

## SDG 2005

### Annual conference of the Spectroscopy and Dynamics Interest Group of the RSC Faraday Division

St Aidan's College, University of Durham, Mon 19<sup>th</sup> to Wed 21<sup>st</sup> December 2005

#### **Location and travel**

The accommodation will be in St. Aidan's College (Windmill Hill, Durham, DH1 3LJ). It is located to the south of the city centre off South Road (A177) towards Darlington. Maps and details of how to reach St. Aidan's College can be found on the meeting's web-site: <http://www.dur.ac.uk/eckart.wrede/SDG2005/travel.php>.

The registration desk will be located in the entrance foyer of the college. Parking spaces are available in the car park of the Lindisfarne Centre to which you will be directed after arrival. Late arrivals, *i.e.* after 19.00 on Mon 19 Dec, can only be dealt with if we know *in advance*.

#### **Venues**

This year, the conference will take place at two venues. The tutorial talks on Monday night and the poster session on Tuesday afternoon will be held in the Lindisfarne Centre which is located within the college grounds. The plenary sessions on Tuesday morning and all day Wednesday will take place in lecture theatre PH8 in the Rochester building (Physics) which is about 10 minutes walk from the college.

#### **Day-delegates**

Directions to the Physics Department can be found via the travel web-page (see [link above](#)). We will open the registration desk in the entrance lobby of the Rochester building on Tuesday 20<sup>th</sup> from 08.30.

#### **Registration and payment**

Registration will take place in the entrance foyer of St. Aidan's College from 17.00 on Monday 19<sup>th</sup>, and again on Tuesday 20<sup>th</sup> from 08.30 in the entrance lobby of the Rochester building (Physics). If you have not paid in advance, payment of registration and accommodation fees should be made by cheque (preferred) or cash (if absolutely necessary) at the registration desk. Cheques should be made payable to "Durham University". The level of bursaries, which will be restricted to student members of the SDG (current or future) giving a talk or presenting a poster, has still to be decided and will be deducted from the fee payable or reimbursed.

#### **Talks**

The tutorial talks on Monday night will be held in the Lindisfarne Centre whereas all plenary lectures on Tuesday morning and Wednesday will take place in lecture theatre PH8 (Physics). A data projector and laptop for PowerPoint or Acrobat presentations will be available at all times. ***Be sure to notify the local organiser ([eckart.wrede@durham.ac.uk](mailto:eckart.wrede@durham.ac.uk)) if you wish to use a Mac.***

Please note that the lecture times for all contributing talks is 20 minutes which *includes* time for discussion.

## **Posters**

The poster session will be held in the Lindisfarne Centre on Tuesday afternoon. The poster boards are suitable for A0 size (portrait and landscape; usable size approx. 120×120 cm). Posters can be set-up from Tuesday lunchtime and can be used until the end of the poster session. Velcro strips will be provided. Please make sure that you take down your poster before you leave the college for the plenary sessions on Wednesday morning.

## **Meals and refreshments**

All meals (breakfast, lunch and dinner) will take place in the Dining Hall of St. Aidan's College. Coffee and tea will be served during breaks in room PH122 (Physics).

## **Vacation of rooms and luggage storage**

On Wed 21<sup>st</sup>, the college rooms should be vacated after breakfast (*i.e.* before you leave for the lectures). Luggage can be stored in the Shincliffe room (near the college entrance) until lunchtime. After lunch, please take your luggage down to Physics where it can be left (locked) in PH122.

## **Sponsorship**

This meeting has been made possible with financial support from The Royal Society of Chemistry, Coherent, Elliot Scientific, InnoLas, Kore Technology, Kurt J Lesker, Laser 2000, Laser Components, Leybold Vacuum and Photonic Solutions. Books have been kindly donated by Wiley Academic Publishers.

# **PROGRAMME**

## ***Monday 19 December 2005***

**17:00–19:00 Registration** (Foyer, St. Aidan's College)

18:30 **Dinner** (Dining Hall, St. Aidan's College)

### ***Session 1 (Lindisfarne Centre)***

Chair: Mike Ashfold

19:30 Opening remarks.

