

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Local magnetic moments in doped BaFe₂As₂ JACQUES SOULLARD, ILYA KAPLAN, Universidad Nacional Autonoma de Mexico, RAUL PEREZ-ENRIQUEZ, Universidad de Sonora — We present a comparative calculation of the high critical temperature superconductor doped BaFe₂As₂ with its parent compound at the electron correlation level by the embedded cluster method; the electron correlation is calculated at the second order Møller-Plesset perturbation theory level. For the pure material we consider the Ba Fe₅As₈ cluster, for the doped material the central Fe is substituted by Co or Ni. The analysis of orbital populations in the doped material reveals a charge density increase on the central impurity with respect to the charge density of the central Fe atom of the undoped case. On the other hand, the spin-density analysis allows to determine the distribution of the spin density on the neighboring of the central impurity. Both analysis show how the interaction between the central impurity and its neighboring Fe atoms participates to the formation mechanism of the local magnetic moments.

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Date submitted: 10 Jan 2014

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