New Surface Hopping Methods for Simulating Nonadiabatic Dynamics in Molecules and Clusters

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In this talk, we discuss the quantum-classical dynamics of nonadiabatic transitions from the perspective of trajectory surface hopping. Our approach builds on the semiclassical Liouville formalism for describing the dynamics of generalized phase space distributions representing elements of the electronic density matrix. The result is a new method for trajectory surface hopping "by consensus", where individual trajectories interact and influence each other in a way that captures the underlying features of exact quantum dynamics. We describe modifications to the existing trajectory surface hopping method of Fewest Switches Surface Hopping (FSSH) to incorporate the insights gained from our consensus formalism while retaining the numerical advantages of FSSH. Finally, we describe applications to electronic nonadiabatic dynamics and vibrational predissociation of clusters.

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