# Molecular Dynamics for Strongly Correlated Electron Systems

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We design a quantum molecular dynamics method for strongly correlated electron metals. The strong electronic correlation effects are treated within a real-space version of the Gutzwiller variational approximation (GA), which is suitable for the inhomogeneity inherent in quantum molecular dynamics (MD) simulations. We also propose an efficient algorithm based on the second-moment approximation to the electronic density of states for the search of the optimal variation parameters, from which the effective renormalized interatomic MD potentials are fully determined. By considering a minimal one-correlated-orbital Anderson many-particle model based on tight-binding hopping integrals, this fast GA-MD method is benchmarked against the exact diagonalization solution for the GA variational parameters. The efficiency and accuracy are illustrated via simulated annealing (infinitely damped) MD simulations. This novel method will open up an unprecedented opportunity enabling large-scale quantum MD simulations of strongly correlated electronic materials.