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Embedding quantum-mechanics in an interatomic potential simulation using local energies NOAM BERNSTEIN, Naval Research Laboratory, GABOR CSANYI, University of Cambridge — Atomistic simulations that use quantum-mechanical total-energy models provide high accuracy and reliability at the price of computational expense. Classical approximations such as interatomic potentials are much faster, but less transferable. We couple the two approaches concurrently, to describe part of the system quantum-mechanically and part with interatomic potentials, using a weighted sum of atomic energies. This enables us to compute a *well defined total energy* for the hybrid system with small and controllable errors caused by the boundaries of the QM region. Using tight-binding as a model quantum-mechanical method, we can efficiently evaluate the derivatives of the total energy, including the effects of charge self-consistency, enabling an energy conserving molecular dynamics simulation for a fixed QM region. We show that a localized quantum-mechanical atomic energy can be defined, and that this energy is physically meaningful. We present tests of the method, and discuss convergence with respect to various method parameters, and the effects of moving the QM region during the dynamics.

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