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Ge doping of $FeGa_3$[1] J.C. ALVAREZ-QUICENO, M. CABRERA-BAEZ, UFABC, Brazil, J. MUNÉVAR, H. MICKLITZ, E.M. BITTAR, E. BAGGIO-SAITOVITCH, CBPF, Brazil, R.A. RIBEIRO, M.A. AVILA, G.M. DALPIAN, UFABC, Brazil, J.M. OSORIO-GUILLÉN, UdeA, Colombia — The intermetallic narrow-gap semiconductor $FeGa_3$ is one of the few Fe-based diamagnetic materials. Experimentally, Ge doping induces a ferromagnetic (FM) state. The mechanism responsible for this FM response is still unestablished, but there are proposals of itinerant magnetism to explain this behavior. Our DFT simulations show that inserting holes induces a delocalized FM response, while inserting electrons induces a localized FM response around some Fe atoms. We also modeled different distributions of Ge substitution and observe that the FM response depends on the Ge concentration and also on the Ge distribution on the Ga sites. We observed that the extra electrons become localized in some specific Fe atoms, rather than delocalized over the entire crystal lattice, as expected from an itinerant model. For experimental probing of this scenario, we have performed ^{57}Fe Mössbauer spectroscopy on flux-grown singlecrystalline samples. The resulting resonance peak shape supports a localized model for ferromagnetism, since it is possible to resolve the presence of two distinct Fe isomer shifts (despite a single crystallographic site), expected to correspond to Fe atoms with high and low magnetic moments.

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