

Faraday Division
**First Principles Computation
of Structure and Dynamics**

Small Chemistry Lecture Theatre,
School of Chemistry, Cardiff University
Wednesday 30th January 2008

Free to attend, no registration formalities

Centenary Lecture
Professor Trygve Helgaker
University of Oslo, Norway

First Principles Computation of Structure and Dynamics

PROGRAMME

14:00 Welcome by Professor Peter Knowles, Cardiff University

14:05 Beyond Quantum Transition
State Theory

Professor David Manolopoulos
University of Oxford

14:50 Exploring Isomerisation/
Dissociation Processes
via Molecular Simulations:
application to $H+(H_2O)_n$

Dr Massimo Mella
Cardiff University

15:35 Tea/Coffee

Chairman: Professor David Clary; President, Faraday Division

16:05 Accurate Condensed Phase
Electronic Structure Theory

Dr Fred Manby
University of Bristol

16:45 Centenary Lecture
The Applications of Quantum
Chemistry to Large Systems

Professor Trygve Helgaker
University of Oslo, Norway

17:30 Close and wine reception

For map and directions, please go to www.cardiff.ac.uk/locations/index.html

Future Faraday Discussion meetings

● Faraday Discussion 139: The Importance of Polymer
Science for Biological Systems
26 - 28 March 2008 - University of York, York
*Register by 28 January 2008 to take advantage
of the early booking fees.*

● Faraday Discussion 140: Electrocatalysis:
Theory and Experiment at the Interface
07 - 09 July 2008 - University of Southampton,
Southampton

● Faraday Discussion 141: Water - From Interfaces
to the Bulk
27 - 29 August 2008 - Heriot-Watt University,
Edinburgh

● Faraday Discussion 142: Cold and Ultracold
Molecules
15 - 17 April 2009 - Durham University, Durham

For more information, visit www.rsc.org/faradaydivision

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