

MOLEC XVII 2008 European Conference on Dynamics of Molecular Systems  
St.Petersburg, Russia – August 23-29, 2008

**PROGRAM**

**August 23, Saturday**

16.00 – 18.00 Registration

18.00 Welcome Cocktail

20.30 Dinner

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**August 24, Sunday**

8.00 – 8.30 Breakfast

8.30 – 9.00 Buses to the Pushkin Administration Hall

9.00 – 9.30 Conference Opening

9.30 – 11.30 Session PMI-1

**Chairman: Z. Herman (Institute of Physical Chemistry, Prague, Czech Republic)**

9.30 – 10.05 **R. D. Levine (Hebrew University of Jerusalem, Israel)**  
*Ultrafast purely electronic reorganization in lithium hydride*

10.05 – 10.40 **A. G. Suits (Wayne State University, Detroit, USA)**  
*Roaming atoms and radicals*

10.40 – 11.05 **M. H. M. Janssen (Vrije Universiteit Amsterdam, The Netherlands)**  
*Femtosecond time-resolved photoelectron-photoion coincidence imaging of multi-photon multi-channel dynamics*

11.05 – 11.30 **R. Schinke (MPG Institute for Dynamics and Self-Organization, Göttingen, Germany)**  
*The photodissociation of NO<sub>2</sub> in the second absorption band: Puzzling comparison with experimental results*

11.30 – 11.50 Coffee Break

11.50 – 13.25 Session MC-1

**Chairman: R. McCarroll (Université Pierre et Marie Curie, Paris, France)**

11.50 – 12.25 **K. Liu (IAMS, Academia Sinica, Taiwan)**  
*A fresh look at mode-specific bimolecular reactivity*

12.25 – 13.00 **G. E. Hall (Brookhaven National Laboratory, USA)**  
*Flipping electron spin without touching: collision-induced intersystem*

*crossing in CH<sub>2</sub>*

**13.00 – 13.25 K. McKendrick (Heriot-Watt University, Edinburgh, UK)**  
*Collisional evolution of rotational orientation and alignment of OH(X)*

**13.25 – 14.00 Buses to the Kochubey Palace**

**14.00 – 15.00 Lunch**

**15.00 Bus Excursion to the Downtown St.Petersburg**

**20.00 Dinner**

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**August 25, Monday**

**8.00 – 9.00 Breakfast**

**9.00 – 11.00 Session UC-1**

**Chairman: R. Anderson (University of California, Santa Cruz, USA)**

**9.00 – 9.35 P. Pillet (Laboratoire Aimé Cotton, Orsay, France)**  
*Dynamics of ultracold molecules*

**9.35 – 10.10 E. Tiemann (Leibniz University Hannover, Germany)**  
*Cold collisions and molecular spectroscopy*

**10.10 – 10.35 T. Stoecklin (Institut des Sciences Moléculaires, Talence, France)**  
*Spin depolarisation of N<sub>2</sub><sup>+</sup> (<sup>2</sup>Σ<sup>+</sup>) in ultra cold collisions with <sup>3</sup>He and <sup>4</sup>He in a magnetic field*

**10.35 – 11.00 A. A. Buchachenko (Moscow State University, Russia)**  
*Metal atoms in magnetic traps: Interaction potentials and dynamics*

**11.00 – 11.20 Coffee Break**

**11.20 – 12.55 Session UC-2**

**Chairman: V. Aquilanti (University of Perugia, Italy)**

**11.20 – 11.55 E. Bodo (University of Rome “La Sapienza”, Italy)**  
*Ultra cold ion atom and ion molecule collisions: dynamics, chemical reactions and charge exchange*

**11.55 – 12.30 M. Drabbels (Ecole Polytechnique Fédéral de Lausanne, Switzerland)**  
*Photodynamics of doped helium nanodroplets*

**12.30 – 12.55 S. Y. T. van der Meerakker (Fritz-Haber-Institut MPG, Berlin, Germany)**  
*Crossed beam collision experiments with Stark decelerated beams*

**13.00 – 14.30 Lunch**

**14.30 – 16.30 Session MC-2**

**Chairman: D. Ascenzi (University of Trento, Italy)**

**14.30 – 15.05 D. W. Chandler (Sandia National Laboratory, USA)**

*Kinematic cooling of molecules*

**15.05 – 15.40 S. Cavalli (University of Perugia, Italy)**

*Resonances in reaction dynamics*

**15.40 – 16.05 W. Christen (Humboldt University Berlin, Germany)**

*Cooling and slowing in high-pressure jet expansions*

**16.05 – 16.30 S. Le Picard (Université de Rennes 1, France)**

*Experimental kinetics study of intramultiplet transitions in collisions of  $C(^3P_j)$  with He and  $H_2$  at temperatures down to 7 K*

