

Ab-initio study of the structural, magnetic and hyperfine properties of the ferrite MgFe_2O_4

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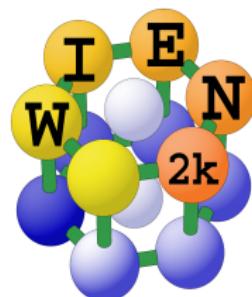
XIX MEETING OF PHYSICS 2020
LIMA - PERÚ



Computational details



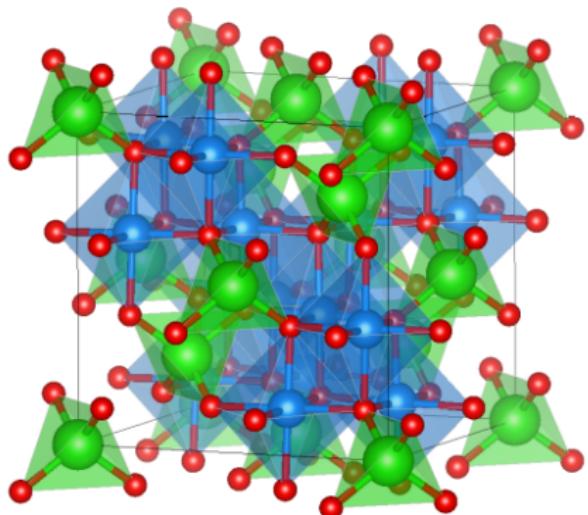
- Electronic structure calculations based on the Density Functional Theory (DFT).
- Exchange-Correlation: GGA-PBE
- DFT+U, $U = 5.0$ eV for 3d-Fe atoms.
- Reciprocal space: $21 \times 21 \times 21$ grid.
- Wien2k: $R_{MT} \times K_{max} = 8$.
- QE: Ecutoff = 80 Ry.



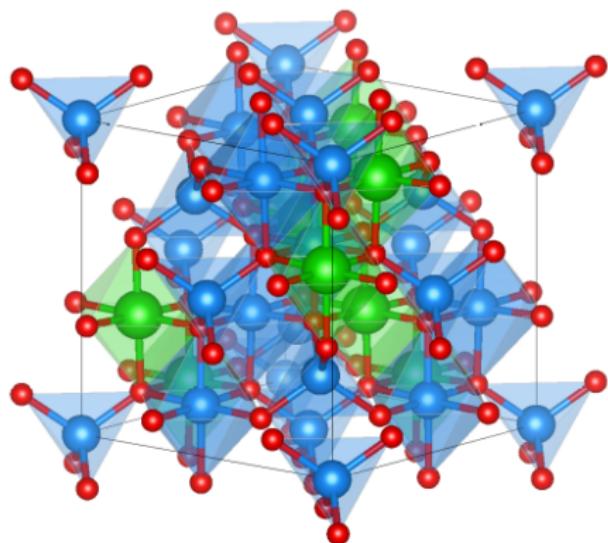
Spinel crystal structure $(\text{Mg}_{1-\delta}\text{Fe}_\delta)[\text{Mg}_\delta\text{Fe}_{2-\delta}]\text{O}_4$