19:35 **Prof. Colin D. Bain (University of Durham).**  
*Surface-specific vibrational spectroscopy.*

20:30 **Prof. Tim P. Softley (University of Oxford).**  
*Chemical Dynamics at Sub-Kelvin Temperatures.*

21:30 The bar will be open until 23:00.

## ***Tuesday 20 December 2005***

08:00 **Breakfast**

Please allow 10 minutes to walk from the college to the Physics building.

**Session 2 (Lecture Theatre PH8)**

Chair: Stuart Mackenzie

- 09:10 **Prof. Brooks H. Pate (University of Virginia).**  
*Shake, Rattle, Roll: Applications of True Broadband Fourier Transform Microwave Spectroscopy to Isomerization Reactions.*
- 10:00 **Nicholas R. Walker, S. Francis and A.C. Legon (University of Bristol).**  
*Microwave Spectrum and Structure of  $N_2-CuF$ .*
- 10:20 **Paolo Barletta, J.M. Munro, B.C. Silva, J. Tennyson (University College London).**  
*Ab initio spectroscopy of  $H_3^+$  and  $D_2H^+$  near dissociation.*
- 10:40 **Sarah Wilsey (Imperial College London).**  
*The National Service for Computational Chemistry Software (NSCCS).*
- 10:50–11:20 **Coffee (PH122)**

**Session 3 (PH8)**

Chair: Matt Costen

- 11:20 **Dr. André Fielicke (Fritz-Haber Institute, MPG Berlin).**  
*Probing the structures of pure metal clusters and metal cluster complexes.*
- 12:10 **Stuart Mackenzie (University of Warwick).**  
*Elucidating the role of geometrical structure in determining the reactivity of metal clusters.*
- 12:30 **Tom E. Salter, V.A. Mikhailov, C.J. Evans, A.M. Ellis (University of Leicester).**  
*Infrared spectroscopy of alkali metal-solvent clusters.*
- 13:00–14:00 **Lunch (St. Aidan's College)**

**Session 4 (Lindisfarne Centre):**

- 14:00 Poster set-up
- 14:15–18:15 **Poster session**
- 16:15 **Tea**
- 17.15 **AGM** (room to be announced)
- 19:00 **Dinner** (Dining Hall)
- 20:30 The bar will be open until midnight.
- 21:00 Quiz (Junior Common Room)

**Wednesday 21 December 2005**

- 08:00 **Breakfast**  
Please allow 10 minutes to walk from the college to the Physics building.

**Session 5 (Lecture Theatre PH8)**

Chair: Ken McKendrick

- 09:10 **Dr. Vasilos Stavros (University of Warwick).**  
*Coherent control of electronic, vibrational and rotational dynamics.*
- 10:00 **Nicholas T. Form, J.B.C. Whitaker and A. Barman (University of Leeds).**  
*Dial-a-Product: The Coherent Control of Nitrotoluene Dissociation.*

10:20 **Michael A. Parkes**, S. Ali, V. Mikhailov, C.A. Mayhew and R.P. Tuckett  
(**University of Birmingham**).

*Vacuum-UV photofragmentation and ion-molecule reactions of cyclic- $C_4F_8$ .*

10:40 **Bríd Cronin**, M.G.D. Nix, A.L. Devine, R.N. Dixon and M.N.R. Ashfold.  
(**University of Bristol**).

*High resolution photofragment translational spectroscopy studies of the UV photodissociation of pyrroles.*

11:00–11:30 **Coffee** (PH122)

### **Session 6 (PH8)**

Chair: Andy Ellis

11:30 **David López Durán**, M.P. de Lara Castells, P. Villarreal Herrán, G. Delgado Barrio, F.A. Gianturco, C. di Paola and J. Jellinek  
(**Consejo Superior de Investigaciones Científicas, Madrid**).

