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Electronic and optical properties of tantalum pentoxide polymorphs from first principles calculations[1] JIHANG LEE, EMMANOUIL KIOUPAKIS, Materials Science and Engineering, University of Michigan, WEI LU, Electrical Engineering and Computer Science, University of Michigan — Tantalum oxide has been extensively studied due to its attractive properties as dielectric films, anti-reflection coatings, and resistive switching memory. Although various crystalline structures of tantalum pentoxide (Ta_2O_5) have been reported, the structural and electronic/optical properties still remain a controversial issue. We investigate the electronic and optical properties of crystalline and amorphous Ta_2O_5 structures using first-principles calculations in the GW approximation. The calculated band gaps of the crystalline structures are too small to explain the experimental measurements. The amorphous structure exhibits a strong exciton binding energy and an optical band gap ($\sim$ 4eV) similar to experiment. We determine the atomic orbitals that form the conduction band of each polymorph and analyze the dependence of the band gap on the atomic geometry. Our results establish the connection between the underlying structure and the electronic and optical properties of Ta_2O_5.

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