
Faraday Division
Programme and Application Form
Call for Posters
Faraday Discussion 127
NON-ADIABATIC EFFECTS IN CHEMICAL DYNAMICS
St Catherine's College, Oxford, UK
5 - 7 April 2004
✓ 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
Register on-line: www.rsc.org/fd127
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advancing the chemical sciences

The Meeting

The Faraday Division of the RSC invite you to participate in the 127th Faraday Discussion, to be held at St Catherine's College, Oxford from 5 - 7 April 2004.

The programme structure of a Discussion meeting is quite different to most other conferences and symposia. As the name suggests, the special feature of these meetings is the emphasis placed on 'discussion'. All registered participants are sent the papers that will be presented in advance of the meeting and are expected to have read them before the meeting starts. Papers are usually grouped together and authors are given five minutes to present their main findings, and then the meeting is thrown open for discussion. The proceedings are recorded and serve as a wonderful record of the contemporary knowledge and understanding in a particular well-defined area. The papers and reported discussion will be published as Faraday Discussions Volume 127 about 6 months after the meeting. The price of the Volume is included in the full member and non-member registration fees and will be sent to those delegates after the meeting. Please note: This does not include the student registration fees, however a copy of the publication may be purchased at the meeting.

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

The Discussion will comprise 4 sessions and a poster session, the first session commencing after lunch on Monday 5 April 2004, and the final session ending at lunchtime on Wednesday 7 April 2004. The papers listed below will be presented and discussed during the course of the meeting although not necessarily in the stated order.

Introductory Lecture: Nonadiabatic Effects in Chemical Dynamics
D G Truhlar
University of Minnesota, USA

Ultrafast Temporary Charge Transfer in Pyrrolidinyl-Benzonitrile and Pyrrolyl-Benzonitrile in the Gas Phase
W Fuß*, W Rettig, W E Schmid, S A Trushin and T Yatsuhashi
Max-Planck-Institut für Quantenoptik, Germany

Regularised Diabatic States and Quantum Dynamics on Intersecting Potential Energy Surfaces
H Köppel
Universität Heidelberg, Germany

A Resonance-Mediated Non-Adiabatic Reaction: $F^*(^2P_{1/2})+HD \rightarrow HF(v'=3)+D$
S-H Lee, F Dong and K Liu*
Institute of Atomic and Molecular Sciences (IAMS), Taiwan

Details and Consequences of the Nonadiabatic Coupling in the $Cl(^2P)+H_2$ Reaction
M H Alexander*, G Capecchi and H-J Werner
University of Maryland, USA

Target Isotope Effects for Vibrationally-Resolved Electron Capture in Low-Energy Collisions of O^{3+} With Molecular Hydrogen
P C Stancil*, J G Wang, A R Turner and D L Cooper
The University of Georgia, Athens, USA

Rapid Timescale Processes and the Role of Electronic Surface Coupling in the Photolysis of Diatomic Ligands from Heme Proteins
P M Champion*, F Rosca, D Ionascu, W Cao and X Ye
Northeastern University, USA

Ultrafast Internal Conversion in Nucleic Acids
B Cohen, C E Crespo-Hernández, P M Hare, C J Marai and B Kohler*
The Ohio State University, USA

** Denotes presenter of paper to whom the affiliation refers*

St Catherines's College
5 -7 April 2004

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NON-ADIABATIC EFFECTS IN CHEMICAL DYNAMICS

APPLICATION FORM

Please type or write clearly (this form may be photocopied)

This form should be completed and returned, with your remittance, to **Christine Hall, Ref: FD127,** RSC, Burlington House, Piccadilly, London W1J 0BA UK fax: +44 (0) 20 7734 1227 not later than **Monday 1 March 2004**.

Title: ☐ Mr ☐ Miss ☐ Ms ☐ Mrs ☐ Dr ☐ Professor **Gender:** ☐ M ☐ F

Name: RSC Membership No:

Organisation:

Mailing Address:

Postcode: Email:

Tel: Fax:

Special Requirements: please give details of any special requirements and/or disability, medical conditions

Please state how you heard about the conference: ☐ Email ☐ Web ☐ Direct Mailing ☐ RSC Newsletter

☐ Others (please state)

PAYMENT *Please delete where appropriate

All payments should be made in **UK Pounds Sterling**

☐ **Cheque** - I enclose a personal/company cheque* made payable to 'Royal Society of Chemistry' for £

☐ **Credit Card** - Please charge my MASTERCARD/VISA/AMERICAN EXPRESS* the sum of £

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Cardholder's Signature: Date:

☐ **Bank Transfer:** (a copy of payment advice must be attached). Payment can be made to the following account:
National Westminster Bank, Kings Parade, 10 Benet Street, Cambridge CB2 3PU
A/C Name: RSC Conferences - 04FD127 A/C No: 24052558 Sort Code: 60-04-23

The RSC 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. A list of participants, which will include email addresses, will be published for distribution at the conference. If you do not wish to be included in this list, please tick the box ☐. 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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Please complete the form by indicating your choice in the boxes and entering your payment in this column. 1102514004

