Magnetism in Transition Metal Ilmenenes

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Abstract

Ilmenene is a new two-dimensional material that has recently been exfoliated from the naturally occurring titanate ore ilmenite (FeTiO3) [1], a material found in abundance on the earth´s surface. With the synthesis of this material, it is a matter of time before other similar systems are obtained from their bulk counterparts. In this work, using density functional theory, we performed calculations of the structural, electronic and magnetic properties of the ilmenenes $TMTiO_3$ (with TM running from V to Zn), being more stable when they are TM ended. The magnetic ground state is antiferromagnetic, except for the Cu and Zn cases which shown ferromagnetic and spin compensated solutions, respectively. The energy differences with respect to the ferromagnetic system are about 0.01 eV/TM-atom, although for the Cr and Cu ilmenenes the differences become considerably larger. The TM local magnetic moments as a function of the atomic number follow the Slater-Pauling type curve. We established a simple electronic model filling the TM levels. However, for the Cr and Cu cases, we find a Janh-Teller like distortion breaking the degeneracy of the dxz and dyz orbitals. Because magnetism in two-dimensional materials is being currently held promising for spintronics, the synthesis of these materials could be interesting for experimentalists.

References

[1] Balan et al., Chemistry of Materials, 30 (2018) 5923-593.

Figures

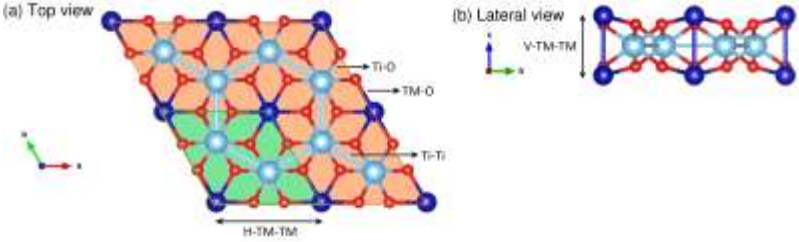

Figure 1: Top (panel (a)) and lateral (panel (b)) view of transition metal ended ilmenene-like systems.

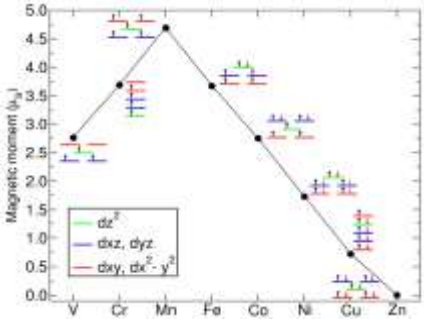

Figure 2: Calculated local magnetic moment at the transition metal atoms. For each compound, the electronic filling model is also shown. Red levels denote the in-plane $dx^2–y^2$ and dxy orbitals; green, the out-of-plane dz^2 orbital: and blue, the orbitals dxz and dyz.