

## Plenary talks (PV)

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**Plenary Talk (SAMOP)**      PV XIII   Wed 9:15   HSZ 02  
**Dynamics of Ground and Excited Electronic States from First Principles** — ●TODD J. MARTINEZ — Department of Chemistry  
Stanford University, Stanford, CA

The ab initio multiple spawning (AIMS) method is now a quite mature method to describe dynamics including quantum effects of both the electrons and the nuclei from first principles. AIMS is specifically focused on the description of nonadiabatic effects, i.e. breakdown of the Born-Oppenheimer approximation. We discuss the role of conical intersections in excited state nonadiabatic dynamics, as determined

from AIMS simulations and validation to experiments. The role of condensed phase environments (solvent and/or protein) is discussed. We highlight the new ability, by leveraging consumer videogame technology (graphical processing units or GPUs), to carry out fully first principles dynamics calculations of solvated proteins and we use this to investigate the validity of mixed quantum mechanical/molecular mechanical (QM/MM) descriptions. A number of applications are used to demonstrate the diversity of behaviors in excited state dynamics, ranging from photoinduced cis-trans isomerization to excited state proton transfer.