Chemical engineering of magnetism in 2D materials

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The recent isolation of two-dimensional (2D) magnets offers tantalizing opportunities for spintronics, magnonics and quantum technologies at the limit of miniaturization. [1] In this presentation, I will provide an overview of our recent results on this fascinating topic. First, we will take advantage of the outstanding deformation capacity of 2D materials to answer the question: Can we use strain engineering to control spin waves propagation? [2] For that, we will focus on the magnetic properties of the air-stable 2D magnetic semiconductor CrSBr, investigating their evolution under mechanical strain using first-principles. Then, we will introduce the modulation of the magnetic properties, magnon dispersion and spin dynamics of this 2D magnet after the deposition of sublimable organic molecules, molecular spin qubits and spin-crossover molecules in a journey towards molecular controlled magnonics. [3, 4, 5] We will delve into the origin of the high T_C of Fe_3GaTe_2 [6] and, finally, we will introduce a coordination-driven chemical strategy to realize altermagnetic spin splitting in 2D planar tetracoordinated Cr-based metal-organic frameworks, enabling the rational design of 2D molecular materials with tunable altermagnetic properties for next-generation spintronic devices.[7]

References

[1] B. Huang *et al*., *Nature*, 546 (2017) 270–273.
[2] D. L. Esteras, A. Rybakov, A.M. Ruiz, J.J. Baldoví, *Nano Lett.*, 22 (2022) 8771–8778.
[3] A. M. Ruiz, G. Rivero-Carracedo, A. Rybakov, S. Dey, J.J. Baldoví, *Nanoscale Adv.*, 6 (2024) 3320–3328.
[4] S. Dey, G. Rivero-Carracedo, A. Shumilin, C. Gonzalez-Ballestero, J.J. Baldoví, *Nano Lett.*, 25 (2025) 10457–10464.
[5] A. Shumilin, S. Dey, D. Coltuneac, L. Stoleriu, J.J. Baldoví, *Adv. Mater.* (2026) Under review; arXiv:2512.17003.
[6] A.M. Ruiz, D.L. Esteras, D. López-Alcalá, J.J. Baldoví, *Nano Lett.*, 24 (2024), 7886–7894.
[7] D. López-Alcalá, A.M. Ruiz, A. Shumilin, J.J. Baldoví, *J. Am. Chem. Soc*. (2026) Under review; arXiv:2512.14623.

Figures

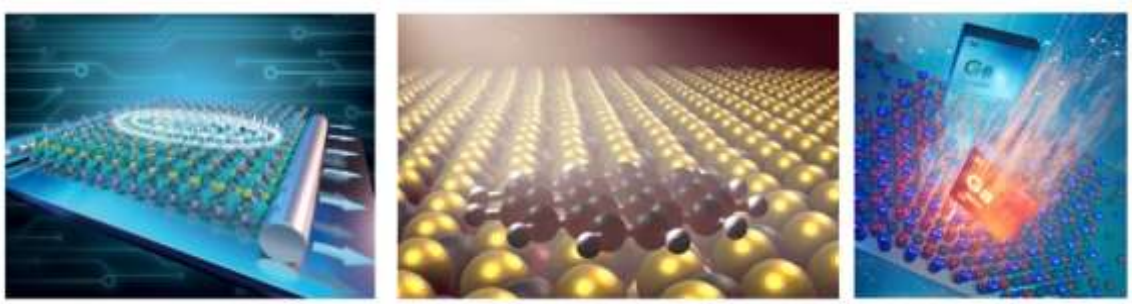

Figure 1: *Artistic representation of (left) magnon straintronics device showing the chemical structure of CrSBr; (center) an irradiated coronene molecule on the surface of a 2D magnetic material; (right) formation of a Fe_3GaTe_2 single-layer representing the enhancement of T_C with respect to Fe_3GeTe_2.*