Master Thesis

# Simulation of molecular wave packets and comparison to time-resolved studies

In the course of this joint master thesis, a collaboration between the groups of Prof. Koch and Prof. Hauser, the highly unusual behavior of indium dimers ($In_2$) in droplets of superfluid helium is studied in theory and experiment (Fig. 1).

While being mostly concerned with the computational aspects of molecular dynamics simulations and electronic structure theory, the interested student will also be exposed to the most recent experimental data regarding the highly topical problem of time-resolved wave packet excitation in a molecular quantum system. Vibrational wave packets, triggered through ultra-short laser pulses, can be thought of as localized nuclear wavefunctions travelling on the molecular potential energy surface (PES). In particularly "exciting" cases – from a scientific point of view – the motion of such a wave packet might involve more than one PES. In other words, electronic and vibrational degrees of freedom are coupled in these systems.

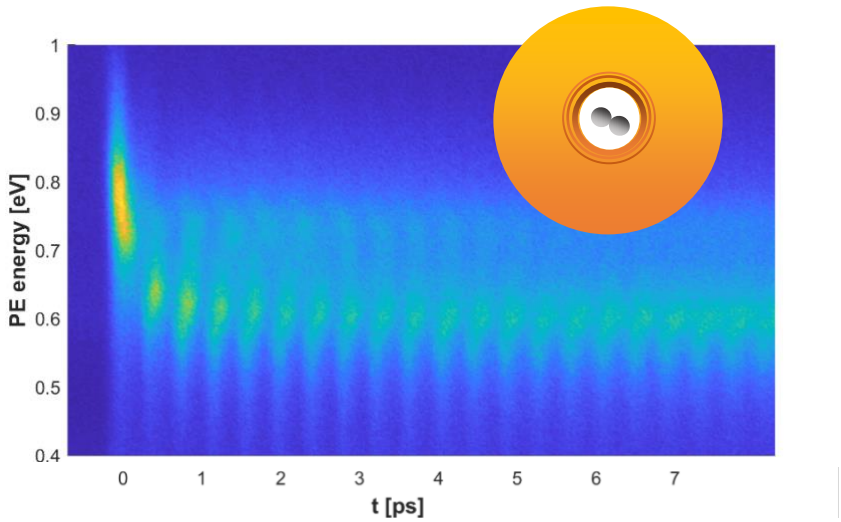


Fig. 1: Vibrational wavepacket dynamics of $In_2$ molecules inside He nanodroplets, measured with femtosecond time-resolved photoelectron spectroscopy. The quantum solvent influence on the coherent nuclear motion is surprisingly low and requires further exploration. For more information see our latest paper (Phys Rev Lett **124**, 115301) or recent press coverage: APS Physics, Der Standard.

The interested candidate will be performing calculations of electronically excited states, using multi-reference configuration interaction and many-body perturbation theory, mostly through the MOLPRO suite of programs. This way, the candidate will get exposed to the latest tools of modern computational chemistry and molecular physics. For the 'grand finale', the investigation of system dynamics, independent and creative code development in Python or MATLAB will be highly appreciated. An extension for the eager student, and particularly useful for ongoing research, could be the introduction of quantum effects caused by the solvent, e.g. through phenomenological approaches or methods based on helium density functional theory.

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