

# Conference on molecular energy transfer



## Programme

Department of Chemistry



and

Jesus College



University of Oxford

## Programme

**SUNDAY 11<sup>TH</sup> SEPTEMBER (AFTERNOON)**

**From 11.00 am** Arrival and registration at Jesus College (rooms available from 2.00 pm)

**1.00 pm – 1.30 pm** Buffet lunch (Jesus College, Hall)

**Please note:** All meals are in the main hall in Jesus College.

*All lunches are self-service between 1.00 pm and 1.30 pm.*

*All dinners are served at 7pm (except on Sunday, when it is at 7.30 pm).  
Attendees are requested to be seated in Hall just before dinner is served.*

All lectures are in the large lecture theatre in the Physical and Theoretical Chemistry Laboratory (PTCL)

**Session 1:** Inelastic Scattering 1 (PTCL – Session chair: Gus Hancock)

**4.10 pm – 4.20 pm** **Welcome**

**4.20 pm – 5.00 pm** P1: **Gerard Meijer** (Fritz-Haber Institute, Berlin, Germany)  
*Collision studies with Stark-decelerated beams*

**5.00 pm – 5.30 pm** I1: **David W. Chandler** (Sandia National laboratory, USA)  
*Collision-Induced alignment of NO( $A^2\Sigma^+$ )*

**5.30 pm – 5.50 pm** C1: **Joseph M. Beames** (University of Pennsylvania, USA)  
*A new spectroscopic window on hydroxyl radicals using UV+VUV resonant ionization*

**6.30 pm – 7.30 pm** Wine Reception (Jesus College, Ship Street Centre)  
*Kindly sponsored by the University of Manchester  
in honour of Professor J.N. Connor*

**7.30 pm (prompt)** Dinner (Jesus College, Hall)

**8.30 pm – 11.00 pm** The College bar will be open after dinner.

## MONDAY 12<sup>TH</sup> SEPTEMBER (MORNING)

**8.00 am** Breakfast (Jesus College, Hall)

**Session 2:** Inelastic Scattering 2 (PTCL – Session chair: Matt Costen)

**9.00 am – 9.40 am** P2: **David H. Parker** (Radboud University Nijmegen, The Netherlands)  
*Imaging studies of inelastic collisions*

**9.40 am – 10.10 am** I2: **Paul J. Dagdigan** (Johns Hopkins University, USA)  
*Theoretical investigation of rotationally inelastic collisions of molecular free radicals*

**10.10 am – 10.30 am** C2: **Géraldine Féraud** (Université Paris-Sud 11, France)  
*Infrared emission from photo-excited gaseous aromatic molecules: competition with molecular dissociation and collisions*

**10.30 am – 11.00 am** Coffee Break (PTCL)

**Session 3:** Photodissociation 1 (PTCL – Session chair: Claire Vallance)

**11.00 am – 11.40am** P3: **Arthur G. Suits** (Wayne State University, USA)  
*Roaming-mediated isomerisation in the photodissociation of nitroaromatics*

**11.40 am – 12.10 pm** I3: **Reinhard Schinke** (MPI for Dynamics and Self-Organization, Germany)  
*Photodissociation of N<sub>2</sub>O: A comprehensive dynamics study*

**12.10 pm – 12.30 pm** C3: **Jim Jr-Min Lin** (IAMS, Academia Sinica, Taiwan)  
*Photochemistry of ClOOCl and formation of the ozone hole*

**1.00 pm – 1-30 pm** Buffet lunch (Jesus College, Hall)

## MONDAY 12<sup>TH</sup> SEPTEMBER (AFTERNOON/EVENING)

### Session 4: **Photodissociation 2** (PTCL – Session chair: Dave Townsend)

**2.20 pm – 3.00 pm**

P4: **Toshinori Suzuki** (Kyoto University, Japan)  
*Ultrafast electronic dynamics in gas and liquid phases studied by time-resolved photoelectron spectroscopy*

**3.00 pm – 3.30 pm**

I4: **Robert E. Continetti** (University of California, San Diego, USA)  
*Spectroscopy and dynamics of the HOCO and DOCO radicals*

**3.30 pm – 3.50 pm**

C4: **Valerie Blanchet** (Université Paul Sabatier & IRSAMC, Toulouse, France)  
*Time-resolved predissociation of CH<sub>3</sub>I excited in the origin level of the B state*

