The formation energies of magnetite vacancies within the density functional theory +U

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Ab-initio calculation of the magnetite point defects properties is a computational physics problem that is relevant for many magnetite applications nowadays. Magnetite is a magnetic iron oxide with strong electronic correlations. The calculation requires a method that able to take it into account.

The properties of isolated point defects of magnetite obtained in previous works are very contradictory. Indeed, the formation energies of A- and B-vacancies obtained within density functional theory (DFT) +U are 3.45 and 2.30 eV [1], respectively, while without correction for the same defects, the values are 2.69 and 0.83 eV [2]. Analysis of the literature data shows that the reason for such contradictions may lie in the high sensitivity of the DFT+U cubic phase magnetite model to the calculation method [1, 3, 4].

The report discusses a set of assumptions (the effective correction term U_{eff}, the size of the supercell, initial approximations to the wave functions and electron density, geometry optimization parameters), which gives adequate values of the formation energies of magnetite cubic phase vacancies within DFT+U. The results are compared with the results of calculations without the Hubbard correction.

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