Electric field induced spin crossover in the mixed-valence polyoxovanadate cage V_{12}

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One of the fundamental challenges in spintronics and quantum information processing is development of an efficient method of spin (qubit/qudit) manipulation on a molecular level. A promising alternative is the use of electric field, which contrary to the magnetic field can be applied locally (for instance by the tip of scanning tunneling microscope), with large strength and can be rapidly modulated.

Mixed-valence polyoxovanadate molecular magnets being susceptible to both electric and magnetic fields may serve as good candidates of molecular spins prone to electric manipulation. In this contribution two isostructural anions $[V_{12}As_8O_{40}(HCO_2)]^{n-}$ (with $n = 3, 5$) featuring two different mixed-valence states with itinerant and localized valence electrons are studied. The impact of the electric field on their magnetic properties is investigated by means of two complementary methods informed by magnetic measurements: effective Hamiltonian calculations and density functional theory. It is demonstrated that the magnetoelectric effect induced by relocation of itinerant electrons takes the form of a spin crossover, is highly anisotropic, depends on the valence state and can be detected even at room temperature. These findings can pave the way to practical applications in which an electric field control over spin state is required.

References:

[1] P. Kozłowski, doi: 10.48550/arXiv.2512.02215 submitted to Phys Rev. B