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First Principles Study on Ta_2O_5 Polymorphs[1] YUNING WU, HAIPING CHENG, Department of Physics, University of Florida, USA, LAN LI, College of Arts and Sciences, Kent State University, USA — Using density functional theory (DFT) with generalized gradient approximations (GGA) and the projector-augmented wave method, we have investigated structure, energetics, elastic tensors and mechanical properties of four crystalline forms of Ta_2O_5 with exact stoichiometry and a model amorphous structure. A virtual crystal potential has also been constructed to address partial oxygen occupancy and compared to models of explicit oxygen vacancies and the oxygen-rich system. Calculations show that mechanical properties of these polymorphs are highly anisotropic. By comparison with experimental data, we find that all crystalline phases and the simulated amorphous phase have Young's modulus higher than the amorphous thin film that is measured experimentally, but the variation among crystalline structures is as high a factor of 2. Electronic properties of three Ta_2O_5 polymorphs have been calculated using a hybrid DFT and Hartree-Fock functional method that improves gap size obtained by GGA. We suggest that further experimental measurements on tantala crystals are needed to understand physical properties of this import material.

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