

European conference on the dynamics of molecular systems



Programme



Department of Chemistry



Jesus College

University of Oxford



Programme

SUNDAY 9TH SEPTEMBER (AFTERNOON)

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

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)

3.40 pm – 4.20 pm Tea in the Physical and Theoretical Chemistry Laboratory

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

4.20 pm – 4.30 pm **Welcome**

4.30 pm – 5.05 pm P1: **David H Parker** (Radboud University, Nijmegen, The Netherlands)
Imaging studies of inelastic collisions

5.05 pm – 5.40 pm P2: **Millard H Alexander** (University of Maryland, USA)
Electronic non-adiabaticity in collisional quenching of OH radicals

5.40 pm – 6.00 pm C1: **Michael P Grubb** (Texas A&M University, USA)
Roaming in the dark: Deciphering the mystery of the NO₃ photolysis mechanism

7.00 pm – 7.30 pm Wine Reception (Jesus College, 2nd Quad, subject to weather)

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

8.30 pm – 11.00 pm Bar open (The Jesus College bar will be open after dinner.)

MONDAY 10TH SEPTEMBER (MORNING)

8.00 am Breakfast (Jesus College, Hall)

Session 2: Photodissociation (PTCL – Session chair: Matt Costen)

9.00 am – 9.35 am P3: **Marc Vrakking** (Max-Born Institute, Berlin, Germany)
Attosecond time-resolved molecular dynamics

9.35 am – 10.00 am I1: **T Peter Rakitzis** (University of Crete, Greece)
Chiral cavity ring down

10.00 am – 10.20 am C2: **W Carl Lineberger** (JILA and University of Colorado, USA)
Energy flow and sequestration in photoexcited ICN⁻

10.20 am – 10.50 am Coffee Break (PTCL)

Session 3: Interstellar/Planetary Chemistry (PTCL – Session chair: Claire Vallance)

10.50 am – 11.25 am P4: **Ewine F Van Dishoeck** (Leiden Observatory, The Netherlands)
Molecular processes in space: from interstellar clouds to planets

11.25 am – 12.00 pm P5: **Harold Linnartz** (Leiden Observatory, The Netherlands)
CHEM-ICE-TRY: Solid state pathways towards molecular complexity in space

12.00 pm – 12.25 pm I2: **Jonathan Tennyson** (University College London, London, UK)
Molecular line lists for the opacity of exoplanets, cool stars, and other atmospheres

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

MONDAY 10TH SEPTEMBER (AFTERNOON/EVENING)

Session 4: Reactive scattering 1 (PTCL – Session chair: Javier Aoiz)

- 2.20 pm – 2.55 pm P6: **Piergeorgio Casavecchia** (Università degli Studi di Perugia, Italy)
Intersystem crossing dynamics in polyatomic multichannel reactions of oxygen atoms with unsaturated hydrocarbons
- 2.55 pm – 3.20 pm I3: **Tomás González-Lezana** (CSIC, Madrid, Spain)
The dynamics behind atom-diatom collisions with competing reaction pathways
- 3.20 pm – 3.40 pm C3: **Eduardo Carrascosa** (University of Innsbruck, Austria)
Towards probing the dynamics of the endothermic S_N2 -reaction $I + CH_3Cl$ using velocity map imaging

3.40 pm – 4.20 pm Tea Break (PTCL)

Session 5: Reactive scattering 2 (PTCL – Session chair: David Parker)

- 4.20 pm – 4.55 pm P7: **Gerrit C Groenenboom** (Radboud University, Nijmegen, The Netherlands)
Cold polar radical-radical collisions
- 4.55 pm – 5.20 pm I4: **Michel Costes** (Université de Bordeaux, Talence, France)
Crossed-beam scattering experiments at energies approaching the cold regime
- 5.20 pm – 5.40 pm C4: **Marcelo de Miranda** (University of Leeds, UK)
New concepts and approaches for precise quantification and exact quantum description of the dynamics of molecular collisions

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

8.00 pm – 11.00 pm Poster Session 1 (JCR - Jesus College)
Bar open

TUESDAY 11TH SEPTEMBER (MORNING)

8.00 am Breakfast (Jesus College, Hall)

Session 6: Biomolecules / Cold collisions (PTCL – Session chair: Stefan Willitsch)

9.00 am – 9.25 am I5: **Jeremy M Hutson** (University of Durham, UK)
The prospects of forming micro-Kelvin molecules by sympathetic cooling with ultracold atoms

9.25 am – 10.00 am P8: **Villy Sundström** (Lund University, Lund, Sweden)
Identification of the mechanism of photoprotection in eumelanin pigments

10.00 am – 10.20 am C5: **Svetlana Kotochigova** (Temple University, Philadelphia, USA)
Reactive collisions and interactions of ultracold dipolar molecules

10.20 am – 11.00 am Coffee Break (PTCL)