(A): tetrahedral site, [B]: octahedral site, δ : inverse grade

Space-group: $Fd\bar{3}m$

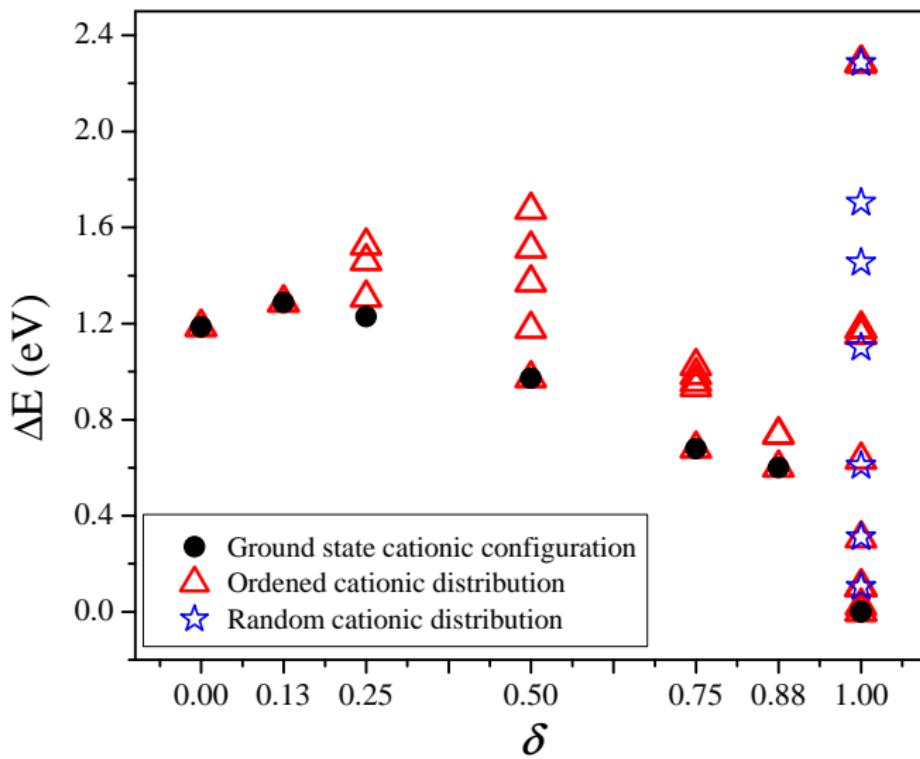


Normal ($\delta=0.0$)

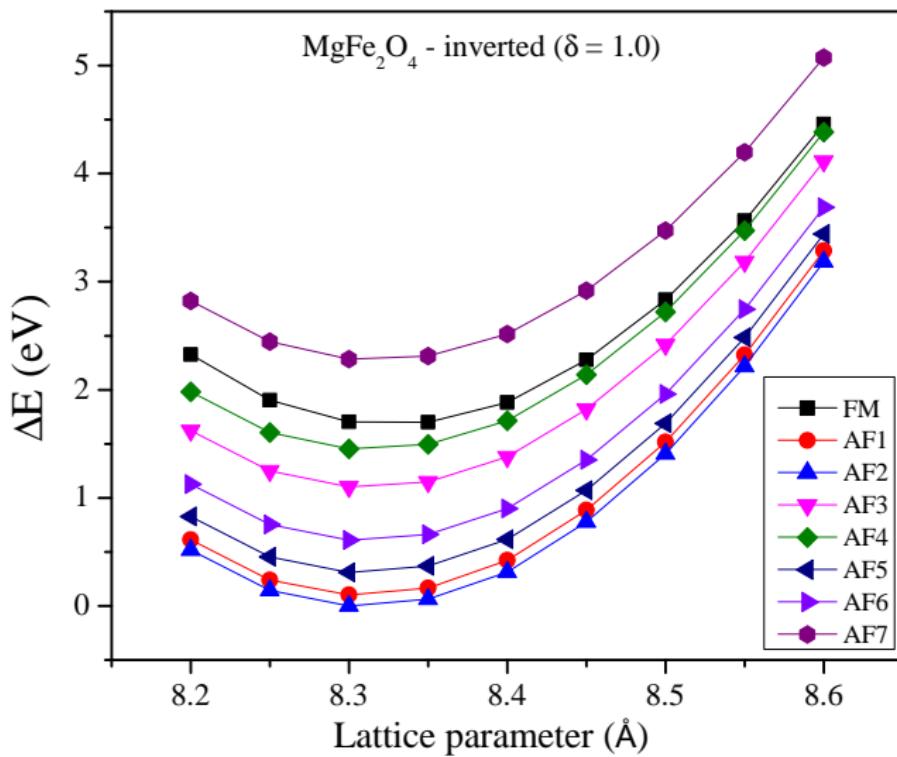


Inverted ($\delta=1.0$)

