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***Ab initio* study of the *thermodynamic properties and the* phonon calculations of Zircon and Reidite** MRUNALKUMAR CHAUDHARI, JINCHENG DU, University of North texas — Zircon and Reidite are the polymorphs of Zirconium Silicate which find its importance geologically, because of its natural hosting to various radioactive elements in the crust of the earth. High permittivity also makes it a promising material for the gate dielectric material in metal-oxide semiconductors. Knowledge of the thermodynamic properties and the phonon based calculations is very critical to understand the high temperature and high pressure properties in order to consider its application as an effective natural storage for the radioactive wastes. These properties are thoroughly studied both computationally and experimentally for zircon, while significantly less attention was paid to reidite in the literature. The thermodynamic properties and phonon calculations of Zircon and Reidite were studied using ab initio based periodic density-functional theory (DFT) based calculations using the generalized gradient approximation (GGA). Various properties such as free energy, internal energy, entropy, heat capacity and thermal displacement as a function of temperature is calculated using the PHONON software. Various phonon based density of states and dispersion curves are calculated and compared with the experimental data. No first principles based computational results were reported up to now. Calculated bulk properties agree very well with the experimental data in the literature.

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