

	<b>Monday 29/08/2016</b>		<b>Tuesday 30/08/2016</b>
08:50 – 09:00	Welcome (O. Smirnova)	09:00 – 09:10	S4: “Imaging and control of molecular dynamics” Introduction: <b>R. Moshhammer</b>
09:00 – 09:10	S1: “Ultrafast Non-adiabatic dynamics, Surface hopping, solvent effects” Introduction: <b>V. Engel</b>	09:10 – 09:30	J. Küpper
09:10 – 09:30	M. Barbatti	09:30 – 09:50	R. Forbes
09:30 – 09:50	B. Lasorne	09:50 – 10:10	M. Richter
09:50 – 10:10	F. Santoro	10:10 – 10:30	J. Feist
10:10 – 10:40	Discussion: <b>V. Engel</b>	10:30 – 11:00	Discussion: <b>R. Moshhammer</b>
10:40 – 11:00	Coffee Break	11:00 – 11:30	Coffee Break
11:00 – 11:10	S2: “Synchrotrons, ultrafast optical and X-ray absorption spectroscopies” Introduction: <b>V. Averbukh</b>	11:30 – 11:40	S5: “Multielectron dynamics in external fields: advances in theory” Introduction: <b>E. Suraud</b>
11:10 – 11:30	O. Travnikova	11:40 – 12:00	L. Madsen
11:30 – 11:50	M.A. Hervé du Penhoat	12:00 – 12:20	A. Scrinzi
11:50 – 12:10	C. Milne	12:20 – 12:40	H. Bachau
12:10 – 12:40	Discussion: <b>V. Averbukh</b>	12:40 – 13:00	S. Patchkovskii
12:40 – 15:00	Lunch + Posters + Coffee	13:00 – 13:30	Discussion: <b>E. Suraud</b>
15:00 – 15:10	S3: “Time-resolved cluster dynamics” Introduction: <b>T. Fennel</b>	13:30 – 15:30	Lunch + Posters + Coffee
15:10 – 15:30	D. Rolles	15:30 – 15:40	S6: “New trends in attosecond spectroscopy” Introduction: <b>M. Ivanov</b>
15:30 – 15:50	M. Krikunova	15:40 – 16:00	J. Mauritsson
15:50 – 16:10	U. Saalman	16:00 – 16:20	A. Brown
16:10 – 16:40	Discussion: <b>T. Fennel</b>	16:20 – 16:40	M. Dahlström
16:40 – 17:00	Coffee Break	16:40 – 17:00	F. Lepine
17:00 – 17:20	<b>I. Sola Reija</b>	17:00 – 17:30	Discussion: <b>M. Ivanov</b>
17:20 – 17:40	<b>S. Mai</b>	17:30 – 18:30	Coffee Break + Posters
17:40 – 18:00	<b>R. Heilemann Myhre</b>		

**Location:**

Lecture Theatre T250, School of Chemistry, Joseph Black Building, King’s Buildings Campus, University of Edinburgh, David Brewster Road, EH9 3FJ Edinburgh  
 Map: <https://goo.gl/maps/GEuDbJod59T2>

## Monday 29/08/2016

08:50 – 09:00 Welcome remarks (**O. Smirnova**)

09:00 – 10:40 Session 1: “Ultrafast Non-adiabatic Dynamics, Surface Hopping, Solvent Effects”.

10-minute introduction, 20-minute talks without questions, followed by 30 minutes’ discussion. Introduction and discussion leader: **V. Engel**.

Speakers:

**M. Barbatti**: “*Dynamics or reaction paths, which is the best quantum chemistry we can do?*”

**B. Lasorne**: “*Diabatic strategies for photochemical quantum dynamics*”

**F. Santoro**: “*Quantum/classical approaches for solvent effects on electronic spectra and ultrafast photoexcited dynamics*”

10:40 – 11:00 Coffee Break

11:00 – 12:40 Session 2: “Synchrotrons, Ultrafast Optical and X-ray Absorption Spectroscopies”

10-minute introduction, 20-minute talks without questions, followed by 30 minutes’ discussion. Introduction and discussion leader: **V. Averbukh**

Speakers:

**O. Travnikova**: “*Hard-X-ray-induced multistep ultrafast dissociation: multistep core-hole-clock approach*”

**M.A. Hervé du Penhoat**: “*Ultrafast dissociation in core-ionized biomolecules*”

**C. Milne**: “*Ultrafast chemical processes probed with X-rays*”

12:40 – 15:00 Lunch + Posters + Coffee

15:00 – 16:40 Session 3: “Time-Resolved Cluster Dynamics”

10-minute introduction, 20-minute talks without questions, followed by 30 minutes’ discussion. Introduction and discussion leader: **T. Fennel**

Speakers:

**D. Rolles**: “*Imaging cluster and nanoplasma dynamics with free-electron lasers*”

**M. Krikunova**: “*TBA*”

**U. Saalman**: “*Dynamical coupling of electrons and ionizing X-ray-induced dynamics*”

16:40 – 17:00 Coffee Break

17:00 – 18:00 Hot Topics, 20 minutes including questions

Speakers:

**I. Sola Reija**: “*Spectator-actor-referee games in electron-nuclear processes*”

**S. Mai**: “*Internal conversion and intersystem crossing dynamics of 2-thiouracil*”

**R. Heilemann Myhre**: “*Coupled cluster methods for transient NEXAFS spectroscopy: the ultrafast  $\pi\pi^*$ - $n\pi^*$  transition in thymine*”

## **Tuesday 30/08/2016**

09:00 – 11:00 Session 4: “Imaging and Control of Molecular Dynamics”

10-minute introduction, 20-minute talks without questions, followed by 30 minutes’ discussion.

Introduction and discussion leader: **R. Moshhammer**

Speakers:

**J. Küpper:** “*Dynamics and reactivities of cold and controlled molecules*”

**R. Forbes:** “*Excited state wavepacket Dynamics in NO<sub>2</sub> probed by strong-field ionization*”

**M. Richter:** “*Sub-laser-cycle control of coupled electron-nuclear dynamics at a conical intersection*”

**J. Feist:** “*Modifications of molecular structure and reactions under strong light-matter coupling*”

11:00 – 11:30 Coffee Break

11:30 – 13:30 S5: “Multielectron Dynamics in External Fields: Advances in Theory”

10-minute introduction, 20-minute talks without questions, followed by 30 minutes’ discussion.

Introduction: **E. Suraud**

**L. Madsen:** “*Time-dependent restricted-active-space self-consistent-field theory*”

**A. Scrinzi:** “*Chemistry in strong fields - the haCC approach*”

**H. Bachau:** “*Stimulated Compton and Raman scattering in hydrogen irradiated by XUV and soft X-ray short and intense laser pulses*”

**S. Patchkovskii:** “*Full-dimensional, quantum treatment of short-time vibronic dynamics in molecular high-harmonics generation process*”

13:30 – 15:30 Lunch + Posters + Coffee

15:30 – 17:30 S6: “New Trends in Attosecond Spectroscopy”

10-minute introduction, 20-minute talks without questions, followed by 30 minutes’ discussion.

Introduction and discussion leader: **M. Ivanov**

**J. Mauritsson:** “*Controlled free-induction decay in the extreme ultraviolet*”

**A. Brown:** “*Stimulating competition between electrons with XUV-initiated HHG*”

**M. Dahlström:** “*Elimination of dipole phase in attosecond pulse characterization*”

**F. Lepine:** “*Time-resolved attosecond and femtosecond photoelectron imaging in large molecules: towards a multiscale approach*”

17:30 – 18:30 Coffee Break + Posters