**Study of Sc0.875Cr0.125N Dilute Magnetic Semiconductor using Density Functional theory**

Anita Rani

Department of Physics, Guru Nanak College, Sri Muktsar Sahib, Punjab-152026

Corresponding author: ranianita64@gmail.com

Abstract: Motivated by the ongoing interest in nitrides as materials for spintronics applications, we have studied effects of doping with magnetic transition-metal Cr on the electronic and magnetic properties of semiconducting scandium nitride at x = 0.125. We have determined the structural, and electronic properties of pure ScN in zinc-blende (ZB) in this paper. The Siesta Initiative of electronic properties of thousand atoms (SIESTA) code within the density functional theory (DFT) and generalized gradient approximation (GGA), due to Perdew-Burke-Ernzerhof (PBE) has been used to estimate the exchange-correlation functional. Our band structure results for ScN shows the semiconductor nature with indirect band gap. The obtained results are in excellent agreement with earlier reported data.