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First-principles investigation of reactive molecular dynamics in detonating TATB IVAN OLEYNIK, AARON LANDERVILLE, University of South Florida, CARTER WHITE, Naval Research Laboratory — TATB is a highly insensitive energetic material (EM) with a unique planar structure similar to that of graphene. Though hydrostatic compression studies have been performed, little is known about the reasons for the high degree of insensitivity that makes TATB an ideal EM for many important military applications. To elucidate the factors responsible for its high insensitivity, we performed first-principles molecular dynamics simulations of TATB bimolecular collisions at different velocities for various crystallographic orientations. We determine threshold collision velocities for each orientation and discuss steric properties of the bulk crystal as they relate to the inferred anisotropic sensitivities. We also investigate the role of bond dissociation energies in the insensitivity of TATB, and discuss the possible contributions of in-plane hydrogen bonding and van-der-Waals forces.

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