

On the Quest for Intrinsic Magnetic Semiconductor Layers: Two-dimensional Transition-Metal Oxides

Andres Ayuela^{1,*}

Faustino Aguilera-Granja^{1,2}

¹ Centro de Fisica de Materiales-CFM-MPC, Donostia International Physics Center DIPC, Paseo Manuel de Lardizabal 5, 20018 San Sebastián, Spain

² Instituto de Física, Universidad Autónoma de San Luis Potosí, 78000 San Luis Potosí, Mexico

Contact@E-mail (swxayfea@sw.ehu.es)

Future nanoscale technological applications in spintronics require research on two-dimensional materials with combined semiconductor and magnetic properties. Semiconductor layers made of boron nitride BN [1] and silicon-carbon sulphides [2] were designed following an isoelectronic strategy from well-known 2D compounds such as graphene [3] and phosphorene [4]. Magnetic properties are currently being added to layers by having some traditional magnetic transition metal in the basic composition [5]. Here, we investigate transition metal dioxides in the form of layers, and we report on the structural and electronic properties of selected late transition metal d-elements [6]. With half-filled d states, the MnO₂ layers are magnetic semiconductors, and for side d-elements the CrO₂ and FeO₂ layers become half metals. These magnetic materials in 2D must be synthesized in order to assess their usefulness in future electronic and spintronic devices.

References

- [1] K. Watanabe, T. Taniguchi, and H. Kanda, *Nature Mater.* **3**, 404 (2004); K. S. Novoselov et al., *Proc. Natl. Acad. Sci. U.S.A.* **102**, 10 451 (2005).
- [2] Z. Zhu, J. Guan, D. Liu, and D. Tománek, *ACS Nano* **9**, 8284 (2015); J.-H. Yang, Y. Zhang, W.-J. Yin, X. Gong, B. I. Yakobson, and S.-H. Wei, *Nano Lett.* **16**, 1110 (2016); T. Alonso-Lanza, F. Aguilera-Granja, J. W. González, and A. Ayuela, *Phys. Rev. Materials* **1** 024001 (2017).
- [3] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, and A. A. Firsov, *Science* **306**, 666 (2004).
- [4] H. Liu, A. T. Neal, Z. Zhu, Z. Luo, X. Xu, D. Tománek, and P. D. Ye, *ACS Nano* **8**, 4033 (2014); A. Castellanos-Gómez, et al., *2D Mater.* **1**, 025001 (2014).
- [5] F. Aguilera-Granja & A. Ayuela, *A. J. Phys. Chem. C*, **124**, 2634 (2019).

Figures

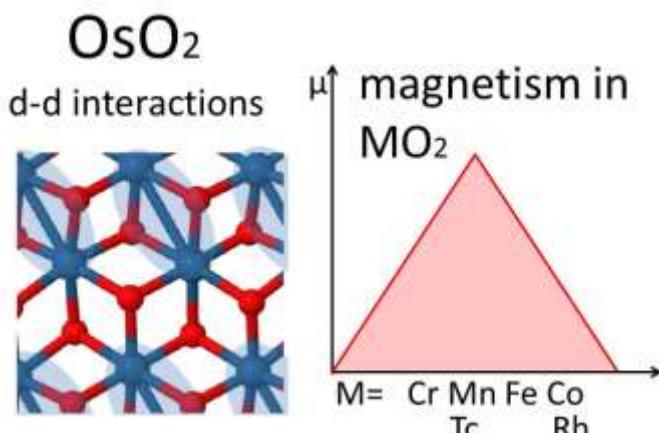


Figure 1: Structural deformations and general magnetic trends found for MO₂ being M a transition metal.