

Abstract Submitted
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Tight binding multi-scale simulations of detonating energetic materials EVAN REED, Lawrence Livermore National Laboratory, RIAD MANAA, LAURENCE FRIED — We present density-functional tight-binding (DFTB) molecular dynamics simulations of shock and detonation waves propagating through a series of explosives ranging from insensitive TATB to sensitive hydrogen azide and identify key differences in behavior. The simulations are performed using the Multi-Scale Shock Method (MSST) which we have extended to maintain thermodynamic equilibrium between electrons and ions to correctly treat electronic heat capacity. This work was performed in part under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Evan Reed
Lawrence Livermore National Laboratory

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