

Sunday 11th September

15:30-17:00 Registration

17:00-17:15 Opening Remarks

40th Anniversary Special Celebration Session

Chair: Gerardo Delgado-Barrio *Instituto de Física Fundamental, CSIC (Spain)*

17:15-18:00 **Francesco A. Gianturco** *Innsbruck Universitaet (Austria)*

Plenary Lecture (PL1) : The puzzle of anions' formation from carbon-rich molecules in the Interstellar medium: how molecular quantum dynamics can help modelling their evolution in astronomical objects

18:00-18:45 **J. Peter Toennies** *Max-Planck-Institut für Dynamik und Selbstorganisation (Germany)*

Plenary Lecture (PL2) : Looking at molecules in very cold and gentle superfluid helium nanodroplets

18:45-19:15 MOLEC Award Ceremony

19:15-20:30 Welcome Reception

Monday 12th September

Session I: Reactive Collisions

Chair: Alexandra Viel *Institute of Physics of Rennes (France)*

09:00-09:35 **F. Javier Aoiz** *Universidad Complutense de Madrid (Spain)*

Plenary Lecture (PL3) : Quantum interferences in chemical reactions: Do they reveal classical mechanisms?

09:35-10:05 **Keli Han** *Dalian Institute of Chemical Physics (China)*

Invited Lecture (IL1) : Reactant coordinate based state-to-state reactive scattering dynamics implemented on GPUs

10:05-10:35 *Coffee Break*

Session II: Ultrafast Phenomena I

Chair: Luis Bañares *Universidad Complutense de Madrid (Spain)*

10:35-11:10 **Fernando Martín** *Universidad Autónoma de Madrid (Spain)*

Plenary Lecture (PL4) : Imaging attosecond molecular dynamics with pump-probe schemes: a theoretical perspective

11:10-11:40 **Anatoli Kheifets** *Australian National University, Canberra (Australia)*

Invited Lecture (IL2) : Time delay in molecular photoionization: Window to ultrafast electron dynamics

11:40-12:10 **Valerie Blanchet** *Université de Bordeaux (France)*

Invited Lecture (IL3) : Toward femtochemistry with circular polarized pulses

12:10-12:30 **Raimund Feifel** *University of Gothenburg (Sweden)*

Oral Presentation (OP1) : Ultrafast molecular three-electron collective Auger decay

12:30-14:30 *Lunch*

Session III: Spectroscopy I

Chair: María Luisa Senent *Instituto de Física Fundamental, CSIC (Spain)*

14:30-15:05 **Timothy J. Lee** *NASA Ames Research Center (USA)*

Plenary Lecture (PL5) : Computing highly accurate spectroscopic line lists for characterization of exoplanet atmospheres and assignment of astronomical observations

15:05-15:35 **Petr Slaviček** *University of Chemistry and Technology Prague (Czech Republic)*

Invited Lecture (IL4) : Nuclear quantum effects in spectroscopy and dynamics: ab initio simulations

15:35-15:55 **Yohann Scribano** *Université de Montpellier (France)*

Oral Presentation (OP2) : Translation-rotation dynamics of confined molecules using an efficient Smolyak Sparse-grid scheme

15:55-16:25 *Coffee Break*

Session IV: Photoinduced Processes

Chair: Raimund Feifel *University of Gothenburg (Sweden)*

16:25-17:00 **King-Chuen Lin** *National Taiwan University (Taiwan)*

Plenary Lecture (PL6) : Roaming signature in photodissociation of some carbonyl compounds

17:00-17:30 **Helen H. Fielding** *University College London (United Kingdom)*

Invited Lecture (IL5) : Time-resolved photoelectron spectroscopy of biological chromophores: from isolated molecules to dimers and liquid jets

17:30-18:00 **Mattanjah S. de Vries** *University of California, Santa Barbara (USA)*

Invited Lecture (IL6) : Photodynamics of nucleobases and their derivatives

18:00-18:20 **Etienne Gindensperger** *Université de Strasbourg – CNRS (France)*

Oral Presentation (OP3) : Spin-vibronic excited-state quantum dynamics in transition metal complexes

