

HALF-DAY SYMPOSIUM

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+(H₂O)_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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ONE-DAY SYMPOSIUM



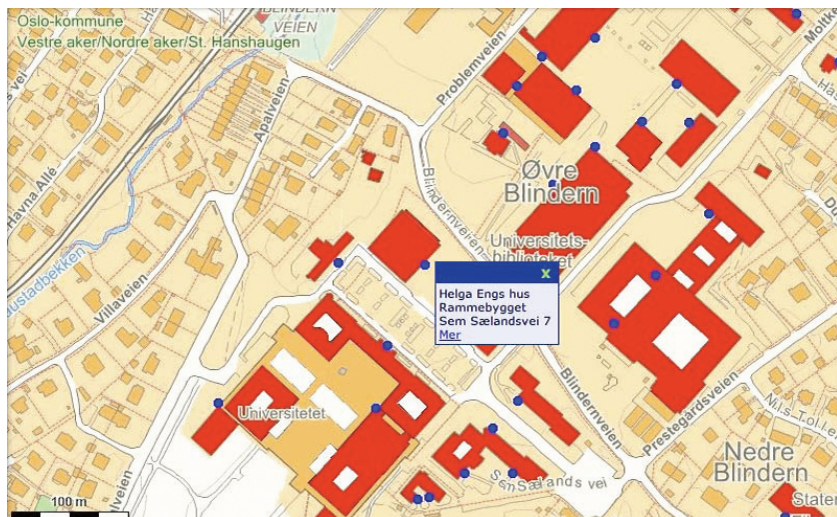
Royal Society of Chemistry Faraday Division in association with the Norsk Kjemisk Selskap, University of Oslo and its Centre for Theoretical and Computational Chemistry

New Frontiers in Theory-based Chemical Research

Lecture Hall 2, Helga Engs Hus
Sem Saelandsvei 7, Blindern

Monday 5th May 2008

Free to attend, no registration formalities



RSC Centenary Lecture
Professor Trygve Helgaker
University of Oslo, Norway

RSC S F Boys-A Rahman Lecture
Professor Mike Robb
Imperial College London, UK

RSC Marlow Medal Lecture
Dr Fred Manby
University of Bristol, UK

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The Faraday Division of the Royal Society of Chemistry in association with the Norsk Kjemisk Selskap, University of Oslo and its Centre for Theoretical and Computational Chemistry invite you to this one day symposium to be held in Oslo.

The Royal Society of Chemistry and the Norsk Kjemisk Selskap gratefully acknowledge the support from the University of Oslo in organising this event.

How to get to the University of Oslo:

The nearest station to the venue is Blindern. It is on lines 3, 4 and 5, direction 'Vest' (West), all departing from Oslo Central Railway Station where the airport express train arrives.

A detailed map can be found at: http://www.uio.no/om_uio/kart/index.html

The RSC is the largest organisation in Europe for advancing the chemical sciences. Supported by a network of 44,000 members worldwide and an internationally acclaimed publishing business, its activities span education and training, conferences and science policy, and the promotion of the chemical sciences to the public. For more information, go to www.rsc.org.

New Frontiers in Theory-based Chemical Research

PROGRAMME

10:15 **Welcome by Professor Anders Elverhøi, Vice Dean of Research, Faculty of Science, University of Oslo**

Chairman: Dr Kenneth Ruud, University of Oslo

10:30 **RSC S F Boys-A Rahman Lecture** **Professor Mike Robb**
How Conical Intersections Control Photostability and Photoisomerisation in Biological Systems *Imperial College London, UK*

11:15 Mesoscopic non-Equilibrium Thermodynamics for Biological Systems **Professor Signe Kjelstrup**
Norwegian University of Science and Technology, Trondheim, Norway

12:00 Lunch

Chairman: Professor Harald Walderhaug, General Secretary, Norwegian Chemical Society

13:45 **RSC Marlow Medal Lecture** **Dr Fred Manby**
Some Recent Developments in Explicitly Correlated Structure Theory *University of Bristol, UK*

14:30 Heterogeneous Catalysis - In Search of the Active Site(s) **Professor Unni Olsbye**
University of Oslo, Norway

15:15 Tea/Coffee

Chairman: Professor Mike Robb, Imperial College London

15:45 Functional Oxides and Nanomaterials: Interactions Between Theory and Experiment **Professor Helmer Fjellvåg**
University of Oslo, Norway

16:30 **RSC Centenary Lecture** **Professor Trygve Helgaker**
Excitation Energies From Density-Function Theory - Some Failures and Successes *University of Oslo, Norway*

17:15 Closing remarks

17:30 Wine reception