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Theoretical study of ThO_2 by first principles calculations

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Abstract

In this paper, the thermodynamic, structural properties and vibrational spectrum of thorium dioxide have been studied using the density functional perturbation theory (DFPT) and density functional theory (DFT) in the framework of first principles calculations. Quantum espresso software, which is an open source computing code, has been used in order to compute the Kohn-Sham equations to obtain the minimum total energy of crystal. The vibrational spectrum of the thorium dioxide was examined along various symmetrical directions, and the results showed the dynamical stability of the crystal system. The quasi-harmonic Debye-Einstein model, as implemented in GIBBS2 Code, was used to calculate the thermodynamic properties of thorium dioxide at high temperatures and pressures. The simulation results showed that the Debye temperature of thorium dioxide decreased with increasing temperature at a constant pressure and increased with increasing pressure at a constant temperature. Increasing the Debye temperature indicated an increase in the crystal stiffness and the average sound velocity. It was observed that the volumetric thermal expansion coefficient and Grüneisen parameter decreased exponentially with increasing pressure at a constant temperature, while increased with increasing temperature at a constant pressure, indicating an increase in heat transfer in the crystal lattice.

Keywords: nuclear fuel, Debye-Einstein thermal model, vibrational entropy, volumetric expansion coefficient

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