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Abstract for an Invited Paper
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First Principles Calculations and Spin Models¹

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Single magnetic molecules are fascinating entities. The individual transition metal ions have well defined spin states associated with localized d-orbitals bonded to ligands, which mediate the effective exchange or magnetic coupling among spins. At low temperatures and magnetic fields the internal complexity of the molecule can often (but not always) be ignored, with only the total collective spin determining the ground state and first few excited states. Using Mn₁₂ and V₁₅ as prototypes, this talk will describe a more reductionist approach and describe first principles electronic structure calculations used to gain insight into the electronic and magnetic structure of the individual transition metal ions and their interactions. Various spin coupling schemes and phenomenological Hamiltonians will be presented and compared to a variety of experimental results. Many colleagues and students from a number of institutions have contributed to this work and will be acknowledged during the talk.

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