MOLECULAR MAGNETISM UNDER ELECTRONS' ORBITAL PHASE CONSTRAINTS

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The large magnetic anisotropy and high blocking temperature of molecule magnets are underlined exclusively by the nature of the zero-field splitting that is directly influenced by the type of crystal field and type of the metal ion's open shell [1]. These systems may exhibit multiple microscopic magnetic states that might not be addressable via conventional parametrization schemes studying the electrons' orbital dynamics as unconstrained.

In order to study all possible microscopic magnetic states and obtain the one that uniquely reflects the compound's magnetic properties, a more complex theoretical approach is required. To this aim, we use the semi-classical multi-electron Hamiltonian formalism and exact diagonalization method to devise an improved post Hartree-Fock method accounting for the effect of constrained electron's orbital dynamics on the occurrence of zero-field splitting. The method was successfully applied to study the unexpected magnetic properties of two Nickel-based single-ion magnets [2] and shows the potential for studying arbitrary mononuclear nanomagnets.

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[2] M. Georgiev and H. Chamati, ACS Omega **8**, 28640 (2023); Sci. Rep. **15**, 11398 (2025).

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