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**Large-Scale Reactive Simulations of Materials in Extreme Conditions** ANDRES JARAMILLO-BOTERO, WILLIAM GODDARD, California Institute of Technology, MSC TEAM — First-principles quantum mechanics methods are inadequate for accurately describing the effects of thermal, mechanical, chemical or radiation excitations that may occur in materials operating under extreme conditions, or impractical to use due to the prohibitive scaling cost of propagating the total Schrodinger equation for a large set of atoms. In the regime of a high number of electronic excitations, the electronic portion of the wave function contains contributions from many stationary states, and the Born-Oppenheimer approximation breaks down. We have been developing a mixed quantum-classical dynamics approach, called the Electron Force Field (eFF), to simulate the non-adiabatic dynamics of materials in extreme conditions. We have demonstrated its application to describe the: thermodynamics of dense hydrogen over 0-100,000 Kelvin; real-time dynamics of Auger fragmentation of diamond nano particles; transient electronic effects in high-strain rate silicon fracture; Coulomb explosion of carbon clusters; dynamics of cascaded valence ionizations in shocked hydrocarbons; and the dynamics of hypervelocity impact of materials. Here, we summarize our recent progress in the theory and application of eFF for modeling and simulation of materials in extreme conditions.

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