18:20-20:00 *Poster Session*

Tuesday 13th September

Session V: Coherence Control I

Chair: Burkhard Schmidt *Free University Berlin (Germany)*

09:00-09:35 **Regina de Vivie-Riedle** *Ludwig-Maximilians-Universität München (Germany)*

Plenary Lecture (PL7) : Quantum dynamics and control of molecular reactions: From gas phase to solution

09:35-10:05 **Cristoph Meier** *Laboratoire Collisions Agrégats Réactivité, , CNRS (France)*

Invited Lecture (IL7) : Femtosecond quantum dynamics and laser control of non-isolated quantum systems

10:05-10:25 **Ágnes Vibók** *University of Debrecen (Hungary)*

Oral Presentation (OP4) : Control by frequency chirped laser-induced conical intersections

10:25-10:55 *Coffee Break*

Session VI: Ultrafast Phenomena II

Chair: Etienne Gindensperger *Université de Strasbourg – CNRS (France)*

10:55-11:30 **Stephen R. Leone** *University of California, Berkeley (USA)*

Plenary Lecture (PL8) : An X-ray spectroscopic revolution in time-resolved molecular dynamics

11:30-12:00 **Marc J. J. Vrakking** *Max Born Institute Berlin (Germany)*

Invited Lecture (IL8) : Novel opportunities for studying atomic, molecular and cluster dynamics intense HHG sources

12:00-12:30 **Leticia González** *University of Vienna (Austria)*

Invited Lecture (IL9) : Challenges to describe intersystem crossing dynamics

12:30-12:50 **Asier Longarte** *Universidad del País Vasco (Spain)*

Oral Presentation (OP5) : Ultrafast excited state dynamics of size selected neutral molecular clusters

12:50-14:50 *Lunch*

15:30 *Visit to Toledo*

Wednesday 14th September

Session VII: Low-Energy Collisions and Reactions I

Chair: Steven Stolte *Jilin University (China)*

09:00-09:35 **Jonathan Tennyson** *University College London (United Kingdom)*

Plenary Lecture (PL9) : Low temperature chemistry using the R-matrix method

09:35-10:05 **David W. Chandler** *Sandia National Laboratory (USA)*

Invited Lecture (IL10) : Study of collision induced dissociation of NO₂ using crossed molecular beam scattering

10:05-10:25 **Manuel Lara** *Universidad Autónoma de Madrid (Spain)*

Oral Presentation (OP6) : Dynamics of the S(¹D)+o-D₂ → SD+D reaction at low collision energies: revisiting the SH2 system

10:25-10:55 *Coffee Break*

Session VIII: Low-Energy Collisions and Reactions II

Chair: Jose María Fernández *Instituto de Estructura de la Materia, CSIC (Spain)*

10:55-11:30 **Sebastiaan Y. T. van de Meerakker** *Radboud University (Netherlands)*

Plenary Lecture (PL10) : Taming molecular collisions

11:30-12:05 **Ad van der Avoird** *Radboud University (Netherlands)*

Plenary Lecture (PL11) : Quantum phenomena in molecular collisions

12:05-12:35 **Edvardas Narevicius** *Weizmann Institute of Science (Israel)*

Invited Lecture (IL11) : Observation of scattering resonances in neutral-neutral and neutral-ion collisions

12:35-12:55 **Alexandra Viel** *Institute of Physics of Rennes (France)*

Oral Presentation (OP7) : Bound states and inelastic scattering of $^3\Sigma_u^+ \text{Rb}_2 - \text{He}$

12:55-14:50 *Lunch*

Session IX: Coherent Control II

Chair: Ágnes Vibók *University of Debrecen (Hungary)*

14:50-15:20 **Oriol Vendrell** *Aarhus University (Denmark)*

Invited Lecture (IL12) : Coupled nuclear and electronic wave packet dynamics

15:20-15:40 **Ignacio R. Sola** *Universidad Complutense de Madrid (Spain)*

Oral Presentation (OP8) : Ultrafast population inversion by parallel transfer

15:40-16:00 **Burkhard Schmidt** *Free University Berlin (Germany)*

Oral Presentation (OP9) : Quasi-exact solvability and supersymmetry in molecular quantum mechanics: From pendular to tunneling states

