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Dynamical simulations of strongly correlated electron materials JOEL KRESS, KIPTON BARROS, CRISTIAN BATISTA, Los Alamos National Laboratory, GIA-WEI CHERN, University of Virginia, GABRIEL KOTLIAR, Rutgers University — We present a formulation of quantum molecular dynamics that includes electron correlation effects via the Gutzwiller method. Our new scheme enables the study of the dynamical behavior of atoms and molecules with strong electron interactions. The Gutzwiller approach goes beyond the conventional mean-field treatment of the intra-atomic electron repulsion and captures crucial correlation effects such as band narrowing and electron localization. We use Gutzwiller quantum molecular dynamics to investigate the Mott transition in the liquid phase of a single-band metal and uncover intriguing structural and transport properties of the atoms.

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