

Investigating Photochemistry: Classical Trajectories that Simulate Quantum Excitations

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Room 8335

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Addressing the challenge of designing efficient organic photovoltaics requires theoretical methods that accurately described the coupling between electronic state transitions and nuclear dynamics, and that are computationally efficient for complex many-dimensional systems. In this talk, we introduce a recently developed path-integral based model dynamics, Mapping-Variable Ring Polymer Molecular Dynamics (MV-RPMD) that employs classical molecular dynamics trajectories to capture quantum dynamic effects in photochemical processes. This is achieved by deriving an exact path-integral representation of the canonical partition function for an N-level system using classically analogous, Cartesian phase-space variables to represent both discrete electronic states and nuclear degrees of freedom [1,2]. We demonstrate the numerical accuracy of our method in simulations of model systems that exhibit dynamics in both the adiabatic and nonadiabatic limits. Further, we derive good electronic state population estimators that provide accurate, instantaneous state information necessary for the detailed mechanistic analysis of photochemical reactions [3].

[1] N. Ananth, *J. Chem. Phys.*, 139, 124102 (2013)

[2] N. Ananth and T. F. Miller, III, *J. Chem. Phys.*, 133, 234103 (2010)

[3] J. R. Duke and N. Ananth, Manuscript in Preparation

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