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First-principles calculations of thermodynamic properties and phase transitions in Al_2O_3 and Ga_2O_3 at high temperature and high pressure BIN XU, JIANJUN DONG, Auburn University — Using *ab initio* density functional theory and statistical quasi-harmonic approximation theory, we have calculated thermodynamic potentials of mineral Al_2O_3 materials and the related Ga_2O_3 materials over a wide range of temperature and pressure (T-P) conditions. The equilibrium T-P phase diagrams are predicted to understand the trend of pressure induced phase transitions in group IIIB oxides. Furthermore, we theoretically explored the possible new high-pressure structures of Ga_2O_3. Finally, we derived experimentally measurable thermal properties, such as lattice thermal expansion, heat capacity, and isothermal compressibility. Our calculated thermal properties are in excellent agreement with available experiments.

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