MOLIM 2017, Molecules in Motion

International Workshop on Molecular Quantum Dynamics and Kinetics
(Working Group 2 of MOLIM, Time-dependent method developments)

ETH Zürich, Hönggerberg Campus, HCI Building,
Vladimir-Prelog-Weg, Lecture Hall HCI J7

https://molim2017.ethz.ch, http://cost-molim.eu/

Tuesday 18 April through Thursday 20 April 2017

Tuesday, 18 April 2017	
Session 1, Chairperson Martin Quack	
after 11:30	Welcome coffee and sandwich lunch for speakers (in front of Lecture Hall)
12:30 – 12:50	**Martin Quack** *Welcome and Introduction*
12:50 – 13:30	**L1 Bill Poirier** *Exact Quantum Dynamical Treatment of Hydrogen-material Interactions*
13:30 – 14:10	**L2 Jürgen Stohner** *Progress in synthesis, enantio-separation and determination of the absolute configuration of small chiral molecules*
14:10 – 14:50	**L3 Emilio Martínez-Núñez** *Using chemical dynamics simulations to discover reaction mechanisms and solve the kinetics in reactive systems*
14:50 – 15:30	**L4 Thomas Baumert** *Control of bound electrons in molecules with tailored light fields and of free electrons with chiral potentials*
15:30 – 16:00	Coffee Break
Session 2, Chairperson Attila G. Császár	
16:00 – 16:40	**L5 Tamás Szidarovszky** *Laser-induced alignment dynamics of polyatomic molecules*
16:40 – 17:20	**L6 Stuart C. Althorpe** *Quantum statistics + classical dynamics: what is it?*
17:20 – 18:00	**L7 Alberto García-Vela** *Quantum Coherent Control of the Behavior of a Resonance State*
18:00 – 18:40	**L8 Gilberte Chambaud** *Catalytic oxidation reaction on modified graphene surface*
19:00 – 22:00	Conference Dinner and Welcome Dinner

Wednesday, 19 April 2017	
Session 3, Chairperson Sonia Grubišić or Gilberte Chambaud	
08:30 – 09:10	**L9 Edit Mátyus** *Rovibrational Transitions of the Methane-Water Dimer from Intermolecular Quantum Dynamical Computations*
09:10 – 09:50	**L10 Majdi Hochlaf** *Vibrational quantum localization*
09:50 – 10:30	**L11 Lauri Halonen** *Simple chemical processes on water, ice and quartz surfaces*
10:30 – 11:00	Coffee Break
Session 4, Chairperson Jiří Vaníček	
11:00 – 11:40	**L12 Ioannis Thanopulos** *Non-Markovian quantum emitter dynamics in a plasmonic environment*
11:40 – 12:20	**L13 Klaus Braagaard Møller** *Ultrafast electronic and nuclear dynamics in photo-excited transition-metal complexes*
12:20 – 13:00	**L14 Gunnar Nyman** *Classical Wigner model based on a Feynman path open polymer*
13:00 – 14:00	Lunch on Campus
Session 5, Chairperson Bill Poirier	
14:00 – 14:40	**L15 Frédéric Merkt** *High resolution spectroscopy of few electron molecules*
14:40 – 15:20	**L16 Roberto Marquardt** *Full Quantum Calculations of the Diffusion of Particles on Surfaces*
15:20 – 16:00	**L17 Maria Louisa Senent** *Far infrared spectral features of Ethylene Glycol isotopologues*
16:00 – 16:30	Coffee Break
Session 6, Chairperson Frédéric Merkt	
16:30 – 17:10	**L18 Jiří Vaníček** *Geometric integrators of arbitrary order of accuracy for molecular quantum dynamics in electromagnetic fields*
17:10 – 17:50	**L19 Antonio J. C. Varandas** *Reaction dynamics within the Born-Oppenheimer approximation and beyond*
17:50 – 18:30	**L20 Françoise Remacle** *Ultrafast Non Equilibrium Dynamics Induced By Attopulses*
19:00	Dinner (start before 19:00) on Campus
19:30 – 21:00	**Posters and Discussions (near Lecture Hall)**

Thursday, 20 April 2017	
Session 7, Chairperson Roberto Marquardt	
08:30 – 09:10	**L21 Fabien Gatti** *Multi-dimensional quantum mechanical treatment of an electron transfer in plant cryptochrome and to the control of the ring opening in spiropyrane molecules*
09:10 – 09:50	**L22 Nađa Došlić** *Photochemical Study of 1- and 2-Naphthols and their Water Clusters*
09:50 – 10:30	**L23 Niels Engholm Henriksen** *Laser-induced Quantum Control of Molecular Processes*
10:30 – 11:00	Coffee Break
Session 8, Chairperson Ruth Signorell	
11:00 – 11:40	**L24 Rita Prosmiti** *Quantum computations of nanoconfined molecules*
11:40 – 12:20	**L25 Octavio Roncero** *Reactive Collisions at Cold Temperatures of Interstellar Cloulds*
12:20 – 13:00	**L26 Graham Worth** *Quantum molecular dynamics simulations of polyatomic molecules in a manifold of coupled states*
13:00 – 14:00	Lunch on Campus
Session 9, Chairperson Isabelle Kleiner or Jürgen Stohner	
14:00 – 14:40	**L27 Magnus Gustafsson** *Classical dynamics methods for radiative processes in gases: strengths and weaknesses*
14:40 – 15:20	**L28 Ruth Signorell** *Low-energy electron transport in water: Aerosol droplets, molecular clusters, and liquid bulk*
15:20 – 16:00	**L29 Roland Mitric** *Non-adiabatic energy transport dynamics in molecular assemblies and nanostructures*
16:00 – 16:30	Coffee Break
Session 10, Chairperson Sergey Yurchenko or Martin Quack	
16:30 – 17:10	**L30 Christopher J. Stein** *Vibrational Density Matrix Renormalization Group*
17:10 – 17:50	**L31 Leticia González** *Light triggered dynamics in DNA building blocks*
17:50 – 18:30	**L32 Georg Seyfang** *Intramolecular vibrational energy redistribution in HCCCN*
19:00	**Dinner (on Campus, starts before 19:00 and informal Speakers Dinner)**
Friday, 21 April 2017	
Departure after Breakfast	