

Title: Libra: A Modular Toolbox for Simulating Nonadiabatic Molecular Dynamics.

Abstract:

Rational design of highly-efficient solar energy conversion materials relies on the fundamental understanding of the photoexcited states dynamics, including charge transfer and energy relaxation, photoisomerization. To understand the mechanisms of these processes at the atomistic level, efficient approaches for simulating coupled electronic-nuclear evolution are necessary. Specifically, quantum-classical nonadiabatic molecular dynamics (NA-MD) methods are of great interest. Numerous techniques for NA-MD simulations are proposed yearly.

To facilitate the development, testing, and benchmarking of the novel and existing NA-MD methods, we have developed an extensive library (Libra) of classical and quantum dynamical modules. The core library is interfaced with the third-party packages, making it useful for applied studies as well. My presentation will focus on the latest methodological and practical developments within the Libra code and its derivatives. The capabilities of the codes making them suitable for the methodology development and practical applications will be showcased on examples of model and atomistic simulations.