# MOLIM 2018, Molecules in Motion

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

**Academy of Athens, East Hall, Athens, Greece**

https://molim2018.ethz.ch, http://cost-molim.eu/

**Monday 8 October to Wednesday 10 October 2018**

| **Monday, 8 October 2018** | |
|---|---|
| 09:00 – 09:45 | **Welcome Coffee** |
| 09:45 – 10:15 | **Welcome Session: Chairperson Ioannis Thanopulos**<br>**Speakers Attila G. Császár, Martin Quack, Ioannis Thanopulos, Constantinos G. Vayenas, Anthony Kounadis, President of the Academy of Athens** |
| **Session 1, Chairperson Martin Quack** | |
| 10:15 – 11:00 | **L1 Hans Jakob Wörner**<br>*Probing chiral dynamics on femtosecond and attosecond time scales* |
| 11:00 – 11:45 | **L2 Jürgen Stohner**<br>*Small Chiral Molecules for the Investigation of Chiroptical Properties* |
| 11:45 – 12:30 | **L3 Lionel Poisson**<br>*Ultrafast relaxation dynamics of isolated diarylethenes* |
| 12:30 – 13:15 | **L4 Majed Chergui**<br>*Electronic and nuclear dynamics in molecular systems* |
| 13:15 – 15:00 | Lunch Break and Posters |
| **Session 2, Chairperson Ioannis Thanopulos** | |
| 15:00 – 15:45 | **L5 Stefan Willitsch**<br>*Studies of chemical kinetics and dynamics with cold and controlled molecules* |
| 15:45 – 16:30 | **L6 Johannes Deiglmayr**<br>*Cold ion-molecule chemistry within the orbit of a Rydberg electron* |
| 16:30 – 17:00 | Coffee Break |
| **Session 3, Chairperson Attila G. Császár** | |
| 17:00 – 17:45 | **L7 Nicolina Pop**<br>*Dissociative recombination and vibrational excitation of molecular cations with electrons: Application to $H_2^+$, $HD^+$, $H_3^+$ and $BeT^+$* |
| 17:45 – 18:30 | **L8 Octavio Roncero**<br>*Low temperature reactive collisions of polyatomic molecules: looking for an appropriate method including quantum effects* |
| **Session 4, Public Lecture, Chairperson Martin Quack** | |
| 18:45 – 19:45 | **L9 Jürgen Troe**<br>*Electron attachment and detachment processes: practical and theoretical aspects* |

| Tuesday, 9 October 2018 | |
|---|---|
| **Session 5, Chairperson Stefan Willitsch** | |
| 09:00 – 09:45 | **L10 Attila G. Császár**<br>*To tunnel or not to tunnel* |
| 09:45 – 10:30 | **L11 Jeremy O. Richardson**<br>*Ring-polymer instanton theory: a practical ab initio approach for simulating tunneling* |
| 10:30 – 11:00 | Coffee Break |
| **Session 6, Chairperson Rita Prosmiti** | |
| 11:00 – 11:45 | **L12 Constantinos G. Vayenas**<br>*Electrons, positrons and neutrinos in rotational motion* |
| 11:45 – 12:30 | **L13 Edit Mátyus**<br>*Theoretical developments for precision spectroscopy* |
| 12:30 – 13:15 | **L14 Lauri Halonen**<br>*Recent advances in molecular dynamics simulations of a variety of formic acid systems* |
| 13:15 – 15:00 | Lunch Break and Posters |
| **Session 7, Chairperson Majdi Hochlaf** | |
| 15:00 – 15:45 | **L15 Sonja Grubišić**<br>*Parameterization and validation of an accurate force-field for molecular dynamics simulations of organic and biomolecular systems* |
| 15:45 – 16:30 | **L16 Rita Prosmiti**<br>*Assessing guest-host interactions in clathrate hydrate systems* |
| 16:30 – 17:15 | **L17 Niels Engholm Henriksen**<br>*Laser-induced Quantum Control of Molecular Processes* |
| 17:15 – 18:00 | **L18 Csaba Fábri**<br>*Coherent inhibition and enhancement of tunneling in ammonia isotopomers* |
| 20:00 | Conference Dinner |

| Wednesday, 10 October 2018 | |
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| **Session 8, Chairperson Constantinos G. Vayenas** | |
| 09:00 – 09:45 | **L19 Nimrod Moiseyev**<br>*Quantum effects in cold molecular collisions from spatial polarization of electronic wave function* |
| 09:45 – 10:30 | **L20 Zlatko Bačić**<br>*Quantum Dynamics of Light Molecules Inside Fullerene Cages: Translation-Rotation Eigenstates, Spectroscopy, and Symmetry Breaking* |
| 10:30 – 11:00 | Coffee Break |
| **Session 9, Chairperson Zlatko Bačić** | |
| 11:00 – 11:45 | **L21 Markus Koch**<br>*Ultrafast photoexcitation dynamics of atoms and molecules inside a quantum solvent* |
| 11:45 – 12:30 | **L22 Nađa Došlić**<br>*Assessing the Performance of Surface Hopping Methods* |
| 12:30 – 13:15 | **L23 Jiří Vaníček**<br>*On-the-fly ab initio semiclassical evaluation of time-resolved electronic spectra* |
| 13:15 – 15:00 | Lunch Break |
| **Session 10, Chairperson Nađa Došlić** | |
| 15:00 – 15:45 | **L24 Majdi Hochlaf**<br>*Quantum tunneling dynamical behaviour on weakly bound complexes* |
| 15:45 – 16:30 | **L25 Felix Iacob**<br>*Analytic formula to fit ab initio calculated potential energy curves* |
| 16:30 – 17:00 | Coffee Break |
| **Session 11, Chairperson Ioannis Thanopulos** | |
| 17:00 – 17:45 | **L26 Kaido Sillar**<br>*The importance of quantum effects in adsorption. Ab initio prediction of adsorption isotherms for small molecules in metal-organic frameworks (MOFs)* |
| 17:45 – 18:30 | **L27 Liudmil Antonov**<br>*Switching the proton transfer mechanism in 10-hydroxybenzo[h]quinolines by structural modifications* |
| 18:30 – 19:15 | **L28 Fabien Gatti**<br>*Joined experimental/theoretical study of the control of the ring opening in spiropyrane molecules: role of the quantum interferences* |
| 19:15 – 19:30 | **L29 Short Surprise Lecture** |
| 19:30 – 19:45 | **Closing Remarks by Martin Quack** |
| 20:00 | Informal Dinner |