# ANALYSIS OF STRUCTURAL, ELECTRONIC, MECHANICAL AND THERMODYNAMIC PROPERTIES OF Ir3TiC COMPOUND USING DFT

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| **ABSTRACT**  Antiperovskite materials are a class of materials of great interest due to their unique physical, chemical and thermodynamic properties [1]. These materials are electronically inverted perovskites and have emerged as a growing class of versatile materials, thus providing materials scientists with an effective and fruitful area of research. In our study, the compound Ir3TiC, an antiperovskite compound, was theoretically analysed. Our study is a purely theoretical study, no experimental parameters were used. The compound has pm3m space group and has cubic structure [2]. The structural, electronic, mechanical and thermodynamic properties of the compound were analysed by the DFT method using the first principles method. Firstly, the structural parameters were determined using geometrical optics. The lattice constant, Bulk modulus and the first derivative of the Bulk modulus were determined by fitting the Murnaghan equation [3]. They were compared with the theoretical and experimental parameters available in the literature. Elastic constants were obtained by Stress-Strain method. The elastic constants were found to be structurally stable by determining their conformity with Born criteria. Young's modulus, Shear modulus, Bulk modulus, Paugh ratio, Caushy pressure and Poisson's ratio, anisotropy value, melting temperature, Debye temperature were obtained from elastic constants. Pugh ratio, Caushy pressure and Poisson's ratio indicated that the compound has a ductile structure. Electronic band structure calculations are important for understanding the physical properties of the crystal structure. By analysing the electronic properties, information such as the nature of the band gap and carrier density is obtained. Electronic band structure calculations showed that the compound is mechanical in nature. In addition, finally, parameters such as Bulk modulus, volume, Heat capacity were determined by detailed analysis of thermodynamic properties.  **References:**  [1] Mehmood, M., Nasir Rasul, M., Hussain, A., Amir Rafiq, M. b, Iqbal, F., Manzoor, A., Azhar Khan, M., Investigation of structural, electronic, elastic, magnetic and thermodynamic properties of antiperovskites XCRh3 (X = Cd, Ta, W, Re, Os, Ir, Pt, Au, Hg, Ce, Pr, Nd, Pm, Sm, Eu, Tb), Physica B: Condensed Matter, 649, 414442, 2023.  [2] Cherrad, D.,Selmani, L., Maouche, D. and Maamache, M. First principles calculations on elasticity, electronic structure and bonding properties of antiperovskites ANTi3 (A = Al, in and Tl), Journal of Alloys and Compounds, 509, 12, 4357–4362, 2011.  [3] Birch,F., The effect of pressure upon the elastic parameters of isotropic solids, according to Murnaghan’s theory of finite strain, Journal of Applied Physics, 9, 279–288, 1938. |

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