**3.50 pm – 4.20 pm**

**Tea Break** (PTCL)

### Session 5: **Non-adiabatic effects 1** (PTCL – Session chair: Tim Softley)

**4.20 pm – 5.00 pm**

P5: **Alec Wodtke** (Max Planck Institute, Gottingen, Germany)  
*Electronically non-adiabatic chemical dynamics at metal surfaces*

**5.00 pm – 5.30 pm**

I5: **John Tully** (Yale, USA)  
*Chemical dynamics at metal surfaces: The role of electronic excitations*

**5.30 pm – 5.50 pm**

C5: **Chuanyao Zhou** (Dalian Institute of Chemical Physics, China)  
*Photochemistry of methanol on TiO<sub>2</sub>(110)*

**7.00 pm (prompt)**

**Dinner** (Jesus College, Hall)

**8.00 pm – 11.00 pm**

**Poster Session 1** (JCR - Jesus College)  
Bar open

## TUESDAY 13<sup>TH</sup> SEPTEMBER (MORNING)

**8.00 am** Breakfast (Jesus College, Hall)

**Session 6:** Non-adiabatic effects 2 (PTCL – Session chair: Andrew Orr-Ewing)

**9.00 am – 9.40 am** P6: **Michael A. Collins** (ANU, Canberra, Australia)  
*Ab initio diabatic potential energy matrix and dynamics for  $OH(A^2\Sigma^+) + H_2/D_2$*

**9.40 am – 10.10 am** I6: **Xueming Yang** (Dalian Institute of Chemical Physics, China)  
*Dynamics of resonances and barriers in the  $F+H_2$  chemical reaction*

**10.10 am – 10.30 am** C6: **Miguel González** (Universitat de Barcelona, Spain)  
*Quasi-classical trajectory-Gaussian binning study of  $OH + D_2 \rightarrow HOD(v_1', v_2', v_3') + D$  angle-velocity and vibrational distributions at 0.28 eV and influence of vibrational excitation of reactants*

**10.30 am – 11.00 am** Coffee Break (PTCL)

**Session 7:** Reactive scattering 1 (PTCL – Session chair: Jonathan Connor)

**11.00 am – 11.40 am** P7: **Richard N. Zare** (Stanford University, USA)  
*Plans for preparing  $M$ -entangled molecules*

**11.40 am – 12.10 pm** I7: **Roland Wester** (University of Innsbruck, Austria)  
*On the dynamics of chemical reactions of negative ions*

**12.10 pm – 12.30 pm** C7: **F. Javier Aoiz** (Universidad Complutense, Madrid, Spain)  
*The dynamics of  $Cl + O_3$  reaction: A theoretical study and comparison with experimental results.*

**1.00 pm – 1-30 pm** Buffet lunch (Jesus College, Hall)

## TUESDAY 13<sup>TH</sup> SEPTEMBER (AFTERNOON/EVENING)

### Session 8: **Reactive scattering 2** (PTCL – Session chair: Grant Ritchie)

**2.20 pm – 3.00 pm** P8: **Kopin Liu** (IAMS, Taipei, Taiwan)  
*Unfolding the polarization-dependent differential cross sections in the reaction of Cl + CHD<sub>3</sub>(v<sub>1</sub>=1)*

**3.00 pm – 3.30 pm** I8: **Ian Sims** (University of Rennes, France)  
*Experimental investigations of radical-molecule reactions using low temperature supersonic flows and applications to atmospheric and astrophysical chemistry*

**3.30 pm – 3.50 pm** C8: **Marc Briant** (IRAMIS/SPAM, CEA-Saclay, France)  
*Photophysics and photochemistry of calcium dimer on helium cluster*

### 3.50 pm – 4.20 pm **Tea Break** (PTCL)

### Session 9: **Biomolecules 1** (PTCL – Session chair: Valerie Blanchet)

**4.20 pm – 5.00 pm** P9: **Rienk van Grondelle** (Vrije Universiteit, Amsterdam)  
*How nature harvests solar light*

**5.00 pm – 5.30 pm** I9: **Philipp Kukura** (University of Oxford, UK)  
*Towards efficient dynamics: Observing and controlling conical intersection dynamics in retinals*

**5.30 pm – 5.50 pm** C9: **Ruth Livingstone** (Heriot-Watt University, Edinburgh, UK)  
*Time-resolved photoelectron spectroscopy of indole and 5-hydroxyindole*

