XXZ anisotropy in J_{eff}=1/2 triangular lattice antiferromagnets: a microscopic map from trigonal distortion

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Pseudospin-1/2 triangular-lattice antiferromagnets (TLAFs) are a central platform for studying geometrical frustration and quantum magnetism. A widely used minimal description is the antiferromagnetic XXZ model, which can be realized by spin–orbit-entangled J_{eff} = 1/2 Kramers doublets, as in high-spin Co^{2+} compounds [1]. Of particular current interest is the possible emergence of a quantum spin-supersolid phase [2, 3], whose stability is governed primarily by the exchange anisotropy $\alpha = J^{zz}/J^{\perp}$. In this talk, I show that, in an axial (trigonal) limit of the J_{eff} = 1/2 Kramers doublet with an (approximately) isotropic bare exchange in the physical-spin basis, α is bounded within the universal range $1/4 \leq \alpha \leq \infty$. Thereby, excluding an ideal XY limit ($\alpha = 0$), while still allowing the Ising limit ($\alpha = \infty$). I then apply this framework to prototypical Co-based pseudospin-1/2 XXZ TLAFs $Na_2BaCo(PO_4)_2$ and $K_2Co(SeO_3)_2$. This analysis reveals the microscopic origin of experimentally observed huge difference of α between these two systems [4, 5]. Furthermore, our first-principles-based modelling shows that alkaline-metal substitution systematically modifies the trigonal crystal field, providing a direct chemical route to tune α. I will also briefly comment on possible magnetoelectric effects in these compounds.

References

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