*Raman spectra of  $(He)_N - Br_2(X)$  clusters: The role of boson/fermion statistics in a quantum solvent.*

11:50 **Adrian L. Boatwright** and A.J. Stace (**University of Nottingham**).

*A systematic shift in the electronic spectra of substituted benzene molecules in helium droplets.*

12:10 **Denis E. Bergeron**, A. Musgrave, V.L. Ayles, R.T. Gammon, J.A.E. Silber and T.G. Wright (**University of Nottingham**).

*REMPI Spectroscopy of Nitric Oxide-Based van-der-Waals Complexes.*

12:30 **Nicola M. Tonge**, E.C. Mac Mahon and M.C.R. Cockett (**University of York**).

*Collision-Free Chemistry: Spectroscopy and Reactivity of Fluorobenzene<sup>+</sup>-(NH<sub>3</sub>)<sub>n</sub>.*

13:00–14:00 **Lunch** (St. Aidan's College)

### **Session 7 (PH8)**

Chair: Stephen Ashworth

14:10 Susan Chung and **Michael Hippler** (**University of Sheffield**).

*Blue-shifting hydrogen bonding between chloroform and sulfur dioxide studied by ab initio theory and IR gas phase spectroscopy.*

14:30 **Sudarshana Saha** and C.M. Western (**University of Bristol**).

*Double resonance and ab initio study of a new  $^1\Delta_g$  state of the  $C_3$  radical.*

14:50 **Sven P.K. Koehler**, M. Allan, K.G. McKendrick (**Heriot-Watt University**).

*Interpreting Interfacial Reaction Dynamics with Liquid Surface Structure Simulations.*

15:10 **Dan Murdock**, L.A. Burns, P.H. Vaccaro (**Yale University**).

*Tunneling Dynamics of Tropolone Probed by Two-Color Resonant Four-Wave Mixing.*

15:30 R.V. Olkhov and **Ian W.M. Smith** (**University of Cambridge**).

*Total and state-to-state rate coefficients for inelastic and reactive collisions of  $CN(X^2\Sigma^+, v = 2)$  in selected rotational levels in collisions with  $N_2$  and  $C_2H_2$ .*

15:50 Close.

16:00 **Tea** (PH122)

## POSTERS

1. Sarah Wilsey (Imperial College London)  
*EPSRC National Service for Computational Chemistry Software.*
2. N.L. Elliott and C.M. Western (University of Bristol)  
*Analysis of perturbed spectra of SO from multiple sources using PGOPHER.*
3. C. M. Western (University of Bristol)  
*PGOPHER: A program for simulating rotational structure.*
4. I.M. Ballingall, A. Alagappan, M.L. Costen, K.G. McKendrick (Heriot-Watt University)  
*Probing Inelastic Collisions of CN Radicals with Frequency Modulated Spectroscopy.*
5. J. Klos, F.J. Aoiz, J.E. Verdasco, M. Brouard, S. Marinakis (Heriot-Watt University)  
*Spotting rotational rainbows: The He-NO case.*
6. Sang Ali (University of Birmingham)  
*Vacuum-UV fluorescence spectroscopy of BCl<sub>3</sub>.*
7. M.J. Simpson, C.A. Mayhew, R.P. Tuckett (University of Birmingham)  
*The reaction of gas-phase anions with fluorinated ethenes.*
8. J.M. Beames, R. Wada, Andrew Orr-Ewing (University of Bristol)  
*Detection of Atmospheric NO<sub>2</sub> by Cavity Ring Down Spectroscopy.*
9. Ryuichi Wada and Andrew J. Orr-Ewing (University of Bristol)  
*Quantitative measurements of iodine monoxide by cavity ring down spectroscopy.*
10. A.L. Devine, M.G.D. Nix, R.N. Dixon, M.N.R. Ashfold (University of Bristol)  
*UV dissociation dynamics of phenol studied by H atom photofragment translational spectroscopy.*
11. C.J.B. Lloyd, D.M. Smith, M.E. Wood (University of Bristol)  
*Infrared spectroscopy of hex-3-ene-1,5-diyne: a precursor of Bergman cyclisation.*
12. E.L. Flynn, A.M. Heath, A. Trottier, E. Wrede (University of Durham)  
*Reactive Scattering of Rydberg Atoms: A novel technique to study ion-molecule reactions.*
13. A. Marcela Coroiu, I. Antón García, David H. Parker, Gerrit Groenenboom, Jonathan Barr, Inmaculada Torres Novalbos, Benjamin J. Whitaker (University of Leeds)  
*Velocity map imaging study of the photodissociation of NO<sub>2</sub> in the range 200–205 nm.*
14. Scott M. Brereton, Andrew M. Ellis, Sheng Fu Yang (University of Leicester)  
*The generation of pulsed helium nanodroplet beams.*
15. V.L. Ayles, D.E. Bergeron, A. Musgrave, R.T. Gammon, J.A.E. Silber and T.G. Wright (University of Nottingham)  
*REMPI Spectroscopy of NO<sub>2</sub>.*
16. C.J. Hammond, K.L. Reid and A.K. King (University of Nottingham)  
*Photoelectron Spectroscopy of Di-Substituted Benzenes Using Velocity Map Imaging.*