16:00-16:30 *Coffee Break*

Session X: Atmospheric Chemistry

Chair: David Lauvergnat *Université de Paris-Sud (France)*

16:30-17:05 **R. Benny Gerber** *Hebrew University of Jerusalem (Israel)*

Plenary Lecture (PL12) : Mechanisms and dynamics of atmospherically relevant molecular reactions on surfaces of liquid water and of ice.

17:05-17:25 **Basile F.E. Curchod** *University of Bristol (United Kingdom)*

Oral Presentation (OP10) : Non-adiabatic molecular dynamics simulations of photochemical isoprene oxidation intermediates

17:25-18:00 *Meeting of International Steering Committee*

18:00-20:00 *Poster Session*

Thursday 15th September

Session XI: He Droplets and Clusters

Chair: Anatoly M. Privilov *Saint-Petersburg State University (Russia)*

09:00-09:35 **Henrik Stapelfeldt** *Aarhus University (Denmark)*

Invited Lecture (IL13) : Laser-induced alignment of molecules in He-nanodroplets: Revivals, long-time coherence and breaking-loose

09:35-10:05 **María Pilar de Lara Castells** *Instituto de Física Fundamental, CSIC (Spain)*

Invited Lecture (IL14) : Ab-initio-assisted modelling of the soft, ^4He droplet-mediated, deposition of metallic nanoparticles

10:05-10:25 **Pablo Villareal** *Instituto de Física Fundamental, CSIC (Spain)*

Oral Presentation (OP11) : Theoretical investigations on doped rare gas clusters with neutral or ionic atomic and diatomic impurities

10:25-10:55 *Coffee Break*

Session XII: Dynamics of Complex Systems

Chair: Paolo Tosi *Università di Trento (Italy)*

10:55-11:30 **George C. Schatz** *Northwestern University (USA)*

Plenary Lecture (PL13) : Plasma enhanced dry reforming: Theoretical studies

11:30-11:50 **Sebastian Fernández-Alberti** *Universidad Nacional de Quilmes/CONICET (Argentina)*

Oral Presentation (OP12) : Excited state dynamics in carbon nanorings

11:50-12:10 **Anthony J. H. M. Meijer** *University of Sheffield (United Kingdom)*

Oral Presentation (OP13) : Investigating the mechanism of vibrationally controllable electron transfer using Density Functional Theory

12:30-14:30 *Lunch*

Session XIII: Processes at Surfaces

Chair: Anthony J. H. M. Meijer *University of Sheffield (United Kingdom)*

14:30-15:05 **Rainer D. Beck** *Ecole Polytechnique Fédérale de Lausanne (Switzerland)*

Plenary Lecture (PL14) : State-to-state scattering of methane from a Ni(111) surface

15:05-15:25 **Daniel Farías** *Universidad Autónoma de Madrid (Spain)*

Oral Presentation (OP14) : Phonon dynamics of graphene on metals

15:25-15:45 **Luca M. Martini** *Università di Trento (Italy)*

Oral Presentation (OP15) : Reactivity of fatty acid methyl esters with OH produced by a plasma Jet

15:45-16:15 *Coffee Break*

Session XIV: Spectroscopy II

Chair: José A. Fernández *Universidad del País Vasco (Spain)*

16:15-16:50 **Dieter Gerlich** *Technische Universität Chemnitz (Germany)*

Plenary Lecture (PL15) : Molecular ions in cryogenic traps

16:50-17:20 **Volker Engel** *University of Würzburg (Germany)*

Invited Lecture (IL15) : Wave-packet approach to two-dimensional vibronic spectroscopy

17:20-17:40 **Jose María Fernández** *Instituto de Estructura de la Materia, CSIC
(Spain)*

Oral Presentation (OP16) : Probing molecular collisions by
Raman spectroscopy

20:00 *Conference Dinner*

End of the Conference