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Electronic and optical properties of Ga_2O_3 from first principles KELSEY MENGLE, EMMANOUIL KIOUPAKIS, University of Michigan — Wide band-gap semiconductors such as Ga_2O_3 are used in numerous applications including high voltage/temperature electronics, deep-UV emission, and transparent contacts. We have investigated the electronic and optical properties of Ga_2O_3 with first-principles calculations based on density functional theory. The electronic and optical properties are calculated with many-body perturbation theory using the GW and Bethe-Salpeter equation methods. The semicore states of Ga are treated as valence electrons to accurately determine the band gap and band structure. We will present results for the structural, electronic, and optical properties of the various Ga_2O_3 polymorphs, including β-Ga_2O_3. This research was supported by the National Science Foundation through Grant No. DMR- 1534221. Computational resources were provided by the DOE NERSC facility.

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