Session 7: Reaction dynamics (PTCL – Session chair: Paul Dagdigian)

11.00 am – 11.35 am P9: **Marsha I Lester** (University of Pennsylvania, Philadelphia, USA)
Dynamical outcomes of quenching: Reflections on a conical intersection

11.35 am – 12.00 pm I6: **Pascal Honvault** (Univ. de Bourgogne, and UFR ST, Univ. de Franche-Comté, France)
 $N + OH \rightarrow NO + H$: New theoretical results and comparison with experiment

12.00 pm – 12.20 pm C6: **Petr Slaviček** (Institute of Chemical Technology, Prague, Czech Republic)
Is there intermolecular Coulomb decay in liquid water and water clusters? Dynamical perspective

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

TUESDAY 11TH SEPTEMBER (AFTERNOON/EVENING)

Session 8: Condensed phases 1 (PTCL – Session chair: Grant Ritchie)

2.20 pm – 2.55 pm

P10: **Andrew J Orr-Ewing** (University of Bristol, UK)
Vibrationally resolved chemical reaction dynamics in solution

2.55 pm – 3.20 pm

I7: **Graham A Worth** (University of Birmingham, UK)
Following and controlling fundamental photochemistry: Quantum dynamics simulations using the MCTDH method

3.20 pm – 3.40 pm

C7: **Nils Huse** (CFELS and University of Hamburg, Germany)
Elucidating charge delocalization in aqueous polypyridyl Fe(II) compounds during photo-induced intersystem crossing via time-resolved spectroscopy in the X-ray water window

3.40 pm – 4.20 pm

Tea Break (PTCL)

Session 9: Condensed phases 2 (PTCL – Session chair: Kenneth McKendrick)

4.20 pm – 4.55 pm

P11: **David Manolopoulos** (University of Oxford, UK)
Chemical reaction rates from ring polymer molecular dynamics

4.55 pm – 5.20 pm

I8: **Huib J Bakker** (FOM Institute AMOLF, Amsterdam, The Netherlands)
Ultrafast dynamics and nanoclustering of water molecules at a membrane surface

5.20 pm – 5.40 pm

C8: **Jaroslav Kočíšek** (Academy of Sciences, Prague, Czech Republic)
Sticky ice: The first step to heterogeneous chemistry

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 12TH SEPTEMBER (MORNING)

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

Session 10: **Fullerenes** (PTCL – Session chair: W. Carl Lineberger)

9.00 am – 9.35 am P12: **Eleanor E B Campbell** (University of Edinburgh, Edinburgh, UK)
Angular-resolved fs photoelectron spectroscopy of fullerenes: giant atoms or hot metal spheres?

9.35 am – 10.00 am I9: **Vadim K Ivanov** (St.Petersburg State Polytechnic University, Russia)
Electronic structure and photoionization processes in clusters, fullerenes and endofullerenes

10.00 am – 10.20 am C9: **Benjamin J Irving** (University of Sheffield, UK)
H₂ formation on non-ideal graphene substrates in interstellar space

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

Session 11: **New Horizons** (PTCL – Session chair: Philipp Kukura)

11.00 am – 11.35 am P13: **Jochen Küpper** (DESY and University of Hamburg, Germany)
Controlling large molecules at high repetition rates: Toward the “molecular movie”

11.35 am – 12.00 pm I10: **Manfred Faubel** (Max-Planck-Institute for Dynamics and Self-Organization, Goettingen, Germany)
Liquid microjet synchrotron radiation photoelectron spectroscopy of chemical state change in aqueous solutions

12.00 pm – 12.20 pm C10: **Grant Paterson** (Heriot-Watt University, Edinburgh, UK)
Interfacial collisions dynamics of OH with organic liquid surfaces

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

WEDNESDAY 12TH SEPTEMBER (AFTERNOON/EVENING)

2.00 pm – 6.00 pm **Conference excursion**
Coach departs from outside Trinity College gates in Broad Street at 2pm

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

8.00 pm – 11.00 pm **Poster Session 2** (JCR – Jesus College)
Bar open

THURSDAY 13TH SEPTEMBER (MORNING)

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

Session 12: **Femtochemistry 1** (PTCL – Session chair: Brian Howard)

9.00 am – 9.35 am P14: **David Villeneuve** (NRC, Ottawa, Canada)
Following simple chemical reactions using homodyne high harmonic spectroscopy

9.35 am – 10.00 am I11: **Henrik Stapelfeldt** (Aarhus University, Denmark)
Laser induced alignment of molecules dissolved in helium nanodroplets

10.00 am – 10.20 am C11: **Francesca Calegari** (National Research Council (IFN -CNR), Milan, Italy)
Probing the ultrafast dynamics of highly-excited states in N₂ molecules excited by attoseconds XUV pulses

