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The effect of pressure on the electric field gradient in $CeAgSb_2$
AZAM POURGHAZI, ZAHRA NOURBAKHSH, University of Isfahan, UNIVERSITY OF ISFAHAN TEAM — $CeAgSb_2$ is a rare example of a ferromagnetically ordered heavy-fermion compound. It presents an opportunity to investigate the physical behavior of a system near a ferromagnetic quantum-critical point. In the vicinity of the quantum critical point, a non-Fermi-liquid character and/or unconventional superconductivity has been found by several workers. In this work, to obtain direct information about the ground-state electronic structure of $CeAgSb_2$ the total energy per primitive unit cell as a function of its volume is calculated, using density functional approach within GGA. We have found a ferromagnetic ground state for $CeAgSb_2$ at zero pressure. Furthermore, we have calculated the electric field gradient (EFG), which is a direct measure of anisotropy in the charge distribution throughout the crystal. We have found that in this 4f metallic compound, EFG increases with pressure. Similar behavior has been reported for sp and 5f metals. We have also found that the value of EFG at Ag and Ce sites are smaller than its value at Sb(I) and Sb(II) sites. The EFG is larger at Sb(I) than it is at Sb(II) site as expected due to the anisotropy of the electric field at Sb(I) position. The sign of EFG's are positive at Ce and Sb(II) sites and negative at other sites.

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