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DFT calculations of hyperfine parameters of Fe-doped MgO

Emission Mossbauer spectroscopy using the radioactive probe $^{57}Mn \rightarrow {}^{57}Fe$ has been performed by the Mossbauer Collaboration at ISOLDE. Among the materials studied have been semiconductors such as MgO, ZnO which are potentially interesting for dilute magnetism [1-4].

In order to better interpret experimental results, hyperfine parameters were obtained using first principle calculations in the frame work of density functional theory (DFT) and the full potential linearized augmented plane wave method (FP-LAPW) [5]. Various implantation sites were proposed and studied using two different approximations: Pedrew-Burke-Ernzerhof (PBE) and the PBE+U with a Hubbard-like coulomb term [6]. The Fe2+ state resulting from damage can be described by considering the effect of Coulomb correlations (U) in the oxygen p-band in addition to the correlation in the d-shell of the transition metal (Fe). We find that our calculations show good agreement with experimental results.

Finally, a discussion on density of state and electrical properties of Fe-doped MgO will be presented. This work demonstrates the benefit of ab initio calculations in helping to resolve outstanding questions arising from experiment.

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Author: MOKHLES GERAMI, Adeleh (K.N Toosi University of Technology (IR))

Co-authors: GUNNLAUGSSON, Haraldur (Aarhus University); JOHNSTON, Karl (Universitaet des Saarlandes (DE)); Prof. VAEZ ZADEH, M (Dept. of physics, K.N.Toosi University of Technology, P.O.Box 15875-4416, Tehran, Iran)

Presenter: MOKHLES GERAMI, Adeleh (K.N Toosi University of Technology (IR))