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Vibrational properties and electron-phonon coupling in Ga2O3 from first principles EMMANOUIL KIOUPAKIS, KELSEY MENGLE, GUANG-SHA SHI, Materials Science and Engineering, University of Michigan — $\beta-$Ga2O3 is a wide band-gap semiconductor that is used in an increasing number of applications, such as power electronics and deep-UV emission. One feature of this material is its low thermal conductivity, which although detrimental for power electronics, it may enable applications in thermoelectric devices. We investigated the vibrational and electron-phonon coupling properties of Ga2O3 with first-principles calculations based on density functional theory, density functional perturbation theory, and the GW method. We will discuss calculated results for the phonon properties (frequencies, heat capacity, sound velocities, isotope effects), electron-phonon coupling, and transport coefficients (Seebeck coefficient, electrical conductivity, and estimated electronic figure of merit ZTe). Our results demonstrate the applicability of β-Ga2O3 for thermoelectric applications under appropriate doping and temperature conditions. This research was supported by the National Science Foundation through Grant No. DMR-1534221 and the GRFP through Grant No. DGE 1256260. Computational resources were provided by the DOE NERSC facility under Contract No. DE-AC02-05CH11231 and by XSEDE, supported by NSF grant ACI-1053575.

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