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 Slavíček 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)*
XXI European Conference on the Dynamics of Molecular Systems

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 NO$_2$ 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-D$_2$ $\rightarrow$ 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 $^3\Sigma_u^+$ Rb$_2$ - 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*
Thursday 15th September

Session XI: He Droplets and Clusters

Chair: Anatoly M. Pravilov *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, $^4$He 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*