Electronic structure of Fe_3O_4 and Fe_2SiO_4 spinels

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Verwey transition in magnetite (Fe_3O_4) is one of the most fascinating phenomena in the solid state physics [1]. Recently, the mechanism of the Verwey transition based on the interplay between the electron correlations of the *3d* states on iron and the electron-phonon interaction was developed [2]. In the low-temperature monoclinic phase, the insulating state with a small gap ~ 0.15 eV results from the coupling between the charge-orbital ordering induced by the strong on-site Coulomb interaction and lattice distortion described by the phonon order parameters [3]. In this presentation, we compare the electronic structures of Fe_3O_4 and the Fe_2SiO_4 spinel. Both compounds crystalize in the same spinel (pyrochlore) structure and differ from each other only by the type of atom (Si replaces Fe) in the tetrahedral position. It results in radically different electronic properties of Fe_2SiO_4. Due to higher occupation of the *3d* states, this compound is a Mott insulator with the magnetically ordered state below the spin-Peierls phase transition at T_c ~ 12 K. Using the LDA+U method, we found that the ferromagnetic metal at $U = 0$ transforms into the antiferromagnetic insulator with the gap ~ 2 eV at U ~ 4 eV [4]. The antiferromagnetic order breaks the crystal symmetry and induces the tetragonal distortion of the high-symmetry cubic phase. The differences between the electronic structures and phase transitions in Fe_3O_4 and Fe_2SiO_4 are discussed.

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