JOHANNES GUTENBERG UNIVERSITÄT MAINZ

# Seminar: Hard Condensed Matter Theory

**Room: Galileo room, 01-128 (Staudinger Weg 7)**
**Time: Tuesday, 10.12.2019, 14:00**


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# Spin Dynamics in Molecular Magnetic Materials: From First Principles to Machine Learning.


Molecular magnetic materials are among the most promising building blocks for quantum computing architectures and spintronic devices. Regardless the targeted application, the main fundamental challenge in the field concerns the extension of the spin life-time at ambient temperature. The interaction between spin and lattice's vibrations, namely the spin-phonon interaction, is the main limitation to the spin life-time. The microscopic mechanism by which spins relax is still debated due to both its inherent complexity and the lack of quantitative models that can consistently explain the vast phenomenology of spin relaxation.

In this seminar I will show the development of a series of computational approaches to tackle the challenge of predicting spin-lattice (T1) relaxations. Our formalism is based a spin Hamiltonian description of magnetism and exploits the Redfield equations in order to describe the dissipative effect of phonos on the molecular spin degrees of freedom. This formalism is then mapped onto electronic structure theory, such as Density Functional Theory and Complete Active Space SCF, in order to determine all the parameters of the model in a full first-principles fashion.

This formalism is used to describe spin-phonon interactions to the first order and present a quantitative and full first principles description of the direct relaxation process in a molecular qubit in high external fields[1]. The model includes the DFT calculation of the phonons over the entire Brillouin zone, the calculation of all the spin-phonon coupling coefficients coming from spin-spin dipolar interactions, hyperfine interaction and the Zeeman interaction.

The use of first principles provides an unbiased and rigorous approach to spin dynamics but requires large computational resources. I will also show our recent progresses in the development of a machine learning methods to predict general conformation-property landscapes[2,3]. These models are trained to reproduce the accuracy of ab-initio methods and can be used to speed-up spin-phonon dynamics simulations of several orders of magnitudes.



[1] A. Lunghi, S. Sanvito, Sci. Adv. **5**, eaax7163 (2019).
[2] A. Lunghi, S. Sanvito, Sci. Adv. **5**, eaaw2210 (2019).
[3] A. Lunghi, S. Sanvito, arXiv:1911.02263 (2019)


**All interested are cordially welcome!**


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