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Tight binding multi-scale simulations of detonating energetic materials[1] EVAN REED, Lawrence Livermore National Laboratory, M. 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.

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