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Thermodynamic properties of ZrSiO4 polymorphs from DFT based *ab initio* phonon calculations[1] JINCHENG DU, MRUNAL CHAUDHARI — Zircon and Reidite are the polymorphs of $ZrSiO_4$minerals that are natural hosts of various radioactive elements in the crust of the earth. Its high permittivity also makes it a promising material for the gate dielectric material in metal-oxide semiconductors. Knowledge of the thermodynamic properties at high temperature and high is very important to consider its application as an effective natural storage for the radioactive wastes and high technology ceramics. These properties are thoroughly studied both computationally and experimentally for zircon, while significantly less attention was paid to reidite in the literature. We report studies of thermodynamic properties of Zircon and Reidite from phonon spectra calculations using *ab initio* based periodic density-functional theory (DFT) calculations. Various thermodynamic properties such as free energy, internal energy, entropy, enthalpy, heat capacity and thermal displacement as a function of temperature are calculated. Phoon dispersion curves and density of states are calculated and compared with the experimental data. Calculated bulk properties agree very well with the experimental data in the literature.

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