

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 <i>Welcome and Introduction</i>
12:50 – 13:30	L1 Bill Poirier <i>Exact Quantum Dynamical Treatment of Hydrogen-material Interactions</i>
13:30 – 14:10	L2 Jürgen Stohner <i>Progress in synthesis, enantio-separation and determination of the absolute configuration of small chiral molecules</i>
14:10 – 14:50	L3 Emilio Martínez-Núñez <i>Using chemical dynamics simulations to discover reaction mechanisms and solve the kinetics in reactive systems</i>
14:50 – 15:30	L4 Thomas Baumert <i>Control of bound electrons in molecules with tailored light fields and of free electrons with chiral potentials</i>
15:30 – 16:00	Coffee Break
Session 2, Chairperson Attila G. Császár	
16:00 – 16:40	L5 Tamás Szidarovszky <i>Laser-induced alignment dynamics of polyatomic molecules</i>
16:40 – 17:20	L6 Stuart C. Althorpe <i>Quantum statistics + classical dynamics: what is it?</i>
17:20 – 18:00	L7 Alberto García-Vela <i>Quantum Coherent Control of the Behavior of a Resonance State</i>
18:00 – 18:40	L8 Gilberte Chambaud <i>Catalytic oxidation reaction on modified graphene surface</i>
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 <i>Rovibrational Transitions of the Methane-Water Dimer from Intermolecular Quantum Dynamical Computations</i>
09:10 – 09:50	L10 Majdi Hochlaf <i>Vibrational quantum localization</i>
09:50 – 10:30	L11 Lauri Halonen <i>Simple chemical processes on water, ice and quartz surfaces</i>
10:30 – 11:00	Coffee Break

Session 4, Chairperson Jiří Vaniček

11:00 – 11:40	L12 Ioannis Thanopoulos <i>Non-Markovian quantum emitter dynamics in a plasmonic environment</i>
11:40 – 12:20	L13 Klaus Braagaard Møller <i>Ultrafast electronic and nuclear dynamics in photo-excited transition-metal complexes</i>
12:20 – 13:00	L14 Gunnar Nyman <i>Classical Wigner model based on a Feynman path open polymer</i>
13:00 – 14:00	Lunch on Campus

Session 5, Chairperson Bill Poirier

14:00 – 14:40	L15 Frédéric Merkt <i>High resolution spectroscopy of few electron molecules</i>
14:40 – 15:20	L16 Roberto Marquardt <i>Full Quantum Calculations of the Diffusion of Particles on Surfaces</i>
15:20 – 16:00	L17 Maria Louisa Senent <i>Far infrared spectral features of Ethylene Glycol isotopologues</i>
16:00 – 16:30	Coffee Break

Session 6, Chairperson Frédéric Merkt

16:30 – 17:10	L18 Jiří Vaniček <i>Geometric integrators of arbitrary order of accuracy for molecular quantum dynamics in electromagnetic fields</i>
17:10 – 17:50	L19 Antonio J. C. Varandas <i>Reaction dynamics within the Born-Oppenheimer approximation and beyond</i>
17:50 – 18:30	L20 Françoise Remacle <i>Ultrafast Non Equilibrium Dynamics Induced By Attopulses</i>
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 <i>Multi-dimensional quantum mechanical treatment of an electron transfer in plant cryptochrome and to the control of the ring opening in spiropyrane molecules</i>
09:10 – 09:50	L22 Nađa Došlić <i>Photochemical Study of 1- and 2-Naphthols and their Water Clusters</i>
09:50 – 10:30	L23 Niels Engholm Henriksen <i>Laser-induced Quantum Control of Molecular Processes</i>
10:30 – 11:00	Coffee Break

Session 8, Chairperson Ruth Signorell

11:00 – 11:40	L24 Rita Prosimi <i>Quantum computations of nanoconfined molecules</i>
11:40 – 12:20	L25 Octavio Roncero <i>Reactive Collisions at Cold Temperatures of Interstellar Clouds</i>
12:20 – 13:00	L26 Graham Worth <i>Quantum molecular dynamics simulations of polyatomic molecules in a manifold of coupled states</i>
13:00 – 14:00	Lunch on Campus

Session 9, Chairperson Isabelle Kleiner or Jürgen Stohner

14:00 – 14:40	L27 Magnus Gustafsson <i>Classical dynamics methods for radiative processes in gases: strengths and weaknesses</i>
14:40 – 15:20	L28 Ruth Signorell <i>Low-energy electron transport in water: Aerosol droplets, molecular clusters, and liquid bulk</i>
15:20 – 16:00	L29 Roland Mitric <i>Non-adiabatic energy transport dynamics in molecular assemblies and nanostructures</i>
16:00 – 16:30	Coffee Break

Session 10, Chairperson Sergey Yurchenko or Martin Quack

16:30 – 17:10	L30 Christopher J. Stein <i>Vibrational Density Matrix Renormalization Group</i>
17:10 – 17:50	L31 Leticia González <i>Light triggered dynamics in DNA building blocks</i>
17:50 – 18:30	L32 Georg Seyfang <i>Intramolecular vibrational energy redistribution in HCCCN</i>
19:00	Dinner (on Campus, starts before 19:00 and informal Speakers Dinner)

Friday, 21 April 2017**Departure after Breakfast**