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Excited State Quantum-Classical Molecular Dynamics[1] PREDRAG KRSTIC, ROBERT HARRISON, BOBBY SUMPTER, Oak Ridge National Laboratory — The development of a new theoretical, algorithmic, and computational framework is reported describing the corresponding excited state many-body dynamics by applying multiphysics described by classical equations of motion for nuclei and Hartree-Fock/Multi-Configuration Hartree-Fock and multiresolution techniques for solving the quantum part of the problem (i.e. the motion of the electrons). We primarily have in mind reactive and electron-transition dynamics which involves molecular clusters, containing hundreds of atoms, perturbed by a slow ionic/atomic/molecular projectile, with possible applications in plasma-surface interactions, cluster physics, chemistry and biotechnology. The validation of the developed technique is performed at three-body systems. Application to the transition dynamics in small carbon clusters and hydrocarbons perturbed by slow carbon ions resolves some long-standing issues in the ion-surface interactions in fusion tokamaks.

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