**16.30 – 16.55 Coffee Break**

**16.55 – 19.00 Session PMI-2**

**Chairman: V. K. Ivanov (Polytechnical University, St.Petersburg, Russia)**

**16.55 – 17.20 W. Sandner (Max Born Institute, Berlin, Germany)**

*Atomic and molecular ionization dynamics in ultra-strong laser fields:  
Neutral fragments after tunneling*

**17.20 – 17.45 N. A. Cherepkov (State University of Aerospace Instrumentation, Russia)**

*Photoionization of fixed-in-space molecules*

**17.45 – 18.10 G. Meloni (The University of San Francisco, USA)**

*Synchrotron photoionization mass spectrometry identification of combustion  
and atmospheric chemistry intermediates*

**18.10 – 18.35 R. Cireasa (Université Paul Sabatier, Toulouse, France)**

*Oscillatory behaviour in  $NO_2$  photodynamics*

**18.35 – 19.00 S. V. Bobashev (Ioffe Institute, St.Petersburg, Russia)**

*Multi-photon ionization of molecular nitrogen in the vacuum ultraviolet*

**19.00 – 20.30 Dinner**

**20.30 – 23.00 Poster Session I**

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**August 26, Tuesday**

**8.00 – 9.00 Breakfast**

**9.00 – 11.00 Session CMD-1**

**Chairman: D. Sokolovski (Queen's University of Belfast, UK)**

**9.00 – 9.35 E. E. Nikitin (Israel Institute of Technology, Haifa, Israel)**  
*Classical and quantum capture of dipolar molecules by ions*

**9.35 – 10.10 H. Nakamura (IMS, Okazaki, Japan)**  
*Nonadiabatic chemical dynamics*

**10.10 – 10.35 A. K. Belyaev (Herzen University, St.Petersburg, Russia)**  
*Nonadiabatic effects in inelastic processes*

**10.35 – 11.00 C. Petrongolo (University of Siena, Italy)**  
*Renner-Teller quantum dynamics of atom+diatom collisions*

**11.00 – 11.15 Coffee Break**

**11.15 – 13.00 Session VC-1**

**Chairman: R. Schinke (MPG Institute for Dynamics and Self-Organization, Göttingen, Germany)**

**11.15 – 11.50 M. Brouard (Oxford University, UK)**  
*Quantum beat studies of angular momentum polarization in chemical processes.*

**11.50 – 12.25 D. H. Parker (University of Nijmegen, The Netherlands)**  
*Predissociation of the OH and SH radicals*

**12.25 – 13.00 V. Aquilanti (University of Perugia, Italy)**  
*Collisional origin of chiral discrimination: orientation in molecular beams and molecular dynamics simulations*

**13.00 – 14.30 Lunch**

**14.30 – 16.30 Session PMI-3**

**Chairman: M. H. M. Janssen (Vrije Universiteit Amsterdam, The Netherlands)**

**14.30 – 15.05 K.-H. Gericke (University of Braunschweig, Germany)**  
*Two-color-two-photon microscopy – imaging the intrinsic protein fluorescence*

**15.05 – 15.40 C. Jouvét (PPM, Orsay, France)**  
*Photodissociation of protonated aromatic amino acid*

**15.40 – 16.05 Q. Timerghazin (University of Alberta, Edmonton, Canada)**  
*Fluorescent probes in biochemistry - can computational chemistry help?*

**16.05 – 16.30 N. P. Gristan (Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia)**  
*Ultrafast hydrogen atom and acryl group transfer*

**16.30 – 16.55 Coffee Break**

**16.55 – 18.35 Session PMI-4**

**Chairman: A. Aguilar-Navarro (University of Barcelona, Spain)**

**16.55 – 17.20 A. M. Privilov (St.Petersburg State University, Russia)**  
*Spectral and kinetic evidences of the  $MI_2$ (ion-pair states) complexes,*  
 *$M = Rg, SF_6$ .*

**17.20 – 17.45 O. Boyarkin (Ecole Polytechnique Fédéral de Lausanne, Switzerland)**  
*Probing quantum states of water below and above the dissociation limit*

**17.45 – 18.10 Jong-Ho Choi (Korea University, Seoul, Korea)**  
*Reaction dynamics of transient chemical species*

**18.10 – 19.00 MOLEC Award**

**19.00 – 20.30 Dinner**

**20.30 – 23.00 Poster Session II**

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**August 27, Wednesday**

**8.00 – 9.00 Breakfast**

**9.00 – 11.00 Session MC-3**

**Chairman: K. McKendrick (Heriot-Watt University, Edinburgh, UK)**

**9.00 – 9.35 A. J. Orr-Ewing (University of Bristol, UK)**  
*Adiabatic and nonadiabatic dynamics of reactions of Cl atoms with alkanes*

**9.35 – 10.10 Dock-Chil Che (Osaka University, Japan)**  
*Dynamics of the  $OH+HBr$  four-atom reaction by using electrostatic hexapole state-selection and VUV-LIF product detection*

**10.10 – 10.35 A. Aguilar-Navarro (University of Barcelona, Spain)**  
*Theoretical and experimental RFGIB study of some ion-molecule reactions*

