Coupling Advanced Sampling and Quantum Simulation Methods

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Abstract:
Discovery and design of materials and molecules require the ability to compute multiple properties and to carry out simulations at different length and time scales. We will present recent algorithmic developments aimed at coupling advanced sampling methods with first principles molecular dynamics and the latter with many body perturbation theory calculations. In particular we will discuss coupling between the following codes, developed within the MICCoM center (http://miccom-center.org/): SSAGES (http://miccomcodes.org/), Qbox (http://qboxcode.org/) and WEST (http://www.west-code.org/) and their use on commodity clusters and high performance architectures.