Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Excited statemolecular dynamics in polarizable environments JOSIAH BJORGAARD, KIRILL VELIZHANIN, SERGEI TRETIAK, Los Alamos Natl Lab — Many experimental measurements of molecular systems are performed in solutions, where the solvent forms a polarizable environment around the solute. The effects of this on important molecular processes such as vibrational relaxation or chemical reaction are often significant. In this talk, recent developements in efficiently simulating solvation effects in quantum molecular dynamics for excited electronic states are presented. These methods fall into the category of multiscale quantum mechanics/continuum methods. To adequately describe polarization of the solvent by the electronically excited states of molecules, state-specific methods have been pursued which allow for polarization effects based on the excited state charge density. Variational formulations of solvation models in linear response time-dependent density functional theory are described which allow analytical gradients and efficient molecular dynamics propagation. Further, recently developed simulation methods for nonequilibrium solvation effects are demonstrated.

Josiah Bjorgaard
Los Alamos Natl Lab

Date submitted: 02 Dec 2015 Electronic form version 1.4