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**High Pressure Structural Phase Transition and Electronic Properties of NdX (X = P, As, Sb) Compounds : A First Principles Study**
SANJAY KUMAR SINGH, RAJESHWAR SINGH, Doaba Group of Colleges, Applied Science Department, S. B. S. Nagar, Punjab-144514, India, R.P. SINGH, Department of Physics, S. S. V. Degree College, Hapur, C. C. S. University - Meerut, India — The structural and phase transition properties of NdX (X = P, As, Sb) under high pressure have been investigated using an *ab-initio* full potential linear augmented plane wave plus local orbitals approach within the framework of density functional theory as implanted in the WIEN2k package. In this approach the generalized gradient approximation is chosen for the exchange-correlation functional energy optimization for calculating the total energy. At ambient conditions NdX stabilize in NaCl (B1 phase) structure. Under compression, it undergoes first-order structural transition from *Fm-3m* to *P4/mmm* (body centre tetragonal) phase at 30.0, 24.06 and 15.1 GPa which is found to be in good agreement with the available experimental data 30.0, 24.2 and 15.0 GPa respectively. The structural properties *viz.*, equilibrium lattice constants, bulk modulus and its pressure derivative and volume collapse are also calculated and compared with previous calculations and available experimental data. The local spin-density approximation along with Hubbard-U corrections and spin–orbit coupling has been used for correct prediction of electronic properties.

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