

Abstract Submitted  
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**Coarse gaining of molecular crystals: limitations imposed by molecular flexibility**<sup>1</sup> CATALIN PICU, ANIRBAN PAL, Rensselaer Polytechnic Institute — Molecular crystals include molecular electronics, energetic materials, pharmaceuticals and some food components. In many of these applications the small scale mechanical behavior of the crystal is important such as for example in energetic materials where detonation is induced by the formation of hot spots which are induced thermomechanically, and in pharmaceuticals where phase stability is critical for the biochemical activity of the drug. Accurate modeling of these processes requires resolving the atomistic scale details of the material. However, the cost of these models is very large due to the complexity of the molecules forming the crystal, and some form of coarse graining is necessary. In this study we identify the limitations imposed by the need to accurately capture molecular flexibility on the development of coarse grained models for the energetic molecular crystal RDX. We define guidelines for the definition of coarse grained models that target elastic and plastic crystal scale properties such as elastic constants, thermal expansion, compressibility, the critical stress for the motion of dislocations (Peierls stress) and the stacking fault energy

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