Room temperature magnetism in Zn-ferrite due to structural defects

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Cation site inversion between regular and inverse spinel compositions and oxygen vacancy (V_O) mediated ferromagnetic coupling between Fe spins constitute two major physical mechanisms for the observed ferrimagnetism in $ZnFe_2O_4$ (ZFO) at room temperature [1]. This conclusion is based on experimental results from x-ray magnetic circular dichroism measurements at the Fe $L_{2,3}$ edges and magnetization measurements performed on zinc ferrite nanoparticles and films, with different cation distributions and oxygen vacancy concentrations. Our density-functional-theory calculations indicate that the enhanced ferrimagnetic response observed in some nominally nonmagnetic or antiferromagnetic ferrites can be taken as a further example of the defect-induced magnetism phenomenon. Therefore, we studied the magnetic coupling between the Fe ions in ZFO with and without V_O in more detail. The formation energy of defects is used to analyze the stability of V_O in ZFO for the experimental growth conditions. The Néel temperature (T_N) is determined from Monte Carlo (MC) simulations using the magnetic exchange interactions (J_{ij}) obtained from first-principles method. The correlation energy is treated using GGA+U, where it is found that the J_{ij} change almost linearly with increasing values of U. For T_N comparable to the experimental results, the first neighbor interaction was small and positive as concluded from former experiments. With those J_{ij}, the estimated temperature-dependent saturation magnetization from the MC simulations is in good agreement with recent measurements.

References

[1] C. E. Rodríguez Torres *et al.*, Phys. Rev. B **89**, 104411 (2014)

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