THEODORE MAIMAN SEMINARS
on physics 2019

IMPRS APS | LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN | OSA Student Chapter Munich | MPQ

Nuclear-driven Electronic Coherences in Polyatomic Molecules

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6th of June 2019

11:30 h, Lecture Hall of Max Planck Institute of Quantum Optics

https://www.attoworld.de/

http://www2.mpq.mpg.de/APS/

https://www.en.physik.uni-muenchen.de/

Electronic coherences in molecules has emerged as a 'grand challenge' in molecular sciences due to the role that electronic correlations and dynamics play in structure and bonding. In the field of attosecond science, electronic coherences can be prepared by attosecond pulses, producing purely electronic wavepackets which persist while the atoms are 'frozen' (i.e. a few femtoseconds). Once the atoms unavoidably start to move, the wavepacket could dephase and the electronic coherence would be lost. However, some suggested that nuclear motion could modify or even induce electronic coherences.

Prior theoretical investigations of nuclear-driven electronic coherences by Mukamel, Santra, Levine and others were all based on Molecular Frame (MF) calculations. These made use of coherent X-ray techniques. We make a very simple but important point. For gas phase molecules, the full Hamiltonian necessarily includes the rotational degrees of freedom. These exist only in the Lab Frame (LF), not in the MF. This leads to significant new insights and opportunities, as well as dramatic technical simplifications, for the probing of ultrafast electronic coherences in gas phase molecules. Here we present our study of electronic coherences in a polyatomic molecule (NH_3) driven by nuclear dynamics.