Polaron hopping in nickel ferrite spinel $NiFe_2O_4$

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Transition metal spinel oxides are an important class of materials. Their properties could be principal in several practical applications such as the corrosion process, electrocatalysis or electronic devices. Moreover, these systems are of fundamental interest because of the effects associated with strong electron correlations
Nickel ferrite spinel $NiFe_2O_4$ is a promising material in spin-based devices and non-volatile resistive memory. The polaron hopping conduction mechanism commonly observed in transition metal oxides could be crucial for understanding the fundamentals of the charge transport properties, so it is important to study it in detail. There are many different experimental studies of nickel ferrite, that show major complexity of the charge transport with the possibility of both electron and hole polaron carriers.
Based on successful attempts to describe magnetite [1] and chromite [2], we have built a model of nickel ferrite spinel in the framework of the DFT+U method. The orbital ordering, band gap and charge transport are studied.

[1] Shutikova M I and Stegailov V V 2022 *J. Phys.: Condens. Matter* **34** 475701
[2] Fominykh N A and Stegailov V V 2023 *JETP Lett.* **117** 849–853