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Gutzwiller quantum molecular dynamics simulations of Anderson impurity model[1] JUN LIU, University of Virginia, KIPTON BARROS, JOEL KRESS, Los Alamos National Laboratory, CRISTIAN BATISTA, University of Tennessee, GABRIEL KOTLIAR, Rutgers University, GIA-WEI CHERN, University of Virginia — Molecular dynamics (MD) simulations are crucial to modern computational physics, chemistry, and materials science. We present a formulation of tight-binding quantum molecular dynamics that includes electron correlation effects via the Gutzwiller method. In contrast to the conventional mean-field treatment of the intra-atomic Coulomb repulsion, the Gutzwiller approach captures the crucial correlation effects such as electron localization transition. We perform Gutzwiller quantum MD simulations on the Anderson impurity model and investigate how strong electron correlation affects the structural and dynamical properties of the atoms.

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