**10.35 – 11.00 S. Stolte (Vrije Universiteit Amsterdam, The Netherlands)**  
*Impulsive orientation and alignment of quantum state-selected NO molecules*

**11.00 – 11.20 Coffee Break**

**11.20 – 12.45 Session MC-4**

**Chairman: A. A. Buchachenko (Moscow State University, Russia)**

**11.20 – 11.55 S. Ya. Umanskii (Institute of Chemical Physics, Moscow, Russia)**  
*Multilevel modeling of thin zirconium and hafnium oxide film growth from the gas phase*

**11.55 – 12.20 K. Yamashita (The University of Tokyo, Japan)**  
*An efficient ab initio method for inelastic transport in nanoscale devices and analysis of inelastic electron tunneling spectroscopy*

**12.20 – 12.45 F. Huarte (COSMO Laboratory, Barcelona, Spain)**  
*Molecular dynamics simulations of gas adsorption in carbon nanotubes*

**12.50 – 14.00 Lunch**

**14.00 – 19.00 Excursion to the Hermitage Museum**

**19.00 – 22.00 Conference Dinner**

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## **August 28, Thursday**

**8.00 – 9.00 Breakfast**

**9.00 – 11.00 Session MC-5**

**Chairman: S. Stolte (Vrije Universiteit Amsterdam, The Netherlands)**

**9.00 – 9.35 A. Garcia-Vela (CSIC, Madrid, Spain)**  
*Nonadiabatic photodissociation dynamics in small molecules and clusters*

**9.35 – 10.10 D. Neumark (University of California at Berkeley, USA)**  
*Spectroscopy and time-resolved dynamics in clusters*

**10.10 – 10.35 A. I. Chichinin (Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia)**  
*3D velocity mapping: dynamics of the reaction  $O(^1D) + N_2O \rightarrow 2 NO$  photoinitiated in the  $(N_2O)_2$  dimer*

**10.35 – 11.00 M. Ya. Amusia (Hebrew University of Jerusalem, Israel)**  
*Fullerene shell as a resonator and amplifier for processes in endohedral atoms*

**11.00 – 11.20 Coffee Break**

**11.20 – 12.55 Session PMI-5**

**Chairman: T. Stoecklin (Institut des Sciences Moléculaires, Talence, France)**

**11.20 – 11.55 D. A. Varshalovich (Ioffe Institute, St.Petersburg, Russia)**  
*Big-Bang nucleosynthesis and D/H ratio in interstellar molecular clouds*

**11.55 – 12.30 H. Linnartz (University of Leiden, The Netherlands)**

*Laboratory studies of inter- and circumstellar chemistry*

**12.30 – 12.55 D. Ascenzi (University of Trento, Italy)**  
*Chemistry and physics of molecular ions: from plasma systems to astrochemistry*

**12.55 – 13.00 Conference Photo**

**13.00 – 14.30 Lunch**

**14.30 – 16.35 Session CMD-2**

**Chairman: D. A. Varshalovich (Ioffe Institute, St.Petersburg, Russia)**

**14.30 – 14.55 R. Anderson (University of California, Santa Cruz, USA)**  
*Novel applications of Clebsch-Gordan and 3nj- coefficients in molecular physics*

**14.55 – 15.20 D. Sokolovski (Queen's University of Belfast, UK)**  
*Complex angular momentum approach to chemical reactions: some recent developments and applications*

**15.20 – 15.45 A. J. H. M. Meijer (University of Sheffield, UK)**  
*Accelerated DVR methods for use in chemical physics*

**15.45 – 16.10 V. Kokoouline (University of Central Florida, Orlando, USA)**  
*Theoretical treatment of dissociative recombination of small polyatomic ions*

**16.10 – 16.35 C. Zhu (National Chiao Tung University, Hsinchu, Taiwan)**  
*Semiclassical theory for nonadiabatic transition and tunneling*

**16.35 – 16.55 Coffee Break**

**16.55 – 18.35 Session MC-6**

**Chairman: A. K. Belyaev (Herzen University, St.Petersburg, Russia)**

**16.55 – 17.20 R. McCarroll (Université Pierre et Marie Curie, Paris, France)**  
*Gerade-ungerade symmetry breaking in HD*

**17.20 – 17.45 J. Riedel (IAMS, Academia Sinica, Taipei, Taiwan)**  
*Mode specificity in reactions of Cl with CH<sub>2</sub> stretch-excited CH<sub>2</sub>D<sub>2</sub> (v<sub>1</sub>,v<sub>6</sub>=1):  
A pulsed crossed molecular beam imaging study*

**17.45 – 18.10 D. Babikov (Marquette University, Milwaukee, USA)**  
*Quantum Origin of Anomalous Isotope Effect in Ozone Formation*

**18.10 – Concluding Remarks**

**19.00 – 20.30 Dinner**

**20.30 – Concert**

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**August 29, Friday**

**8.00 – 9.00 Breakfast**

**Departure**