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Physical and chemical properties of the new energetic material Si-PETN YOU LIN, AARON LANDERVILLE, IVAN OLEYNIK, Department of Physics, University of South Florida, CARTER WHITE, Naval Research Laboratory — A new energetic material Si-PETN, having a structure similar to that of PETN, has recently been synthesized (T.M. Klapötke, *et al.*, J. Am. Chem. Soc. 129, 6908 (2007)) and shown to exhibit extreme sensitivity that has precluded investigation of its physical and chemical properties by experiment. Although it is highly unlikely that Si-PETN will be used as munition due to its high sensitivity, it could provide valuable information about the nature of sensitivity in energetic materials. Due to its inherent instability, the equation of state (EOS) for Si-PETN is currently unknown. First-principles van-der-Waals density functional theory was used to obtain the EOS for Si-PETN under hydrostatic compression and anisotropic EOS under uniaxial compressions. Both the EOS and shear stresses were compared to those of PETN. We also investigated the hypervelocity chemistry of initiation reactions in Si-PETN using first-principles reactive molecular dynamics. The bimolecular collisions that should occur behind the shockwave front of shocked Si-PETN were simulated as a function of both collision velocity and orientation. The sensitivity properties of Si-PETN were quantified by determining the threshold collision velocities of reaction initiation for each orientation and compared to those of PETN.

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