MAR13-2012-020282

Abstract for an Invited Paper
for the MAR13 Meeting of
the American Physical Society

Theoretical calculations of spin dynamics and quantum effects in rare earth SMMs

ALEJANDRO GAITA-ARIÑO, Instituto de Ciencia Molecular, University of Valencia

Rare-earth single-molecular magnets constitute a hot emerging topic in molecular magnetism. It also constitutes a promising field to study and eventually remedy the processes that lead to decoherence. In fact, experiments show some success in the design of rare-earth spin qubits with long coherence times. Furthermore, these long-lived quantum states of rare-earth SMMs can in principle be manipulated for quantum information processing. In particular, a simple quantum error correction protocol might be realizable using ElectroNuclear DOuble Resonance. Going further on this path will require a detailed knowledge of the wave function of the low-energy multiplet, and an understanding of how it can be tailored by chemical means. An inexpensive point-charge model has been presented recently that is able to reproduce the main features of the Crystal Field Hamiltonian of both lanthanoids (such as Dysprosium, Holmium, Terbium) and actinoids such as Uranium.