17. A. Boatwright, J.A. Jeffs, A.J. Stace (University of Nottingham)  
*Spectroscopy of Molecules in Helium Nanodroplets.*
18. A.B. Nielsen and A.J. Stace (University of Nottingham)  
*Superefficient charge transfer to oxygen.*
19. G. Wu and A.J. Stace (University of Nottingham)  
*IRMPD spectra and Metal Dication Complexes.*
20. B. Wu, B.J. Duncombe, D. Rawson, A.J. Stace (University of Nottingham)  
*Coulomb Explosion of  $Mg^{2+}$ /Alcohol Complexes.*
21. G.P. Maguire, S.R. Procter and T.P. Softley (University of Oxford)  
*Time-varying electric field deceleration of  $H_2$  Rydberg molecules.*
22. G.R. Lloyd, S.R. Procter and T.P. Softley (University of Oxford)  
*Ionisation of hydrogen Rydberg molecules in the vicinity of a metal surface.*
23. M.T. Bell, D. Carty, S.R. Procter and T.P. Softley (University of Oxford)  
*Deceleration and Trapping of CH Radicals: Progress Towards Ultra-cold Chemistry.*
24. N.A. Macleod, T. de Boer, L.C. Snoek and J.P. Simons (University of Oxford)  
*Protonated amino acids and peptides in the gas phase. A combined experimental and computational study.*
25. Ruth M. Burke, William E. Boxford, Caroline E. Dessent (University of York)  
*The interaction of cations with multiply charged anions.*
26. Nicola M. Tonge, Ewan C. MacMahon and Martin C.R. Cockett (University of York)  
*Collision-Free Chemistry: Spectroscopy and Reactivity of Fluorobenzene<sup>+</sup>-(NH<sub>3</sub>)<sub>n</sub>.*
27. M.L. Anderson, M.S. Ford, T. Drewello, S.R. Mackenzie (University of Warwick)  
*Ion Cyclotron Resonance Studies of the Catalytic Properties of Small Transition Metal Cluster Ions.*
28. John Bomphrey, Stuart Mackenzie, Phil Woodruff (University of Warwick)  
*Molecular surface science: Ion cyclotron resonance studies of metal cluster-adsorbate binding energies.*
29. Mark S. Ford and Stuart R. Mackenzie (University of Warwick)  
*MATI Spectroscopy of Transition Metal Clusters.*
30. D.J. Harding, T.R. Walsh, S.R. Mackenzie (University of Warwick)  
*Structural Isomerism in Small Transition Metal Clusters.*
31. M. Mazurenka, L. Wilkins, J.V. Macpherson, P.R. Unwin and S.R. Mackenzie (University of Warwick)  
*Extension of EW-CRDS to study electrochemical reactions.*

## DELEGATES

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