

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Where are the extra electrons in Co and Ni-substituted BaFe₂As₂? HIROKI WADATI, ILYA ELFIMOV, GEORGE SAWATZKY, Department of Physics and Astronomy, University of British Columbia — In the literature, the substitution of Co or Ni for divalent Fe in pnictides is frequently referred to as an electron doping. Chemical intuition on the other hand, advocates the isovalent nature of the substitution with little effect on the electron density distribution in the rest of the material in a dilute limit. Here we report on the results of a detailed density functional study of a periodic impurity model of various substitutes in BaFe₂As₂. By integrating the total occupied density of states, we demonstrate that the number of electrons situated inside the muffin-tin sphere of the substitute is consistent with isovalent substitution. This suggests that Fermi surface changes seen in the angle-resolved photoemission spectroscopy measurements are mainly due to impurity scattering rather than “electron doping”.

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Date submitted: 18 Nov 2009

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