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Ab Initio Calculations on Magnetic, Electronical and Lattice Dynamical Properties of superconductor CeFeAsO CIHAN PARLAK, RESUL ERYIGIT, Abant Izzet Baysal University — Recent reports of superconductivity in LaFeAsO has led to considerable interest as this provides an alternative noncuprate route to high Tc superconductivity with possibly different superconductivity mechanism. After LaFeAsO, other members of the Fe-As oxypnictides family have been investigated and found to be superconducting. We have investigated the properties of CeFeAsO by using first-principles calculations. The calculations have been carried out within the local density functional approximation (LDA) using norm-conserving pseudopotentials and a plane-wave basis. Energetically favored magnetic structure is found to be a striped AFM Fe layer and zigzaged Ce layers with magnetic moments of 2.7 μ_B and 0.8 μ_B respectively. U parameters are estimated to be 3.62 eV and 4.51 eV for Fe and Ce, respectively. We discuss the electronic structure, orbital resolved density of states and Brillouin zone center phonons for both P4/nmm and Cmma phases along a U dependence of Γ point phonon frequencies.

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