First principles calculations of the Cd-doped $ZrIn_2$: a study of electronic properties and electric field gradients

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Due to their stimulating technological applications, the about 80 binary Indium Transition-Metals (In-TM) alloys are presently attracting considerable attention. The fundamental properties of these alloys as displayed by their atomic compositions, structures and charge densities, however, were extensively studied so far only for a few members of this group of alloys. The present contribution deals with $ZrIn_2$, a member of the Zirconium-Indium system ($ZrIn_2$, $ZrIn_3$, ZrIn, Zr_2In and Zr_3In), for which only few experimental and theoretical studies are available up to now. The electric field gradients (EFG) at Cd impurities on the two In sites (8*e*) of $ZrIn_2$ (space group $I4_1/amd$) have recently been determined by perturbed angular correlation (PAC) spectroscopy [1]. Here we report first principle calculations of the EFG tensor and the electronic structure of Cd-doped $ZrIn_2$. The lattice parameters that correspond to the minimum energy, the total and the partial components of the EFG tensor at Cd on the two In sites were determined and are compared to the experimental PAC results. All calculations were developed at "SsolarIII" in CBPF and at IPEN computational clusters using WIEN2k code.

[1] H. Saitovitch, P.R.J. Silva, J.Thadeu Cavalcante, M. Forker, Journal of Alloys and Compounds 505 (2010) 157-162.