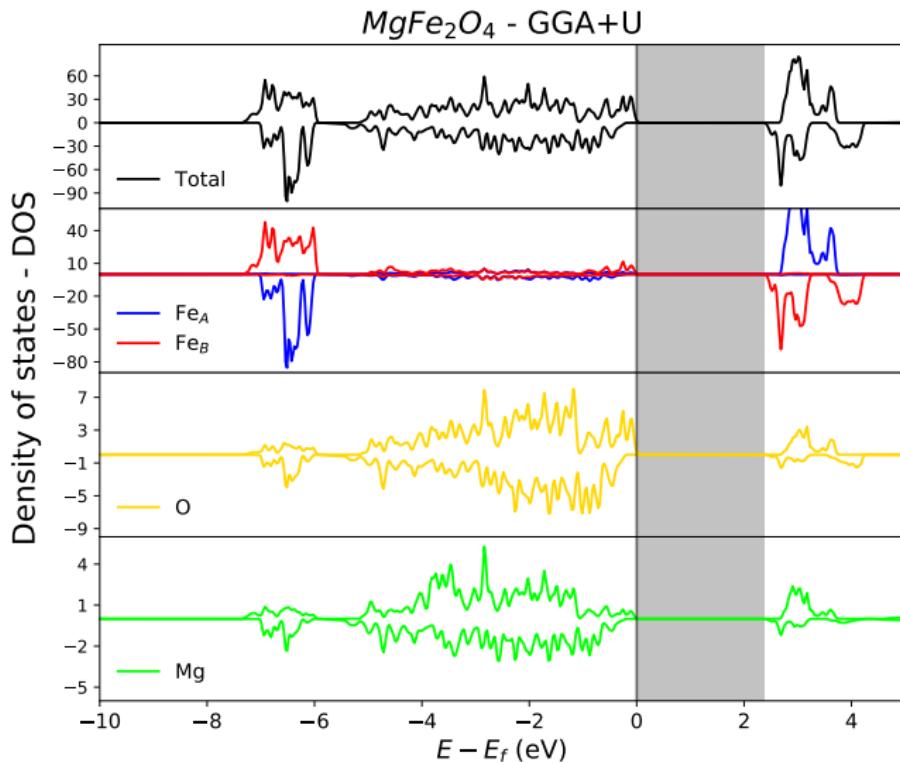
Structural and magnetic ground state



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Electronic structure: $E_g = 2.3\text{eV}$



Hyperfine parameters

- Isomer shift:

$$IS = \alpha[\rho_a(0) - \rho_s(0)]$$

$$IS(A) = 0.30 \text{ m/s}, IS[B] = 0.40 \text{ m/s}$$

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$$QS = \frac{eQ_N V_{zz}}{2} \left(1 + \frac{\eta^2}{3}\right)^{1/2} ; \quad \eta = \left| \frac{V_{xx} - V_{yy}}{V_{zz}} \right|$$

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- Hyperfine magnetic field:

$$B_{hf} = a\mu^{3d} + b\mu^{4s}$$

$$B_{hf}(A) = 52.7 \text{ T}, B_{hf}[B] = 55.2 \text{ T}$$

DFT and experimental measurements

- Equilibrium lattice parameter - X-Ray diffraction:

$$DFT : a = 8.37\text{\AA} \quad , \quad Exp : a = 8.30\text{\AA}$$

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$$DFT : M_T = 0.0\mu_B \quad , \quad \mu_{Fe} = \pm 4.1\mu_B$$

$$Exp : M_T(\delta = 0.7) = 2.4\mu_B \quad , \quad M_T(\delta = 0.9) = 1.0\mu_B \quad \Rightarrow M_T(\delta = 1.0) \approx 0.0\mu_B$$

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- Hyperfine parameters - Mössbauer spectroscopy

$$DFT: IS(A) = 0.30 \text{ m/s} , \quad IS[B] = 0.40 \text{ m/s} , \quad B_{hf}(A) = 52.7 \text{ T} , \quad B_{hf}[B] = 55.2 \text{ T}$$

$$Exp: IS(A) = 0.34 \text{ m/s} , \quad IS[B] = 0.47 \text{ m/s} , \quad B_{hf}(A) = 52.4 \text{ T} , \quad B_{hf}[B] = 54.3 \text{ T}$$

Thank You!



Doctoral and postdoctoral position in the Electronic Structure of Condensed Matter Group at the Institute of Physics La Plata (IFLP).
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