REGISTRATION

Payment | For office use only

Early Bird: Before 6 February 2004

☐ Member of the RSC	£215.00
☐ Non-member	£275.00
☐ Member - with a personal subscription to the Faraday Discussions Volume	£185.00
☐ Student Member	£120.00
☐ Student Non-member	£150.00

Standard: Before 1 March 2004

☐ Member of the RSC	£265.00
☐ Non-member	£325.00
☐ Member - with a personal subscription to the Faraday Discussions Volume	£235.00
☐ Student Member	£135.00
☐ Student Non-member	£165.00

ACCOMMODATION

The full package includes bed and breakfast on 5 & 6 April, lunch and dinner on 5 April, lunch and conference banquet on 6 April

☐ Single *en suite* package	£250.00
☐ Single standard package	£210.00

All prices quoted are per person

ADDITIONAL ACCOMMODATION

Payment | For office use only

Bed and breakfast Sunday 4 April 2004

☐ Single *en suite* room	£67.00
☐ Single standard room	£47.00

All prices quoted are per person per night

MEALS FOR NON-RESIDENTS

☐ Lunch 5 April	£17.50
☐ Dinner 5 April	£22.00
☐ Lunch 6 April	£17.50
☐ Conference Banquet 6 April	£56.00

LUNCH 7 APRIL

☐ Lunch 7 April £17.50

NOTE: VAT at the prevailing rate is included in the fees as appropriate

TOTAL PAYMENT

Terms and Conditions

No reservations for accommodation, meals, or social events will be made if payment is not received prior to the start of the conference. All registrations received by the closing date will be acknowledged. If an acknowledgement is not received within 14 days, please contact the RSC Conference Office.

Cancellations received before **5 March 2004** will be subject to an administrative charge of 25%. It will not be possible to offer any refunds on cancellations (including those for accommodation, meals or social events) received after **5 March 2004**, although a change in attending delegate can be made at any time. Changes to bookings for accommodation, meals or social events cannot be accepted after **5 March 2004**.

Signed ..... Date .....

Non-Adiabatic Effects in Chemical Dynamics

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

STUDENT BURSARIES

Financial support from Schlumberger and the RSC is available for postgraduate students and postdoctoral researchers.

Please note that any request for bursaries received after the closing date of 2 February cannot be considered. All applicants will be notified as soon as possible after the closing date.

- Members of the RSC are given priority in awarding bursaries (an application form for student membership is available on request)
- Student members of the RSC are also eligible for the Skinner Poster Prize of £170

NAME AND TITLE:

ADDRESS:

POSTCODE: TEL: E-MAIL:

POSITION (PLEASE TICK): ☐ POSTGRADUATE STUDENT ☐ POST DOCTORAL RESEARCHER

RSC MEMBERSHIP NO: EXTENT OF SUPPORT REQUIRED UP TO £:

SIGNED (APPLICANT): DATE: / / 2004

NAME OF SUPERVISOR:

BRIEF SUPPORTING STATEMENT FROM SUPERVISOR:

SIGNED (SUPERVISOR): DATE: / / 2004

SIGNED (HEAD OF DEPARTMENT): DATE: / / 2004

To be completed and returned to Christine Hall, RSC, Burlington House, Piccadilly, London W1J 0BA UK fax: +44 (0) 20 7734 1227 by 2 February 2004.

Poster Session

A poster session will be held on the evening of Monday 5 April 2004. Offers of additional papers for poster presentation are now invited. The title and a brief abstract (one page A4 maximum) should be submitted, no later than Monday 2 February 2004 to Christine Hall, FD127, RSC Conference Office, Burlington House, Piccadilly, London W1J 0BA UK
fax: +44 (0) 20 7734 1227 email: conferences@rsc.org

Please Note: The presenting author should be marked with an asterisk (*)

The **Skinner Prize (£170)** will be awarded to an undergraduate or postgraduate student presenting a poster, and whose poster is considered to be the best.

Student Bursaries

Financial support from Schlumberger and the RSC is available to assist students and young researchers is available. Applicants must be members of the RSC or presenting a poster. To apply for a bursary, please complete and return the form by 2 February 2004.

Acknowledgements

The organisers wish to thank the following for their contribution to the success of this conference:

European Office of Aerospace Research and Development, Air Force Office of Scientific Research, United States Air Force Research Laboratory, EPSRC combined computing project CCP6, Gaussian Inc and Schlumberger.

Sponsorship and exhibition opportunities are still available, please contact Christine Hall for further information using the details below.

Organising Committee

Mark Child (Chairman), Gabriel Balint-Kurti, Lorenz Cederbaum, David Cooper, Hanspeter Helm, David Klug and Michael Robb.

Further Information

Full details regarding registration, the submission of poster abstracts, accommodation and how to apply for a student bursary can be found on the web site: **www.rsc.org/fd127**
Or contact Christine Hall on:

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conferences@rsc.org

fax: +44 (0) 20 7734 1227

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