Distorsion and electronic structures in two-dimensional magnetic ilmenenes systems

R.H. Aguilera-del-Toro[1]
M. Arruabarrena[2]
A. Leonardo[1,3]
A. Ayuela[1,2]

[1]*Donostia International Physics Center (DIPC), 20018 Donostia, Spain*
[2]*Centro de Física de Materiales–Materials Physics Center (CFM-MPC), 20018 Donostia, Spain*
[3]*Department of Applied Physics II, University of the Basque Country UPV/EHU, Bilbao, Spain*

rodrigo.aguilera@dipc.org

Ilmenene is a new 2D material that recently has been exfoliated from ilmenite ($FeTiO_3$)[1]. With the synthesis of this 2D material, the door is open to design other similar ilmenene systems. In this work, using density functional theory, we performance calculations of the structural, electronic and magnetic properties of the ilmenenes $TMTiO_3$, TM ended (with TM running from V to Zn). The ground state of magnetic states is antiferromagnetic, except for Zn with a spin compensated solution. The difference with the ferromagnetic system is around 0.01 eV/TM-atom, although for Cr and Cu ilmenenes differences are considerably larger. We established a simple electronic filling model for all materials, except for Cr and Cu, for which we find a Janh-Teller type distortion, breaking the degeneracy of the dxz and dyz orbitals. Magnetism in two-dimensional materials is promising for spintronics, and the synthesis of these materials would confirm the presence of structural distortions as well as the antiferromagnetic coupling.

References

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

Figures

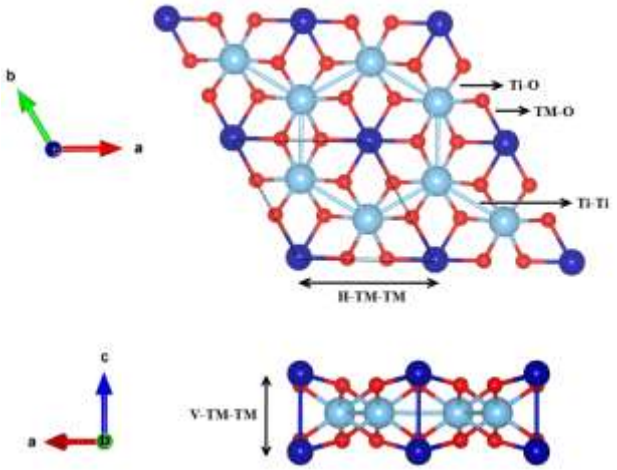

Figure 1: Top and side view of ilmenenes $TMTiO_3$, TM ended, where TM = V – Zn.

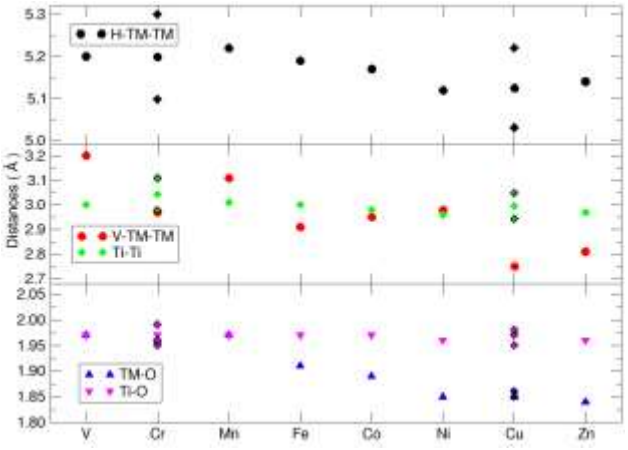

Figure 2: Interatomic distances (Following notation in Figure 1). The rhombus symbols denote distortions in the geometries due to the Jahn-Teller effect.