CFEL SCIENCE

# SEMINAR

***22nd October 2014 - 2:00 p.m.***

CFEL-bldg. 99, seminar room IV


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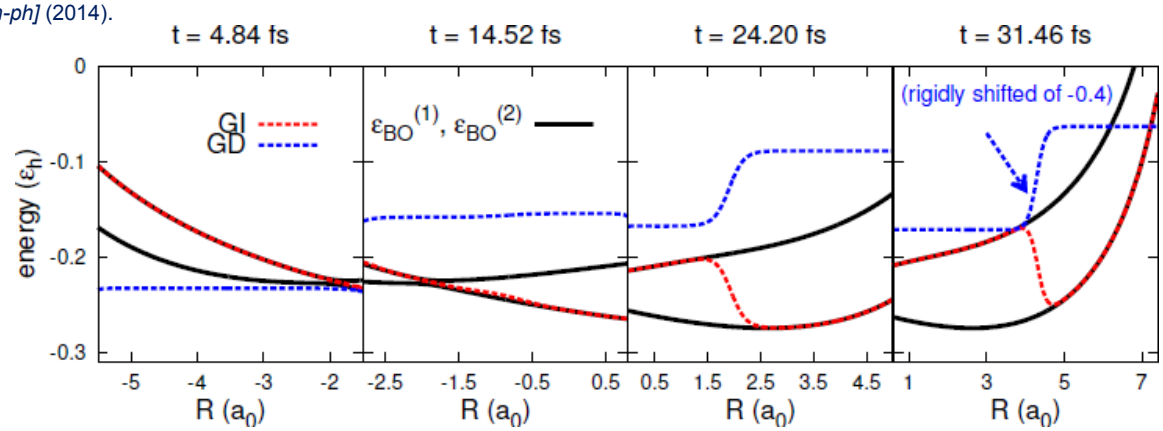
## Evolving classical nuclei on a single time-dependent potential in electronic non-adiabatic processes

The Born-Oppenheimer (BO), or adiabatic, approximation is among the most fundamental approximations in Condensed Matter Physics and Theoretical Chemistry. The theoretical framework provided by the adiabatic treatment of the coupled electron-nuclear dynamics in molecular systems helps us in visualizing dynamical processes as a set of nuclei moving on a *single* potential energy surface that represents the effect of the electrons in a given eigenstate. Yet, this is an approximation, and many interesting phenomena, such as vision, charge separation in organic photovoltaic materials or Joule heating in molecular junctions, take place in conditions beyond its range of validity. Nevertheless, the basic construct of the adiabatic treatment, the BO potential energy surfaces, is employed to describe non-adiabatic processes and the full problem is represented in terms of adiabatic states and transitions among them in regions of strong non-adiabatic coupling. But the concept of *single* potential energy is lost.

The alternative point of view [1] arising in the framework of the exact factorization of the electron-nuclear wave function [2] will be presented. A *single*, time-dependent, potential energy (shown in the figure) provides the force [3] driving the nuclear motion, also in non-adiabatic situations, and is adopted as starting point for the development of approximations to the quantum mechanical formulation of the dynamical problem towards the derivation of a quantum-classical [4] method, that combines the quantum treatment of electronic dynamics with the classical nuclear motion.


[1] A. Abedi, F. Agostini, Y. Suzuki and E. K. U. Gross, *Phys. Rev. Lett.* **110** 263001 (2013)
[2] A. Abedi, N. T. Maitra and E. K. U. Gross, *Phys. Rev. Lett.* **105** 123002 (2010); *J. Chem. Phys.***137** 22A530 (2012)
[3] F. Agostini, A. Abedi, Y. Suzuki and E.K.U. Gross, *Mol. Phys.* **111** 3625 (2013); F. Agostini, A. Abedi, Y. Suzuki, S. K. Min, N. T. Maitra and E. K. U. Gross, *arXiv:1406.4667 [physics.chem-ph]* (2014).
[4] A. Abedi, F. Agostini and E. K. U. Gross, *Europhys. Lett.* **106** 33001 (2014); F. Agostini, A. Abedi and E. K. U. Gross, *arXiv:1406.5126 [physics.chem-ph]* (2014).


Host: Robin Santra – Theory Division