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Structural, electronic, and magnetic properties of ilmenite $FeTiO_3$

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Abstract:

The electronic structure and magnetic properties of ilmenite $FeTiO_3$ were studied by first principle calculations [1]. Ilmenite is a wide-band-gap semiconductor with a 2.5 eV band gap [2], which is exploited to realize multifunctional devices [3]. The ilmenite structure is based on a hexagonal-close-packed oxygen lattice with metal atoms Fe and Ti occupying two-thirds of the available octahedral sites. Each octahedron shares three edges with octahedra inside the layer, a face with an octahedron of the second type of cation in the adjacent layer, and the opposite face with a vacant octahedral site. In other words, layers of Fe and Ti alternate with a cation ordering of Ti-Fe-V-Fe-Ti, V: vacant sites along the c axis.
We present calculations related to the structural properties: total energies, lattice constants, and bulk moduli. We also report the total and local magnetic moments and the spin-polarized densities of states. We considered both the ferromagnetic state and an antiferromagnetic configuration found stable in ilmenite in which the Fe^{2+} spins are ferromagnetically aligned within a bilayer but antiferromagnetically coupled between bilayers: no differences in magnetic moment and electron charge of iron were found between the magnetic configurations.

[1] P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka, and J. Luitz, WIEN2k, An Augmented Plane Wave Local Orbitals Program for Calculating Crystal Properties (Technische Universität Wien, Wien, Austria, 2002).
[2] D. S. Ginley and M. A. Butler, J. Appl. Phys. 48, 2019 (1977)
[3] H. Hojo, K. Fujita, K. Tanaka, and K. Hirao, Appl. Phys. Lett. 89, 142503 (2006)