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Ab initio study on rare-earth iron-pnictides RFeAsO (R =Pr, Nd, Sm, Gd) in low-temperature *Cmma* phase[1] RESUL ERYIGIT, Abant Izzet Baysal University, TANJU GUREL, ESRA ERTURK, Namik Kemal University, A.V. LUKOYANOV, Institute of Metal Physics, Ural Branch of Russian Academy of Sciences and Ural Federal University, GUVEN AKCAY, Abant Izzet Baysal University, V.I. ANISIMOV, Institute of Metal Physics, Ural Branch of Russian Academy of Sciences and Ural Federal University — We present density functional theory calculations on iron-based pnictides RFeAsO (R =Pr, Nd, Sm, Gd). The calculations have been carried out using plane-waves and projector augmented wave (PAW) pseudopotential approach. Structural, magnetic and electronic properties are studied within generalized gradient approximation (GGA) and also within GGA+U in order to investigate the influence of electron correlation effects. Low-temperature *Cmma* structure is fully optimized by GGA considering both non-magnetic and magnetic cells. We have found that spin-polarized structure improves the agreement with experiments on equilibrium lattice parameters, particularly c lattice parameter and Fe-As bond-lengths. Electronic band structure, total density of states, and spin-dependent orbital-resolved density of states are also analyzed in the frameworks of GGA and GGA+U and discussed. For all materials, by including on-site Coulomb correction, rare earth 4f states move away from the Fermi level and the Fermi level features of the systems are found to be mostly defined by the 3d electron-electron correlations in Fe.

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