High performance single-molecule magnets, Orbach or Raman relaxation suppression?

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Abstract

The current figure of merit to evaluate Single Molecule Magnet (SMM) performance is the blocking temperature (T-B). The best SMMs showT(B)values close to liquid nitrogen boiling point (77 K) while their Orbach effective demagnetization barriers (U-eff) are significantly larger, exceeding 2000 K in some cases. As current high performance SMMs approach the axial limit, new strategies to suppress demagnetization by vibrational tuning have been suggested. In this article, we analyse a set of 17 current high performance SMMs to identify which demagnetization mechanism is limiting the blocking temperature. For the best systems (T-B> 50 K), the limiting mechanism is thermally assisted tunneling and the blocking temperature will depend on the exponential parametersU(eff)and tau(0). Strategies focusing on Raman (vibrational) suppression are expected to have a limited effect for this group. In contrast, systems with lower blocking temperatures (T-B< 50 K) would benefit from such strategies, although they are not expected to surpass current recordT(B)values. The Orbach limit for the blocking temperature can be conveniently estimated usingab initioCASSCF methods. Finally, a recent proposal for a hypothetical high performance SMM is analysed under the presented framework, showing its potential to improve record blocking temperatures.

Palabras clave

KeyWords Plus:ENERGY BARRIERS; BASIS-SETS; ANISOTROPY; ORIGIN

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