Multi-Scale Modeling of Crystalline Energetic Materials

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ABSTRACT

The large discrepancy in length and times at which characteristic processes of energetic materials are of relevance pose a challenge for current simulation techniques. From anisotropic properties which can be modeled at equilibrium, the typical applications of these systems include processes which include shock compression and vibrational coupling to reaction coordinates to heat transfer and the propagation of defects.

We present a systematic study of crystalline energetic materials of different sensitivity and analyze its properties at different theoretical levels. Information like equilibrium structures, vibrational frequencies, conformational rearrangement and mechanical properties like stiffness and elastic properties can be calculated within the density functional theory (DFT) with different approximations. Dynamical properties, which are obtained by computations at finite temperatures can be obtained by atomistic force field based Newtonian dynamics, from here other macroscopic properties are extracted. Current advances in the area as well as the limitations and failures of each methodology are discussed.