

MAR15-2014-020843

Abstract for an Invited Paper
for the MAR15 Meeting of
the American Physical Society

Combining Molecular Dynamics and Density Functional Theory

EFTHIMIOS KAXIRAS¹, Harvard University

The time evolution of a system consisting of electrons and ions is often treated in the Born-Oppenheimer approximation, with electrons in their instantaneous ground state. This approach cannot capture many interesting processes that involve excitation of electrons and its effects on the coupled electron-ion dynamics. The time scale needed to accurately resolve the evolution of electron dynamics is atto-seconds. This poses a challenge to the simulation of important chemical processes that typically take place on time scales of pico-seconds and beyond, such as reactions at surfaces and charge transport in macromolecules. We will present a methodology based on time-dependent density functional theory for electrons, and classical (Ehrenfest) dynamics for the ions, that successfully captures such processes. We will give a review of key features of the method and several applications. These illustrate how the atomic and electronic structure evolution unravels the elementary steps that constitute a chemical reaction.

¹in collaboration with: G. Kolesov, D. Vinichenko, G. Tritsarlis, C.M. Friend, Departments of Physics and of Chemistry and Chemical Biology