Abstract Submitted
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First-principles study of phase stability and phase transition in Ga_2O_3[1] JIANJUN DONG, BIN XU, Department of Physics, Auburn University — Gallium oxide (Ga_2O_3) is a promising opto- and/or electronic wide-band-gap semiconductor. For example, it has been considered as a gate dielectric oxide for MOS device based on GaN or GaAs. In addition to the ground-state monoclinic β-phase, a rhombohedral α-phase metastably exists at ambient conditions. The conditions of stability of either phase are not well understood. In this talk, we will present our recent *ab initio* calculation results of thermodynamic properties of the α and β phase. We have computed Gibbs free energies of the two phases based on the total energy density functional theory (DFT) and the statistical quasi-harmonic approximation (QHA), calculated the thermal equations of states, and estimated the equilibrium phase boundary. We have further calculated the pressure dependence of Raman and IR frequencies in the two phases. Our results will be compared with some recent experimental data.

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