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Influence of point defects on charge transport in nickel ferrite NiFe2O4

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Nickel ferrite spinel $NiFe_2O_4$ promising material in spin-based devices and non-volatile resistive memory. In this work we consider electronic structure of pristine and defective nickel ferrite. The orbital ordering, band gap and charge transfer are studied in the framework of density functional theory with account of strong electronic correlations (DFT+U method). The possibility of changing the type of polaron transport in the presence of oxygen vacancies and nickel antisites has been demonstrated. The corresponding non-adiabatic activation barriers of polaron transport is considered. The resulting hopping energies are in general agreement with experimentally observed activation energies. The highlighted influence of point defects on the polaron conductivity mechanism could be a suitable explanation for the large variability of activation energies in previous experimental works.
The extended version of these findings has been published in the journal Computational Materials Science.

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