# Magnetic order and magnetic anisotropy in two-dimensional transition metal Ilmenenes

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Abstract

Iron ilmenene is a new two-dimensional material that has recently been exfoliated from the naturally occurring iron titanate found in ilmenite ore, a material that is abundant on the earth's surface [1]. In this work, we theoretically investigate the structural, electronic and magnetic properties of 2D transition-metal-based ilmenene-like titanates [2]. The study of magnetic order reveals that these ilmenenes usually present intrinsic antiferromagnetic coupling between the 3d magnetic metals decorating both sides of the Ti–O layer. Furthermore, the ilmenenes based on late 3d brass metals, such as $CuTiO_3$ and $ZnTiO_3$, become ferromagnetic and spin compensated, respectively. Our calculations which include spin–orbit coupling reveal that the magnetic ilmenenes have large magnetocrystalline anisotropy energies when the 3d shell departs from being either filled or half-filled, with their spin orientation being out-of-plane for elements below half-filling of 3d states and in-plane above. These interesting magnetic properties of ilmenenes make them useful for future spintronic applications because they could be synthesized as already realized in the iron case.

References

[1] A. Puthirath Balan *et al.*, *Chem. Mater.*, **30**, 5923-5931, 2018
[2] R.H. Aguilera-del-Toro, M. Arruabarrena *et al.*, *Nanoscale Adv.*, **5** 2813-2819, 2023

Figures

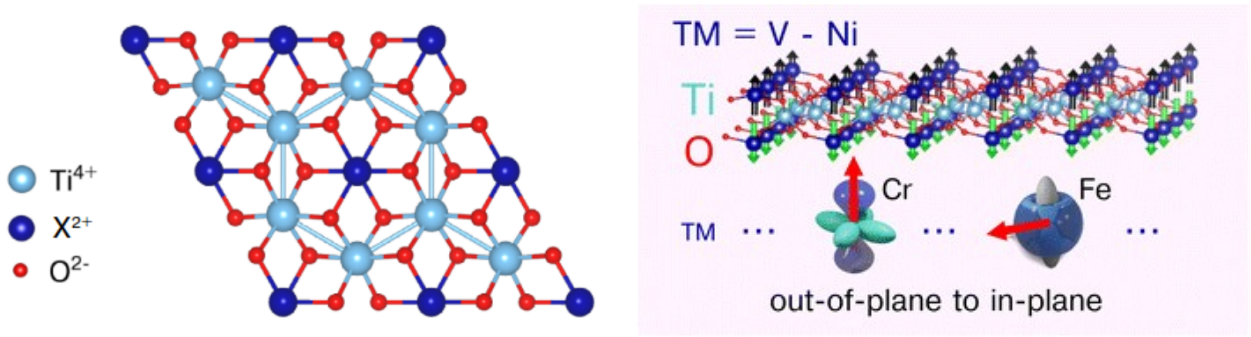


**Figure 1:** (Left) Top view of a single Transition metal Ilmenene layer. (Right) Schematic representation of the magnetic ground state of a TM Ilmenene layer. The spin-density models for CrTiO3 and FeTiO3 are depicted at the bottom, showing their respective out-of-plane and in-plane magnetic anisotropy.