Abstract Submitted
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First Principles Study on Ta_{25} Low- and High-Temperature Phases[1] YU-NING WU, Department of Physics, University of Florida, USA, LAN LI, College of Arts and Sciences, Kent State University, USA, HAI-PING CHENG, Department of Physics, University of Florida, USA — Low- and high-temperature phases of Tantalum pentoxide (Ta_2O_5) have been studied by density functional method. Our calculations have been carried out using the projector-augmented wave method and a plane wave basis set. Tantalum pen-oxide, Ta_2O_5 is considered as a potential alternative to SiO_2 because of its high breakdown voltage, its high dielectric constant, and its excellent step coverage characteristics. It is also a dielectric material for optical coating application that is important to high precision instrumentation. We have studied structure, electronic properties, and phonon spectra, as well as elastic modulii, including bulk modulus, Young's modulus and Poisson's ratio. Four different isomorphs will be presented. Furthermore, SiO_2-doped Ta_2O_5, which is used as mirror coatings in current interferometric gravitational wave detectors, has also been investigated. Our results help to understand the properties of this material in different phases.

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