

## 2<sup>nd</sup> WG1 Meeting: “Ultrafast electron dynamics in molecules”

### 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*” (cancelled due to illness)

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

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**: “*Dynamics of ultrafast cluster charging as revealed by THz streaking*”

**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*” (moved to session 1)

**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