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Temperature renormalization of the electronic and phonon properties of $TiSe_2$ YANG-HAO CHAN, Institute of Atomic and Molecular Sciences, Academia Sinica, PENG CHEN, TAI-CHANG CHIANG, Department of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, MEI-YIN CHOU, Institute of Atomic and Molecular Sciences, Academia Sinica — We present first-principles studies of the phonon dispersions and the electronic structure of bulk $TiSe_2$ as a function of temperature. Above the charge-density-wave (CDW) transition temperature the high-symmetry normal-phase structure is stabilized by anharmonic effects. The transition temperature of the CDW phase is computed to be around 150 K with self-consistent phonon theory [1]. We have also investigated finite-temperature effects on the electronic structure with the molecular dynamics (MD) method. In contrast to zero-temperature band structure which shows a band overlap, MD-averaged band structure shows a small band gap of 76 meV at 300 K. Our results reveal a flat band along the kz direction as observed in ARPES experiments, which is missing in zero temperature calculations. We demonstrate the importance of finite temperature effects on $TiSe_2$ and show that fluctuations of the low-energy CDW phase have significant effects on room-temperature properties. [1] T. Tadano and S. Tsuneyuki, Phys. Rev. B **92**, 054301(2015).

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