# A mesoscopic constitutive law for an energetic molecular crystal fully informed by molecular dynamics calculations

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*A mesoscopic modeling of 1,3,5-triamino-2,4,6-trinitrobenzene, a very anisotropic energetic molecular crystal, is proposed and validated on MD simulations. The two dominant deformation modes observed at nanometric scale and limited stress (less than one GPa) are a buckling instability and a non-symmorphic twinning (irreversible) transformation. A thermodynamically consistent continuum model is detailed, with a non-linear elasticity in pressure constructed to reproduce a cold equation of state. The twinning-buckling phase transition observed in MD is modeled by using a Phase-Field by Reaction-Pathway (PFRP) formalism. To validate the present constitutive law, we study the response of the single crystal under constant strain-rate uniaxial compressions for various directions in the basal plane and present one to one comparisons between both techniques. Finally, an upscale is performed and simulations using the mesoscopic constitutive law are presented for time and space scales non reachable in MD.*