# A DENSITY FUNCTIONAL THEORY ANALYSIS OF THE PRESSURE-INDUCED MECHANICAL STABILITY OF KNiF3 PEROVSKITE COMPOUND

**Belgin KOÇAK**

**Vocational School of Higher Education, Department of Electronics and Automation, Ostim Technical University, Ankara, Turkey**

**ORCID.0000-0002-4395-4467**

**Yasemin ÖZTEKİN ÇİFTCİ**

**Faculty of Science, Department of Physics, Gazi University, Ankara, Turkey**

**ORCID.0000-0003-1796-0270**

|  |
| --- |
| **ABSTRACT**  In this study, we employed density functional theory to evaluate the structural, electronic, and mechanical properties of the KNiF3 cubic perovskite compound, which belongs to the *Pm3m* space group, under high-pressure conditions ranging from 0 to 100 GPa. The results were calculated employing the GGA-PBE approximation in the Vienna Ab initio Simulation Package (VASP) code. Our findings were compared with existing research, and consistent results were obtained. The mechanical properties that our calculations determine are the following: Cauchy pressure, bulk modulus, Young's modulus, shear modulus, Pugh's ratio, Poisson's ratio, hardness, machinability index, Zener anisotropy factor, sound velocities, and Debye temperature. KNiF3 compound was found to meet the criteria for mechanical stability and exhibited consistent mechanical stability across the entire 0 to 100 GPa pressure range. The computed mechanical properties suggest that KNiF3 is a ductile material, and its ductility increases with pressure. Utilizing the EIAM code, elastic anisotropic mechanical properties were visually represented. The estimation of electronic properties has been performed through spin-polarized calculations. |

# Keywords: KNiF3, density functional theory, structural properties, mechanical stability.