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Electron Localization in Fe_3O_4: an Ab Initio Wannier Study[1]
PERRY SAKKARIS, CAREL BOEKEMA, San Jose State University — Magnetite, Fe_3O_4, is an unusual ferrimagnetic oxide with emergent physical properties that are not yet fully understood. Among these are the metal-insulator transition at the Verwey Temperature T_V (123K) and a spin-glass-like transition at about twice T_V. The "extra" fully spin-polarized 3d electrons that span the t_{2g} bands of the B sublattice show strong electron correlation effects and are mainly responsible for conduction above T_V. We perform a DFT+U calculation to obtain a set of Bloch orbitals describing the t_{2g} bands. We then use the gauge invariance of Wannier functions to transform the Bloch orbitals into a set of Maximally Localized Wannier Functions (MLWFs). The MLWFs are a real space description of the "extra" 3d electrons allowing us to describe their spatial localization and determine the mechanism of conduction above T_V. Wannier studies of Fe_3O_4 may also allow us to determine the extent of electronic coupling to lattice vibrations, which may provide us substantial quantitative clues on the physical mechanism of the Verwey Transition.

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