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An *ab-initio* Investigation: The physical properties of $ScIr_2$ Superconductor *

© Uttam Kumar Chowdhury[1], Tapas Chandra Saha[2]

Department of Physics, Pabna University of Science and Technology,
Pabna-6600, Bangladesh

E-mail: phy.uttam@gmail.com

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Using ab initio technique the physical properties of $ScIr_2$ superconductor have been investigated with T_c-1.03 K with a $MgCu_2$-type structure. We have carried out the plane- wave pseudopotential approach within the framework of the first-principles density functional theory (DFT) implemented within the CASTEP code. The calculated structural parameters confirm a good agreement with the experimental and other theoretical results. Using the Voigt-Reuss-Hill (VRH) averaging scheme the most important elastic properties including the bulk modulus B, shear modulus G, Young′s modulus E and Poisson′s ratio ν of $ScIr_2$ are determined. At ambient condition, the values of Cauchy pressure and Pugh′s ratio exhibit ductile nature of $ScIr_2$. The electronic and optical properties of $ScIr_2$ were investigated for the first time. The electronic band structure reveals metallic conductivity and the major contribution comes from Ir-5*d* states. In the ultraviolet region the reflectivity is high up to 50 eV as evident from the reflectivity spectrum.

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