### 7.00 pm (prompt) **Dinner** (Jesus College, Hall)

### 8.30 pm – 9.30 pm **Concert** (Hertford College Chapel)

### 9.30 pm – 11.00 pm **Bar open** (Jesus College)

## WEDNESDAY 14<sup>TH</sup> SEPTEMBER (MORNING)

**8.00 am** Breakfast (Jesus College, Hall)

**Session 10:** Biomolecules 2 (PTCL – Session chair: Fleming Crim)

**9.00 am – 9.40 am** P10: **Jos Oomens** (FOM Institute for Plasma Physics, The Netherlands)  
*The chemistry of peptide sequencing elucidated by IR spectroscopy*

**9.40 am – 10.10 am** I10: **Wolfgang Domcke** (Technical University, München, Germany)  
*Conical intersections and their role for the photostability of the building blocks of life*

**10.10 am – 10.30 am** C10: **Amir Golan** (Lawrence Berkeley National Laboratory, USA)  
*Ionization of dimethyluracil dimers leads to facile proton transfer in the absence of H-bonds*

**10.30 am – 11.00 am** Coffee Break (PTCL)

**Session 11:** Condensed phase dynamics (PTCL – Session chair: Philipp Kukura)

**11.00 am – 11.40 am** P11: **F. Fleming Crim** (University of Wisconsin, USA)  
*Time-resolved studies of vibrational relaxation and isomerization in liquids and cryogenic matrices*

**11.40 am – 12.10 pm** I11: **Andrew J. Orr-Ewing** (University of Bristol, UK)  
*Taking the plunge: quantum state resolved dynamics of chemical reactions in solution*

**12.10 pm – 12.40 pm** I12: **George C. Schatz** (Northwestern University, USA)  
*Gas phase and gas surface reaction dynamics studies*

**1.00 pm – 1-30 pm** Buffet lunch (Jesus College, Hall)

## WEDNESDAY 14<sup>TH</sup> SEPTEMBER (AFTERNOON/EVENING)

### Session 12: Clusters and interfaces (PTCL – Session chair: Brian Howard)

2.20 pm – 3.00 pm

P12: **David J. Nesbitt** (University of Colorado, USA)  
*Energy transfer dynamics at the gas-liquid and gas-solid interfaces:  
A quantum state resolved perspective*

3.00 pm – 3.30 pm

I13: **Mark A. Johnson** (Yale, USA)  
*Trapping and characterization of reaction intermediates using cryogenic ion  
chemistry*

3.30 pm – 3.50 pm

C11: **David R. Glowacki** (University of Bristol, UK)  
*Formulating models of non-equilibrium dynamics in solution phase organic  
chemistry*

3.50 pm – 4.20 pm

Tea Break (PTCL)

### Session 13: New horizons (PTCL – Session chair: David Nesbitt)

4.20 pm – 5.00 pm

P13: **Daniel M. Neumark** (University of California, Berkeley, USA)  
*Ultrafast x-ray science: applications to femto and atto chemistry*

5.00 pm – 5.30 pm

I14: **Kenneth G. McKendrick** (Heriot-Watt University, UK)  
*Dynamics of gas-liquid interfacial scattering*

5.30 pm – 6.00 pm

I15: **Rainer D. Beck** (École Polytechnique, Lausanne, Switzerland)  
*Steric effects and vibrational bond selectivity in the dissociative  
chemisorption of methane*

6.00 pm – 6.20 pm

C12: **Raluca Cireasa** (IRSAMC, University of Toulouse, France)  
*Dynamic imaging of molecules using high harmonics generation*

7.00 pm (prompt)

Dinner (Jesus College, Hall)

8.00 pm – 11.00 pm

Poster Session 2 (JCR – Jesus College)  
Bar open



## THURSDAY 15<sup>TH</sup> SEPTEMBER (MORNING)

**8.00 am** Breakfast (Jesus College, Hall)

**Session 14:** Femtochemistry (PTCL – Session chair: Daniel Neumark)

**9.00 am – 9.40 am** P14: **Paul Corkum** (NRC, Ottawa, Canada)  
*Laser induced molecular imaging*

**9.40 am – 10.10 am** I16: **Albert Stolow** (NRC, Ottawa, Canada)  
*Towards Polanyi rules for polyatomics via time-resolved photoelectron spectroscopy*

**10.10 am – 10.40 am** I17: **Helen Fielding** (University College, London, UK)  
*Femtosecond dynamics through conical intersections*

