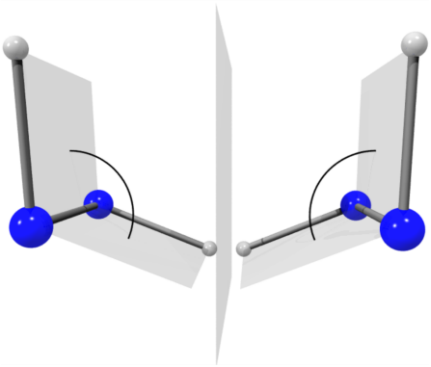

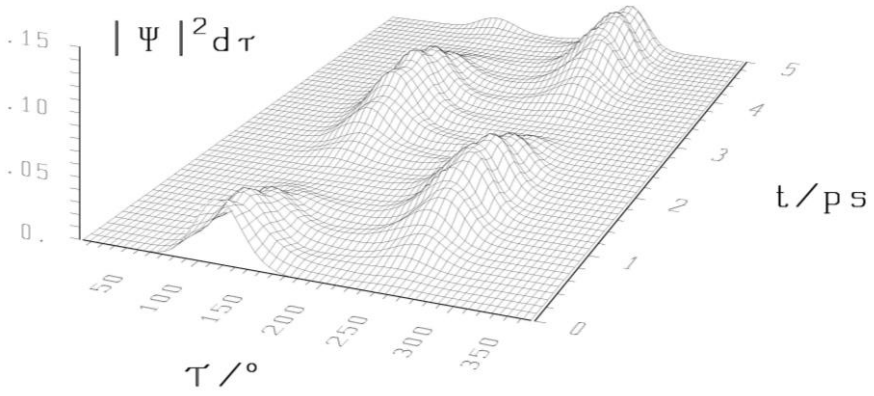

Molecules in Motion

International Workshop of working Group 2 of MOLIM and Leopoldina Symposium on Molecular Quantum Dynamics and Kinetics,

Athens, Greece, with Academy Athens and Berlin Brandenburg Academy of Sciences BBAW

8 – 10 October 2018

First Announcement (Draft)

The 2018 meeting venue is in Athens, the capital of Greece, easily reached by air for all participants from outside Greece and otherwise locally for the Greek participants. The scientific sessions will be held in the wonderful location of the Academy of Athens building. **They will start in the morning of Monday 8 October 2018 (arrival on the 7th) and end in the afternoon or evening of Wednesday 10 October 2018. Accommodation is arranged individually by the participants and hotels with special rates for the meeting are announced on the website. Please reserve hotel now at your earliest convenience and let us know about your interest to participate and updated contact information**.

Quantum dynamical phenomena are of importance in a wide range of fields in the physical, chemical, biological and computational sciences. The present Workshop is highly cross-disciplinary. It encompasses both theoretical and experimental work on Molecular Quantum Dynamics and Kinetics

in the gas and condensed phases, in general, including biological systems, chemical reactions, tunneling and energy flow phenomena in molecules, solids and liquids. The relation to classical dynamical modelling and its limitations will be discussed as well. A strong interaction between experiment and theory is desired. We encourage contributions on all time dependent phenomena where molecular quantum dynamics plays an important role, including inorganic, organic and organometallic reactions, tunneling processes in clusters and nanoparticles, enzyme-catalyzed reactions, and some non-traditional emerging areas, this list being exemplary and non-exhaustive.

The scientific program will include the following topics, among others:

- Classical and Quantum Molecular Dynamics for Modelling Chemical Reactions and Processes
- Molecular Quantum Dynamics in the primary processes of energy flow
- Molecular Quantum Dynamics in isomerization processes and in general unimolecular and bimolecular reactions and in catalysis
- Molecular Quantum Dynamics of stereomutation and parity violation in chiral molecules
- Molecular Quantum Dynamics and Classical Dynamical Modelling in biomolecular systems
- Molecular Quantum Dynamics for developments in quantum technology
- Quantum dynamics of electron motion in molecules on the attosecond time scale
- Tunneling in hydrogen bonded systems
- Kinetic isotope effects
- Vibrational rotational tunneling dynamics in molecules and clusters
- Molecular Quantum Dynamics in diffusion phenomena
- Electron transport in nanosystems
- Advances in theoretical and computational methods and software for modelling chemical reaction dynamics.

Executive Committee (co-chairs)

Frédéric Merkt (ML, ETH Zurich, Leopoldina DCF Swiss Chemical Society and BBAW)
Martin Quack (leader of WG2,ML, ETH Zurich, Leopoldina and BBAW)
Ioannis Thanopulos (TEI of Western Greece and responsible local organizer)
Constantinos G. Vayenas (University of Patras and Academy of Athens)

Further information may be obtained by contacting Ioannis Thanopulos (ithano@eie.gr)

Martin Quack (Martin@Quack.CH) or the other members of the executive committee.

Save the dates now and provide updated contact information to us if you are interested. Further information will be communicated with the second announcement.

This workshop of working group 2 of the COST action MOLIM is held jointly as Leopoldina Symposium and with the BBAW, the Academy of Athens and the Swiss Chemical Society