Electron Localization in Fe$_3$O$_4$: an Ab Initio Wannier Study$^1$

PERRY SAKKARIS, CAREL BOEKEMA, San Jose State University — Magnetite, Fe$_3$O$_4$, 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$_3$O$_4$ 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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