Point defects and electronic structure of Fe_3O_4

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A comprehensive experimental study of magnetite point defects was made by R. Dieckmann and co-authors [1, 2]. The formation energy of the Frenkel pair is one of the important results. Although some ab initio data concerning magnetite point defects have been obtained previously [3, 4], there is still not a single comparison between theoretical and experimental formation energies for defects in magnetite.

Ab initio modelling of point defects in the cubic phase of magnetite faces two problems: the cubic structure becomes unstable below the Verwey temperature and there is no consensus on the electronic structure of the cubic phase (if there is a band gap, what type of symmetry of the wavefunction should be considered and how to describe strong electronic correlations).

The aim of the present study is to refine the magnetite model using the comparison between the DFT+U results and the experimental data on the Frenkel pair formation energy in the magnetite cubic phase together with the data on the lattice constant and the band gap. We show that the comparison of the Frenkel pair formation energy carefully measured at high temperatures with the first-principles calculations allows to determine a consistent DFT+U model of cubic Fe_3O_4.

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