Path-integral Based Approach to Nonadiabatic Processes in Chemistry

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Addressing the challenge of designing photovoltaic and molecular electronic materials requires theoretical methods that accurately describe coupling between electronic state transitions and nuclear dynamics, and for which the computational effort scales well with system size. In this talk, we introduce a recently developed path-integral method, Mapping-Variable Ring Polymer Molecular Dynamics (MV-RPMD), that employs continuous Cartesian variables to represent both electronic and nuclear degrees of freedom [1,2]. We discuss the scope and accuracy of this method in the context of condensed-phase electron transfer processes [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. Duke and N. Ananth, *Manuscript in Preparation*