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Structural variability and electronic properties of bulk and monolayer Si2Te3[1] COREY COMBS, University of Tennessee Knoxville Department of Materials Science and Engineering, Vanderbilt University Department of Physics and Astronomy, XIAO SHEN, Vanderbilt University Department of Physics and Astronomy, University of Memphis Department of Physics and Materials Science, YEVGENIY PUZYREV, LIDA PAN, Vanderbilt University Department of Physics and Astronomy, SOKRATES PANTELIDES, Vanderbilt University Department of Physics and Astronomy, Oak Ridge National Laboratory Materials Science and Technology Division — Silicon telluride, a layered material recently experimentally made to a few atomic layer-thick (1) has intriguing variations of optical and electronic properties, associated with the flexibility of its structure. In Si2Te3, the Te atoms form a hexagonal close packed structure, while Si atoms form Si-Si dimers and fill 2/3 of the allowed sites. There are 4 possible orientations of the Si-Si dimers, 3 in-plane directions 60 degrees to each other and one out-of-plane direction perpendicular to 2D plane. X-ray and electron diffraction data on bulk Si2Te3 suggested that 1/4 of the dimers are vertical while the other 3/4 of the dimers are randomly oriented horizontally. We performed density functional calculations to show that both bulk and monolayer Si2Te3 exhibit large variations in properties, resulting from reorientation of silicon dimers. These variations are up to 5 percent in lattice constant and up to 40 percent in electron band gap. Transition of Si2Te3 from bulk to monolayer configuration also shows an increase in the band gap and lattice constant. We show that these properties are, in principle, controllable by temperature and strain, making Si2T3 a promising candidate as optomechanical and optoelectronic material. (1) Keuleyan, S. et al. Nano Lett. 2015, 15 (4), 2285-2290.

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