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The Physical and Electronic Properties of Lead-free (K1-xNaxNbO3) under Stress-Strain at Temperature and Pressure Change

Piezoelectric material is a type of ceramic that has electrical properties. When it is subject to mechanical force, the piezoelectric material provides a voltage known as piezoelectric effect. This commonly uses piezoelectric which is known as KNN (K1-xNaxNbO3) due to high curie temperature. KNN can also be used to apply in many ways. In this research, we studied further about the physical properties of KNN, by using Density Functional Theory (DFT) within the generalized gradient approximation (GGA) calculation method with PBE developed for solids (PBEsol) functional. We started at a ground state of KNO. From the lattice parameter, we are able to see the equilibrium of four structures of KNO which are tetragonal, orthorhombic, trigonal, cubic. We also calculated band structure and the density of states (DOS).We analyzed the results from the band structure and the density of states (DOS) of each crystal structure to find the trend of physical and electronic properties.

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