Faraday Division

Programme and Application Form

Call for Posters

RS•C

advancing the chemical scier

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

66 B 30

Register on-line: www.rsc.org/fd127

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→HF(∨'= 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(_P)+H_ 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 O³⁺ 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



Nonadiabatic Effects in Photobiology T J Martinez University of Illinois, USA

Spin-Forbidden CO Ligand Recombination in Myoglobin J N Harvey University of Bristol, UK

Structure of the Intersection Space Associated with Z/E Photoisomerization of Retinal in Rhodopsin Proteins A Migani, A Sinicropi, N Ferré, A Cembran, M Garavelli and M Olivucci* Università di Siena, Italy

Non-Adiabatic Intramolecular and Photodissociative Dynamics Studied by Femtosecond Time-Resolved Photoelectron and Coincidence-Imaging Spectroscopy O Gessner, M Z Zgierski, A Stolow*, A M D Lee, D M Wardlaw, J P Shaffer, T Schultz, E t H Chrysostom and C C Hayden National Research Council of Canada, Canada

The Competing Pathways of ICI* Relaxation in a He Supersonic Expansion J P Darr and R A Loomis* Washington University, USA

Photodissociation Dynamics of Pyrrole and Indole: Evidence for Mode Specific Dynamics from Conical Intersections J Wei, A Kuczmann, J Riedel, C Elsner, F Renth and F Temps* Christian-Albrechts-Universität zu Kiel, Germany

Ultrafast Excited State and Energy Transfer Processes in Multinuclear Transition Metal Complexes J Andersson, T Polivka, F Puntoriero, S Campagna and V Sundström* Lund University, Sweden

Dynamics Simulation of an Ultrafast Photoreaction Mechanism in Aromatic Molecules

V Vallet*, A Sobolewski and W Domcke Technical University of Munich, Germany A Novel Algorithm for Non-Adiabatic Direct Dynamics using Variational Gaussian Wavepackets G A Worth*, M A Robb and I Burghardt *King's College London, UK*

Marching Along Ridges. An Extrapolatable Approach to Locating Conical Intersections D R Yarkony Johns Hopkins University, USA

On Diabatization and the Topological D-Matrix: Theory and Numerical Studies of the H+H₂ System and the C_2H_2 Molecule M Baer*, T Ve'rtesi, G J Halász, Á Vibók and S Suhai University of Debrecen, Hungary

Time Resolved Solvent Rearrangement Dynamics T Sanford, D Andrews, J Rathbone, M Taylor, F Muntean, M Thompson, A McCoy, R Parson and W C Lineberger* University of Colorado, USA

Environmental Effects on a Conical Intersection: A Model Study I Burghardt*, L S Cederbaum and J T Hynes Ecole Normale Supérieure, France

Triatomic Dissociative Recombination Theory: Jahn-Teller Coupling Among Infinitely Many Born-Oppenheimer Surfaces V Kokoouline and C H Greene* University of Colorado, USA

Extraordinary Branching Ratios in Astrophysically Important Dissociative Recombination Reactions W D Geppert, R Thomas, A Ehlerding, J Semaniak, F Österdahl, M af Ugglas, N Djuri'c, A Paál and M Larsson* Stockholm University, Sweden

Experimental Maps of Nonadiabatic Coupling in Triatomic Hydrogen U Galster, U Müller and H Helm* Albert-Ludwigs-Universität, Germany

Concluding Remarks J C Tully Yale University, USA

* Denotes presenter of paper to whom the affiliation refers



	St Catherines's College										
		OWES	PAID	INV	ID	REG NO					
	5 -7 April 2004										
	ION-ADIABATIC EFFECTS IN CHEMICAL DYNAMICS										
	APPLICATION FORM	TION FORM Please type or write clearly (this form may be photocopied)									
	is form should be completed and returned, with your remittance, to Christine Hall, Ref: FD127, RSC, urlington House, Piccadilly, London W1J 0BA UK fax: +44 (0) 20 7734 1227 not later than Monday 1 March 2004 .										
	tle: Mr Miss Ms Mrs Dr Professor Gender: M F										
	Name: RSC Membership No: Organisation: Mailing Address:										
j	Postcode: Email:										
	Tel:	Fax									
j	Special Requirements: please give details of any special requirements and/or disability, medical conditions										
j	Please state how you heard about the conference: Email Web Direct Mailing RSC Newsletter										
	Others (please state)										
	PAYMENT *Please delete where appropriate	All pay	ments shoul	d be made i	n UK Poun	ds Sterling					
	Cheque - I enclose a personal/company cheq	ue* made pa	yable to 'Roy	yal Society o	of Chemistry	' for £					
	Credit Card - Please charge my MASTERCARD/V	ISA/AMERICAN	EXPRESS* the	sum of £							
j	Card N°:										
						_					
j											
	Cardholder's Signature:			Dat	e:						
Bank Transfer: (a copy of payment advice must be attached). Payment can be made to the following acc											
	National Westminster Bank, Kings Parade, 10 A/C Name: BSC Conferences - 04ED127	National Westminster Bank, Kings Parade, 10 Benet Street, Cambridge CB2 3PU									
ļ	AVO NAITE, 1100 COTTETETECES - 041 D 127 AVO NO. 24032336 SUIT COUR. 00-04-23										
	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 b We may contact you by mail, telephone, email or fax to tell you about activities, products and services that may be of intere- If you DO NOT wish to receive this information, please put a tick in the box .											
9	The Royal Society of Chemistry VAT Registration num	ber is: GB 342	1764 71		THIS IS NOT	A TAX INVOICE					
/	1										

Please complete the form by indicating your choice in the boxes and entering your payment in this column. 1102514								
REGISTRATION		Payment	~	ADDITIONAL ACCOMMODATION	Payment			
Early Bird: Before 6 February 2	2004 £215.00 £275.00		For office use on	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		For office use on		
Discussions Volume	£185.00			MEALS FOR NON-RESIDENTS				
□ Student Member □ Student Non-member	£120.00 £150.00			Lunch 5 April £17.50				
Standard: Before 1 March 2004	1 March 2004 RSC £265.00			□ Diffier 5 April £22.00 □ Lunch 6 April £17.50 □ Conference Banquet 6 April £56.00				
$\Box \text{ Non-member}$ $\Box \text{ Member - with a personal}$	£325.00			lunch 7 april				
subscription to the Faraday Discussions Volume Student Member Student Non-member	£235.00 £135.00 £165.00			□ Lunch 7 April £17.50 NOTE: VAT at the prevailing rate is included in the fees as appropriate				
ACCOMMODATION				TOTAL PAYMENT				
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			Terms and Conditions No reservations for accommodation, meals, or social ever payment is not received prior to the start of the conference received by the closing date will be acknowledged. If an a not received within 14 days, please contact the RSC Conf Cancellations received before 5 March 2004 will be subje administrative charge of 25%. It will not be possible to of			e if ons ent is		
All prices quoted are per perso			cancellations (including trose for accommodation, meals of sc received after 5 March 2004, although a change in attending o be made at any time. Changes to bookings for accommodatio social events cannot be accepted after 5 March 2004.	lelegate ca n, meals or	រ) រn r			

Signed Date									
Non-Adiabatic Effects in Che St Catherine's College, Oxford, UK	mical Dynamics 5 – 7 April 2004								
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									
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:



+44 (0) 20 7440 3336



fax: +44 (0) 20 7734 1227



RSC Conference Office Burlington House, Piccadilly London W1J 0BA UK

conferences@rsc.org

Registered Charity Nº 207890 12MMIII/MMXXV



