First Principles Study on Ta$_2$O$_5$ Polymorphs

YUNING WU, HAI-PING 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$_2$O$_5$ 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$_2$O$_5$ 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.

$^1$Funding support from NSF/PHY-0855292 and NSF/DMR-0804407, computers from NERSC and UF/HPC.

Yuning Wu
Department of Physics, University of Florida