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Structural, electronic and phase transition properties of ytterbium monopnictides under high pressure: A LSDA+U study[1] SANJAY KUMAR SINGH, P. RANA, U.P. VERMA, School of Studies in Physics, Jiwaji University, Gwalior-474011, Madhya Pradesh, India — In present paper, we have investigated the structural, electronic properties of ytterbium monopnictides (YbX = N, P) and its phase transition behaviour under high pressure by using the full potential linear augmented plane wave plus local orbitals approach within the framework of density functional theory. In the study the generalized gradient approximation (GGA) is chosen for the exchange-correlation functional energy. The equilibrium properties *viz.*, equilibrium lattice constants, bulk modulus, its pressure derivative and total energy are calculated in four different phases *i.e.* B1, B2, B3 (zinc blende), and BCT phases 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. The LSDA + U strategy shows significant impact on the energy levels of the occupied and unoccupied $4f$ states in the electronic structure of both the compounds. The calculation shows YbX to be semi-metallic. The LSDA + U method provides better description of crystal properties of present system. At ambient conditions YbX (X = N, P) stabilize in NaCl (B1) structure characterized by the space group *Fm-3m*. Under compression, both YbN and YbP undergo first-order structural transition from *Fm-3m* (B1) to Pm-*3*m (B2) at 164.0 and 31.0 GPa, respectively.

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