**10.40 am – 11.10 am** Coffee Break (PTCL)

**Session 15:** Cold molecules (PTCL – Session chair: Stuart Mackenzie)

**11.10 am – 11.50 am** P15: **Jun Ye** (JILA, Boulder, USA)  
*Polar molecular gas in the quantum regime*

**11.50 am – 12.20 pm** I18: **Edward Hinds** (Imperial College, London, UK)  
*Improved measurement of the electron electric dipole moment*

**12.20 pm – 12.40 pm** C13: **Martin Bell** (University of Oxford, UK)  
*Ion-molecule cold chemistry using molecular beams with a tuneable velocity*

**1.00 pm – 1-30 pm** Buffet lunch (Jesus College, Hall)

# Conference on molecular energy transfer 2011



## THURSDAY 15<sup>TH</sup> SEPTEMBER (AFTERNOON/EVENING)

2.00 pm – 5.00 pm                      **Conference excursion**  
Coach departs from outside Trinity College gates in Broad Street at 2pm

6.30 pm – 7.00pm                      **Drinks reception** (Jesus College, 2<sup>nd</sup> Quad, subject to weather)

7.00 pm (prompt)                      **Conference banquet** (Jesus College, Hall)

9.00 pm – 11.30pm                      **Bar open** (Jesus College)

## FRIDAY 16<sup>TH</sup> SEPTEMBER      (MORNING)

8.00 am                                      **Breakfast** (Jesus College, Hall)

Conference close                      **Departure**

<b>COMET XXII Oxford 2011</b>							
<b>Outline Programme</b>							
<i>Session Start Time</i>	<i>Sunday 11 Sept</i>	<i>Monday 12 Sept</i>	<i>Tuesday 13 Sept</i>	<i>Wednesday 14 Sept</i>	<i>Thursday 15 Sept</i>	<i>Friday 16 Sept</i>	
	—	<b>Breakfast (Jesus College, 8am)</b>					
9.00 am	—	<i>Session 2</i>	<i>Session 6</i>	<i>Session 10</i>	<i>Session 14</i>		
	— — —	David H. Parker Paul J. Dagdigian Géraldine Féraud	Michael A. Collins Xueming Yang Miguel González	Jos Oomens Wolfgang Domcke Amir Golan	Paul Corkum Albert Stolow Helen H. Fielding	Meeting ends	
	—	<b>Coffee break (PTCL tea room)</b>					—
11.00 or 11-10 am		<i>Session 3</i>	<i>Session 7</i>	<i>Session 11</i>	<i>Session 15</i>	—	
	Registration	Arthur G. Suits Reinhard Schinke Jim Jr-Min Lin	Richard N. Zare Roland Wester F. Javier Aoiz	F. Fleming Crim Andrew J. Orr-Ewing George C. Schatz	Jun Ye Edward Hinds Martin Bell	— — —	
		<b>Lunch (Jesus College, 1.00 pm – 1.30pm)</b>					—
2-20 pm		<i>Session 4</i>	<i>Session 8</i>	<i>Session 12</i>	Excursion	—	
	Registration	Toshinori Suzuki Robert E. Continetti Valerie Blanchet	Kopin Liu Ian Sims Marc Briant	David J. Nesbitt Mark A. Johnson David R. Glowacki	— — —	— — —	
		<b>Tea break (PTCL tea room)</b>				Excursion	—
4-20 pm	<i>Session 1</i>	<i>Session 5</i>	<i>Session 9</i>	<i>Session 13</i>	Excursion	—	
	Gerard Meijer David W. Chandler Joseph M. Beames —	Alec Wodtke John Tully Chuanyao Zhou —	Rienk van Grondelle Philipp Kukura Ruth Livingstone —	Dan M. Neumark Kenneth G. McKendrick Rainer Beck Raluca Cireasa	Excursion	— — — —	
		<b>Dinner (Jesus College, 7pm)</b>				Banquet	—
8.00 pm-11.00 pm	—	Poster 1	Activity	Poster 2	Banquet	—	

*We wish to thank the following for their contributions towards the success of this conference:*



European Office of Aerospace Research and Development, Air Force Office of Scientific Research, United States Air Force Research Laboratory.

## PCCP

The journal Physical Chemistry Chemical Physics of the Royal Society of Chemistry.



Photonic Solutions: Supplier of opto-electronics to the photonics market



Laser 2000: Advanced Solutions for Photonics



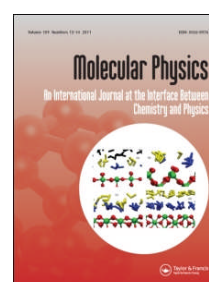
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