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Investigating the role of phonons in magnetic relaxation of molecular nanomagnets with inelastic neutron scattering

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In the quest for quantum technologies, Molecular Magnetism is offering a variety of promising systems. Indeed, Molecular NanoMagnets (MNMs) can either be exploited as classical bits in high-density magnetic memories or as qubits for quantum information processing. One of the most important goals in the current research in this field is to reach a deep understanding of magnetic relaxation and decoherence in MNMs, being this aspect of paramount importance in the design of new systems acting as classical or quantum bits. Despite their crucial role in relaxation dynamics, very limited experimental investigations on phonons in MNMs were performed so far. This motivated a series of Inelastic Neutron Scattering (INS) experiments that we performed with the aim to measure, for the first time, phonon dispersions and density of states (DOS) in MNMs.
In an innovative and challenging experiment we exploited 4-dimensional INS to directly investigate phonon dispersions in a molecular qubit [1]. 4D-INS is a very powerful technique to study phonons, since it enables a direct and immediate access to phonon dispersions by measuring the four-dimensional scattering function in large portions of the reciprocal space. We detected both acoustic and optical branches along different symmetry directions and we compared the results with DFT calculations of phonon energies and polarisation vectors. Both these quantities are in fact necessary for a quantitative evaluation of spin-phonon coupling coefficients, which contain information on the main contributions to relaxation dynamics. We also exploited INS to measure the DOS of Dy-based SMMs with high-energy anisotropy barrier but very different relaxation dynamics. We then combined the so-obtained vibrational properties with relaxation measurements to test a new theoretical approach for the relaxation dynamics of SMMs, able to give more physical insight than phenomenological models, but not as demanding as fully ab-initio calculations.
The results of these studies provided new hints for the design of new and better-performing systems for quantum information processing applications. In particular, we highlighted the role of low-energy non-dispersive phonon modes, which undermine coherence times in molecular qubits due to acoustic-optical phonons anticrossings and make Raman mechanisms more efficient in SMMs. Our latest results also involve the study of phonons with INS in applied hydrostatic pressure and the exploitation of complementary techniques like Inelastic X-ray Scattering.

[1] E. Garlatti, et al., Nat. Commun. 11, 1751 (2020).
[2] A. Chiesa, et al., Phys. Rev. B 101, 174402 (2020).
[3] E. Garlatti, et al., J. Phys. Chem. Lett. 12, 8826-8832 (2021).

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