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Comparative study of pure and Co doped-BaFe2As2 JACQUES SOULLARD, ILYA G. KAPLAN, Universidad Nacional Autonoma de Mexico, RAUL PEREZ-ENRIQUEZ, Universidad de Sonora — We present a comparative study of the high critical temperature superconductor Co doped-$BaFe_2As_2$ at the electron correlation level by the embedded cluster method; the electron correlation is calculated through the second order Møller Plesset perturbation theory. We study successively the pure compound, the Co doped-compound in the antiferromagnetic state and in the non-magnetic state. The Co doping introduces a strong modification of the spin distribution in its neighboring atoms. The analysis of the orbital population reveals that the spin density of the Co impurity becomes 3 times greater than that of the central Fe of the pure compound, increase attributed to a corresponding increase of the d_{z^2} orbital population; a local antiferromagnetic order along the **b** axis of the crystal structure appears. The formation mechanism of the local magnetic moments implies a spin transfer from the (n.n.) and (n.n.n) atoms to the central Co and is relevant to the $J_1 - J_2$ Heisenberg model. The orbital population analysis reveals also that, in the doped compound and in both magnetic cases, the electron charge is associated to a singlet state and may correspond to a holon.

Jacques Soullard
Universidad Nacional Autonoma de Mexico

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