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1st circular

Faraday Discussion 127 NON-ADIABATIC EFFECTS IN CHEMICAL DYNAMICS

St Catherine's College, Oxford, UK 5 – 7 April 2004

Faraday Division



ntroduction

We are pleased to announce that the 127th Faraday Discussion focusing on Non-Adiabatic Effects in Chemical Dynamics will be held at the University of Oxford from **Monday 5 – Wednesday 7 April 2004.**

Electronically non-adiabatic transitions are central to a wide variety of rate processes, ranging from charge transfer collisions in the upper

atmosphere and interstellar material to organic photochemistry. Even a relatively simple reaction such as that between H atoms and water to form OH is known to involve no less than five electronic energy surfaces and current advances in both theory and experiment promise to unravel the detailed state selected dynamics of such events. Electronically non-adiabatic processes play an important role in all transition metal chemistry and may be central to some biological processes such as the chemistry of haemoglobin. There is also considerable topical interest in elucidating observable consequences of



Michael Faraday

the so called 'geometric phase' associated with circumnavigating conical interactions.

New and unpublished experimental and theoretical work will be presented in the following areas:

- Photochemical dynamics
- Fine structure and charge transfer processes
- Surface hopping
- Observable consequences of geometric phase
- Dissociative attachment
- Non-adiabatic processes in biology
- Applications to cold atom collisions

Professor Mark S Child CChem FRSC FRS University of Oxford, UK Chairman, Faraday Discussion 127

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Delegates will arrive on the morning of Monday 5 April 2004, and the Discussion will start after lunch. There will be four discussion sessions in total and the meeting will end on Wednesday 7 April 2004 after lunch. There will be a poster session for submitted contributions on Monday evening and a conference banquet on Tuesday evening.

Call for Papers

Abstracts that fit most closely with the themes of the meeting will be selected for oral presentations. Authors of the selected abstracts will then be invited to submit their work as a full paper, which will form the basis of their short presentation at the meeting. The paper itself must contain new, unpublished work and be submitted several months in advance of the Discussion. The papers selected for presentation and discussion will be refereed and then sent to all participants as preprints four weeks in advance of the meeting.

Offers of papers related to the themes for discussion, are now invited. Please send a brief abstract (1 A4 page maximum) to the address below as soon as possible, and **no later than 5 May 2003**.

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Christine Hall FD127 Royal Society of Chemistry Burlington House, Piccadilly London W1J 0BA UK

tel: +44 (0) 20 7437 8656 fax: +44 (0) 20 7734 1227 email: conferences@rsc.org

Location

Oxford

Oxford is a city in the English countryside and is the home to Britain's oldest University.

St Catherine's College

St Catherine's College, was founded in 1962 by Alan E Bullock (Lord Bullock), although it has its origins in a non-collegiate society established in 1868 as a means for the less well-off to study at Oxford. Designed by Danish architect Arne Jacobsen, the college has a traditional layout in quadrangle style with gardens. Its situation and architecture give a feeling of space and light and peace.

Preprints

Preprints will be issued four weeks in advance of the meeting. The Discussion will be conducted on the assumption that the papers have been read in advance and only five minutes will be allowed for presentation. Most of the time will be devoted to discussion, which is then submitted for publication in the proceedings which will be published by the Society about six months after the conference.

Accommodation

Participants will be accommodated in single *en suite* and single standard rooms at St Catherine's College.

Fees

Registration forms will be distributed with the second circular in November 2003 and details of the registration fees will be posted on the web site in due course.

Faraday Discussion Bursaries

Limited financial support is available for postgraduate students and young researchers from the following sources:

• Faraday Division Student Bursaries – to assist postgraduate students

• Angela and Tony Fish Bequest - to assist postdoctoral researchers

The bursary application form will be enclosed in the second circular. Please note that preference will be given to members of the RSC.

Faraday Discussion Volume

The *Faraday Discussions Volume* documents a long-established series of Faraday Discussion meetings which provide a unique international forum for the exchange of views and newly acquired results in developing areas of physical chemistry, biophysical chemistry and chemical physics. The papers presented are published in the *Faraday Discussions Volume* together with a record of the discussion contributions made at the meeting. Faraday Discussions therefore provide an important record of current international knowledge and views in the field concerned.

RSC Membership

The Royal Society of Chemistry is the UK Professional Body for chemical scientists and an international Learned Society for the chemical scientists, with 46,000 members worldwide. It is a major international publisher of chemical information, supports the teaching of the chemical sciences at all levels and is a leader in bringing science to the public.

For Faraday Discussions the member registration fees at conferences are approximately 25% - 50% less than for non-members and there are additional benefits for student members e.g. The Skinner Prize (£170).

For more information on the benefits of membership and how to join, please contact:

Hilary White Royal Society of Chemistry Thomas Graham House Science Park, Milton Road Cambridge CB4 0WF UK

tel: +44 (0) 1223 432316 fax: +44 (0) 1223 432133 email: whiteh@rsc.org

Organising Committee

Professor Mark S Child (Oxford) (Chairman), Professor Gabriel G Balint-Kurti (Bristol), Professor L S Cederbaum (Heidelberg), Dr David L Cooper (Liverpool), Professor David Klug (Imperial College) and Professor Michael A Robb (Kings College London).

Further Information

The Second Circular and application form will be circulated in November 2003 to those who have returned the slip requesting further information. All enquiries concerning attendance at the Discussion should be addressed to:

Christine Hall FD127 Royal Society of Chemistry Burlington House, Piccadilly London W1J 0BA UK

tel: +44 (0) 20 7437 8656 fax: +44 (0) 20 7734 1227 email: conferences@rsc.org

Any queries regarding scientific matters should be referred to:

Professor Mark S Child University of Oxford Physical and Theoretical Chemistry Lab South Parks Road Oxford OX1 3QZ UK

tel: +44 (0) 1865 275 151 fax: +44 (0) 1865 275 430 email: mark.child@chemistry.oxford.ac.uk

Web Site

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Information will be available on the regularly updated conference web page: www.rsc.org/lap/confs/fara127.htm

NON-ADIABATIC EFFECTS IN CHEMICAL DYNAMICS

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Second Circular and Application Forms

Please send me the 2nd circular and application forms for Faraday Discussion 127

PLEASE WRITE YOUR NAME AND ADDRESS CLEARLY BELOW

NAME:	
AFFILIATION:	
ADDRESS:	
	POSTCODE:
EMAIL:	
TEL:	FAX:

Poster and Oral Presentations

would like to give an oral presentation at the Discussion	
would like to present a poster at the Discussion	

The Royal Society of Chemistry will use the information you supply for the provision and administration of its activities, products, and services and for marketing. It may be necessary to disclose your information to service providers. We may contact you by mail, telephone, email or fax to tell you about activities, products and services that may be of interest to you. If you DO NOT wish to receive this information, please put a tick in the box.





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