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

Session 13: **Femtochemistry 2** (PTCL – Session chair: Steven Stolte)

11.00 am – 11.35 am P15: **R J Dwayne Miller** (DESY and University of Hamburg, Germany)
"Making the molecular movie": First frames.....Now with REGAE music

11.35 am – 12.00 pm I12: **Daan Brinks** (Institute of Photonic Sciences, Barcelona, Spain)
Quantum coherence at room temperature: From single molecules to light harvesting complexes

12.00 pm – 12.20 pm C12: **Alkwin Slenczka** (University of Regensburg, Germany)
Electronic spectroscopy of phthalocyanines and porphyrines inside superfluid Helium nanodroplets

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

THURSDAY 13TH SEPTEMBER (AFTERNOON/EVENING)

Session 14: **He droplets** (PTCL – Session chair: Stuart Mackenzie)

2.20 pm – 2.55 pm

P16: **Paul Scheier** (University of Innsbruck, Austria)
Ion chemistry in doped He nanodroplets

2.55 pm – 3.20 pm

I13: **Gert von Helden** (Fritz-Haber-Institut, Berlin, Germany)
Proteins in the freezer: Embedding mass/charge selected biomolecular ions in liquid helium droplets

3.20 pm – 3.40 pm

C13: **Gediminas Galinis** (University of Leicester, UK)
Molecular superfluidity in helium studied using impulsive alignment

3.40 pm – 4.20 pm

Tea Break (PTCL)

Session 15: **Cold collisions / biomolecules** (PTCL – Session chair: Tim Softley)

4.20 pm – 4.45 pm

I14: **Wim van der Zande** (Radboud University, Nijmegen, The Netherlands)
Flexibility and structure of peptides from far-infrared spectroscopy using free electron lasers

4.45 pm – 5.20 pm

P17: **Stefan Willitsch** (University of Basel, Basel, Switzerland)
Cold chemistry with Coulomb-crystallised atomic and molecular ions in traps

5.20 pm – 5.40 pm

C14: **Ed Narevicius** (Weizmann Institute of Science, Israel)
Observation of quantum effects in sub-Kelvin cold reactions

6.30 pm – 7.00pm

Drinks reception (Jesus College, 2nd Quad, subject to weather)

7.00 pm (prompt)

Conference banquet (Jesus College, Hall)

9.00 pm – 11.30pm

Bar open (Jesus College)

European conference on the dynamics of molecular systems



FRIDAY 14TH SEPTEMBER (MORNING)

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

Conference close _____ **Departure**

MOLEC XIX Oxford 2012

Outline Programme

Session Start Time	Sunday 9 September	Monday 10 September	Tuesday 11 September	Wednesday 12 September	Thursday 13 September	Friday 14 September
8-00 am	—	Breakfast (Jesus College, 8am)				
9-00 am	—	Session 2	Session 6	Session 10	Session 12	Meeting ends
	—	Marc Vrakking (35) Peter Rakitzis (25) Carl Lineberger (20)	Jeremy Hutson (25) Villy Sundstrom (35) Svetlana Kotochigova (20)	Eleanor Campbell (35) Vadim Ivanov (25) Benjamin Irving (20)	David Villeneuve (35) Henrik Stapelfeldt (25) Francesca Calegari (20)	— — —
10-20 am	—	Coffee break (PTCL)				
10-50 am or 11-00 am	—	Session 3	Session 7	Session 11	Session 13	—
	—	Ewine van Dishoeck (35) Harold Linnartz (35) Jonathan Tennyson (25)	Marsha Lester (35) Pascal Honvault (25) Petr Slaviček (20)	Jochen Küpper (35) Manfred Faubel (25) Grant Paterson (20)	Dwayne Miller (35) Daan Brinks (25) Alkwin Slenczka (20)	— — —
1-00 pm	—	Lunch (Jesus College, 1pm)				
2-20 pm	Registration	Session 4	Session 8	Excursion	Session 14	—
	Registration	Piergiorgio Casavecchia (35) Tomas Gonzalez Lezana (25) Eduardo Carrascosa (20)	Andrew Orr-Ewing (35) Graham Worth (25) Nils Huse (20)	Excursion	Paul Scheier (35) Gert von Helden (25) Gediminas Galinis (20)	— — —
3-40 pm	Registration	Tea break (PTCL)		Excursion		—
4-20 pm	Session 1	Session 5	Session 9	Excursion	Session 15	—
	David Parker (35) Millard Alexander (35) Michael Grubb (20)	Gerrit Groenenboom (35) Michel Costes (25) Marcelo de Miranda (20)	David Manolopoulos (35) Huib Bakker (25) Jaroslav Kočíšek (20)	Excursion	Wim van der Zande (25) Stefan Willitsch (35) Ed Narevicius (20)	— — —
7-00 pm	Dinner (Jesus College, 7pm)					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:



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

PCCP

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



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