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Mott metal-insulator transition in a metallic liquid – Gutzwiller molecular dynamics simulations KIPTON BARROS, GIA-WEI CHERN, CRISTIAN D. BATISTA, JOEL D. KRESS, Los Alamos National Laboratory, GABRIEL KOTLIAR, Rutgers University — Molecular dynamics (MD) simulations are crucial to modern computational physics, chemistry, and materials science, especially when combined with potentials derived from density-functional theory. However, even in state of the art MD codes, the on-site Coulomb repulsion is only treated at the self-consistent Hartree-Fock level. This standard approximation may miss important effects due to electron correlations. The Gutzwiller variational method captures essential correlated-electron physics yet is much faster than, e.g., the dynamical-mean field theory approach. We present our efficient Gutzwiller-MD implementation. With it, we investigate the Mott metal-insulator transition in a metallic fluid and uncover several surprising static and dynamic properties of this system.

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