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Investigation on the Electronic Structure and Magnetism of the $FeTiO_3$ Polymorphs from DFT Quantum Simulations

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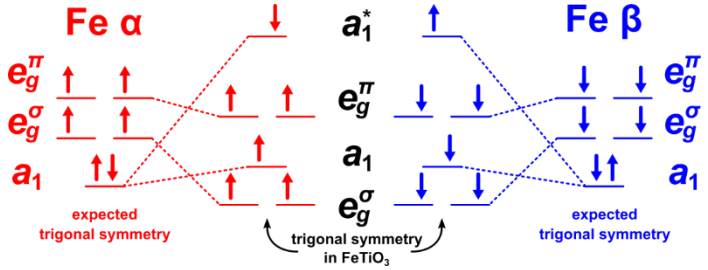
Highlights

- $FeTiO_3$ polymorphs have many technological applications.
- Despite similarities in the R-3 and R3c polymorphs electronic structures, the magnetic exchange mechanisms remain different.

Abstract

Ilmenite $FeTiO_3$ (*R*-3 space group, no. 148) is a layer-type antiferromagnetic semiconductor known for outstanding electronic and magnetic properties. Since the first studies in the late 1950s, different approaches with Ilmenite promoted applications in many fields, such as high-temperature electronics, optoelectronics, spintronics, and photocatalysis. Despite their intriguing electronic and magnetic properties, they remain a subject of discussion[1]. Moreover, in the last decade, the metastable $LiNbO_3$-like structure of the $FeTiO_3$ (*R*3*c* space group, no. 161) became a well-known candidate in the search for green magneto-electric multiferroic materials[2]. However, it is not studied as much as Ilmenite. The magnetic exchange mechanisms of these polymorphs are different. Yet, we found their electronic structures to be quite comparable, having the trigonal symmetry of $[MO_6]$ clusters (M = Fe, Ti) and the spin splitting in Fe atomic orbitals playing a significant role in magnetism (Fig. 1). Crystal orbital isosurfaces and spin density maps corroborate predictions of indirect magnetic exchange mechanisms mediated through Fe-O-Fe (super-exchange) and Fe-O-Ti-O-Fe (super-super-exchange) pathways in the R-3 space group, linked to some extent of spin polarization in oxygen. The Fe-O-Fe indirect magnetic exchange in the R3c space group is not explained by the super-exchange mechanism.

Figure 1. Trigonal symmetry and spin splitting of Fe $3d_{z^2}$ in $FeTiO_3$.



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