Studying 2D magnetic materials with high-throughput automated workflows from Density Functional Theory

Jaime Garrido Aldea [1], Jose Hugo García[1] Aguilar, Stephan Roche [1,3]
[1] ICN2, Instituto Catalan de Nanociencia y Nanotecnología UAB Campus, Bellaterra, 08193, Spain.
[2] Universitat Autònoma de Barcelona, Bellaterra, Campus UAB, 08139 Barcelona, Spain.
[3] ICREA — Institució Catalana de Recerca i Estudis Avançats, 08010 Barcelona, Spain.

jaime.garrido@icn2.cat

The experimental discovery of 2D magnetism in 2017 [1] was the spark that started the advent of 2D magnetic materials as pivotal components for emerging technologies, including spintronics [2], magnetic sensors [3] , and nonvolatile magnetic memories [4]. Despìte the increasing capability of computational resources, the myriad of possible new 2D magnetic materials makes their intensive individual study an intractable task [5]. Moreover, these materials are very difficult to model from first principles due to, for example, the variety of possible magnetic orders (Figure 1), the discrepancy in the results given by the different available methods (Figure 2) or the small energy scales of the crucial anisotropies of these materials. Under these circumstances, IA methods capable of unravelling properties of new materials emerge as a computationally long-term sustainable approach. But, in order to train these models, we need to pave the way for the creation of standardized and reliable datasets of magnetic properties. Some databases of 2D materials exist already [6], but they lack the necessary focus and meticulous attention to magnetic properties to ensure that the results are not only extensive but precise. Additionally, a paramount requirement for the design of high-throughput workflows responsible of creating these databases is the adhesion to the FAIR principles (Findable, Accessible, Interoperable, and Reusable) [7] in order to ensure full transparency and reproducibility in the calculation process. We aim to satisfy all these needs by creating an automated high-throughput workflow that calculates magnetic properties from Density Functional Theory results obtained from SIESTA [9]. Its results are then used to compute exchange constants and anisotropy terms with TB2J [9] that can be used as input for Montecarlo methods that calculate the critical temperature. This workflow is being implemented in the automation infrastructure AIIDA [8]. Its results will serve to identify the critical features required to further increase the Curie temperature of 2D magnets thus opening a new gate for lowpower low-dimensional magnetic memories.

References

[1] B. Huang, G. Clark, E. Navarro-Moratalla, D. R. Klein, R. Cheng, K. L. Seyler, D. Zhong, E. Schmidgall, M. A. McGuire, D. H. Cobden, W. Yao, D. Xiao, P. Jarillo-Herrero and X. Xu, Nature, 2017, 546, 270–273.
[2] S. N. Kajale, J. Hanna, K. Jang and D. Sarkar, Nano Research, 2024, 17, 743–762
[3] Y. Khan, S. M. Obaidulla, M. R. Habib, A. Gayen, T. Liang, X. Wang and M. Xu, Nano Today, 2020, 34, 100902
[4] X. Huang, L. Zhang, L. Tong, Z. Li, Z. Peng, R. Lin, W. Shi, K.-H. Xue, H. Dai, H. Cheng, D. de Camargo Branco, J. Xu, J. Han, G. J. Cheng, X. Miao and L. Ye, Nature Communications, 2023, 14, 2190.
[5] Feliciano Giustino et al, J. Phys. Mater., 3 (2021) 042006
[6] Sten Haastrup et al, 2D Mater., 5 (2018) 042002.
[7] Wilkinson, M., Dumontier, M., Aalbersberg, I. et al., Sci Data, 3 (2016) 160018.
[8] Huber, S.P., Zoupanos, S., Uhrin, M. et al, Sci Data, 7 (2020) 300
[9] Alberto García et al, J. Chem. Phys., 152 (2020) 204108
[10] Xu He et al, Computer Physics Communications, 264 (2021) 107938

Figures

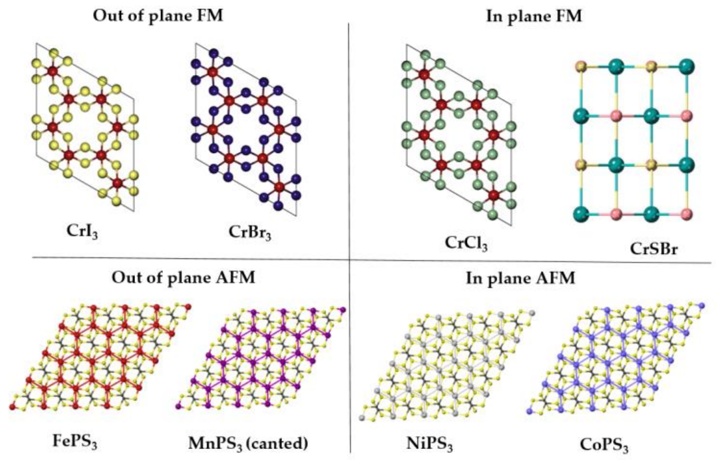

Figure 1. Classification of some important 2D materials in the monolayer limit.

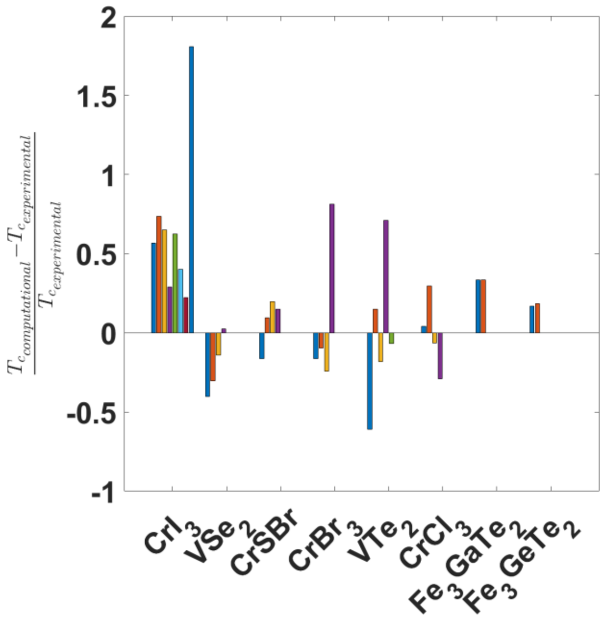

Figure 2. Comparison of calculated critical temperatures of 2D magnets with the experimental value.