Evolutionary Recipe: Designing Single Molecule Magnets for Spintronics

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As semiconductor and ferromagnet-based technologies approach their computational and memory-storage limits, spin-based technologies are emerging as viable alternatives. Magnetic molecules, serving as the smallest magnetic unit, hold promise for applications in spintronics and quantum computing. However, their current use is restricted to very low temperatures. The solution lies in harnessing the main underlying processes responsible for spin relaxation, i.e., the spin-phonon coupling, to design innovative magnetic molecules with extended spin lifetimes at ambient temperature [1]. Coordination compounds demonstrate significant potential in realizing single-ion magnets (SIMs), i.e., single-ion magnetic molecules with a large magnetic anisotropy that show a slow relaxation of their magnetization. Recent breakthroughs have led to the discovery of some SIMs with long spin lifetimes of up to 80 K as the result of 30-year design progress and a few hundred synthesized prototypes [2]. Further improving these systems towards ambient temperature cannot take another 30+ years and it is therefore mandatory to develop a more efficient design strategy.

In this study, we have designed a fully automated computational strategy for the discovery of new SIMs. A thorough screening, based on genetic algorithm efficiently and comprehensively explores the chemical space within cobalt (II) coordination compounds. These compounds have previously demonstrated significant magnetic anisotropy, making them an ideal choice for creating SIMs. We have compiled a reference dataset of ligands from the numerous ones we have identified in crystallography databases. By adding constraints for practical synthesis, we have screened through thousands of potential compounds, successfully identifying ones with even greater magnetic anisotropy than ever found. This investigation represents a strong discontinuity for the molecular magnetism community, which will have access to two orders of magnitude more compounds than ever synthesized so far [3].

References

[1] A. Lunghi, Alessandro, Sci. Adv. 8, eabn7880 (2022).
[2] F. Guo, et al, *Science* 362, 1400 (2018).
[3] P. Sahu, et al., *Coord. Chem. Rev.* 475, 214871 (2023).