Electronic structure study of new family of high-Tc Fe-superconductors based on BaFe2As2 in presence of dopants Co, Ni, Rh and Pd.

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The superconductivity has a long history. One of the most recent discoveries is the superconductivity in the Fe-based family with anti-ferromagnetic state at ambient temperature. In this type of material, the transition to the superconductivity state was found in presence of different dopants. In this report we present the results of calculations for the cluster $Ba_4Fe_5As_8$ in presence of Co, Ni, Rh and Pd as dopants. The methodology of Embedded Cluster Method at the MP2 electron correlation level was employed, which allows us, to reproduce the Madelung potential of the infinite crystal in each site of the cluster. It was calculated the ground state for the pure crystal and in presence of dopants. The population analysis showed two main features: the independence of charge density transfer from the spin density transfer and, the presence of orbitals with electron density but without spin density. It could not be observed the same qualitative behaviour for the spin and charge transfer for both pair of dopants Co and Ni compared to Rh and Pd. However, the observed properties correspond to the RVB mechanism for the superconductivity transition proposed by Anderson for cuprates. This confirms our conclusions obtained for the same material doped by Co and Ni.