Abstract

Role of the Orbital Ordering on Molecular Magnet Mn$_{12}$Ac

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Molecular magnets exhibit many novel nanostructure magnetic properties and potential application, while most of the present studies concentrate on the collective spin dynamics and quantum magnetic tunneling of molecular spin based on a phenomenal Heisenberg spin model, the spin is the only relevant freedom degree. This work focuses on the microscopic origin of the spin interaction in molecular magnets Mn$_{12}$Ac, we find the orbital freedom degree plays roles in the $S = 10$ groundstate and the spin dynamics. Starting from the orbital-degenerate Hubbard model, we obtain the superexchange magnetic coupling matrix for different orbitals between Mn ions by the second-order perturbation approach, orbital-dependent couplings among Mn ions stabilize the $S = 10$ configuration as realistic ground state and the groundstate energy gap by the exact diagonalization. Therefore the anisotropic spin interaction in Mn$_{12}$Ac is attributed to the spatial-symmetry-broken orbital interaction, the orbital dynamics is thus involved in the spin dynamics.