

# Spin dynamics and phonons, insights into potential molecular qubits

*lunedì 9 settembre 2019 15:05 (20 minuti)*

Molecular spins are characterized by an effective electronic and magnetic tunability and this is a very relevant property for quantum computation applications [1]. In particular metal complexes have unpaired electrons located in the d orbitals, whose energy can be easily tuned using proper ligands; hence, metal complexes are very promising candidate to realize qubit devices. An accurate choice of the metal centre and of the ligands is able to substantially increase the spin coherence time [2], that is the basic requirement to implement operative qubits. In this framework, the effects of molecular and lattice vibrations, or phonons, on the spin relaxation mechanisms have been the focus of increasing attention. Thanks to our multitechnique approach, based on alternative current susceptibility, EPR and TeraHertz time-domain spectroscopy, we have evidenced correlation between low energy vibrations and spin relaxation time in molecular qubits [3,4]. Moreover, we have highlighted the role of the rigidity of the molecular structure and of the crystal lattice [4], together with the overall dimensionality [5], on phonons and on the spin dynamics. These recent results are here presented for a series of vanadyl-based compounds, where an appropriate choice of the ligand structure and of the coordination geometry allow to control the spin dynamics.

[1] A. Ghirri, *Magnetochem.* 3, 12 (2017).

[2] K. Bader, *Nat. Comm.* 5, 5304 (2014).

[3] M. Atzori, *JACS* 139, 4338 (2017).

[4] M. Atzori, *Inorg. Chem.* 57, 731 (2017).

[5] T. Yamabayashi, *JACS* 140, 38 (2018).

## Summary

## Topic

1. Phonons, plasmons, magnons and polaritons

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**Classifica Sessioni:** Afternoon Session 1