discussion
11.45	<b>Tom Miller</b> New approaches to simulating biological and molecular catalysts	16.15	<b>Philip Camp</b> Adsorption, self assembly, and friction in oil-based lubricants	11.45	<b>Angelos Michaelides</b> Hydrogen bonding and proton transfer at water/solid interfaces	16.15	<b>Michiel Sprik</b> First principles electrochemistry
12.15	Discussion	16.45	Discussion	12.15	Discussion	16.45	Discussion
12.30	<b>LUNCH</b>	17.00	<b>CLOSE</b>	12.30	<b>LUNCH</b>	17.00	<b>CLOSE</b>

Conference Dinner in honour of Paul Madden's 65<sup>th</sup> birthday