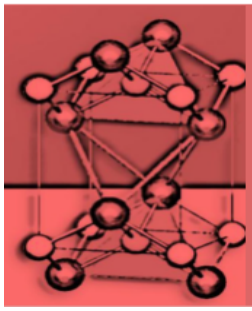

X Workshop on Novel Methods for Electronic Structure Calculations

04th – 06th December 2023
La Plata – Argentina

Spin-lattice couplings and Gilbert damping with *ab-initio* accuracy

Ivan P. Miranda [a]

[a] *Department of Physics and Astronomy, Uppsala University, Box 516, SE-75120 Uppsala, Sweden.*

email:

In the field of ultrafast magnetization dynamics, understanding the interplay between lattice, spin, and electronic degrees of freedom is a necessary step to the description of its origin. The microscopic picture can be initially draw based on the angular momentum and energy flows between those three main actors in play, which can, in turn, be characterized by their respective couplings. For systems with magnetic order, where a collective motion of spins exists, both magnetic moments and lattice degrees of freedom are coupled via the electronic medium, which can influence, for instance, both magnon and phonon spectrum and lifetimes.

Although a formalism to describe the magnetization dynamics accounting for the spin-lattice coupling (SLC) is known from many years ago [1], there is still a gap in the literature regarding the parameters for real materials, obtained with ab-initio accuracy. On the other hand, the coupling between the spins degree of freedom and the electronic system is related to the Gilbert damping (GD) parameter, which regulates the rate of energy dissipation from the former. I'll discuss the new theoretical developments to calculate both SLC and GD quantities from first principles, in the framework of a real-space linear muffin-tin orbital (LMTO) method.

The formulations are derived to provide input parameters for the phenomenological Landau-Lifshitz-Gilbert dynamics, in the atomistic description. Results and implications for elemental ferromagnetic materials (e.g., Fe, Co, Ni) will be also presented and examined.

[1]. V. P. Antropov, M. I. Katsnelson, B. N. Harmon, M. van Schilfgaarde, and D. Kusnezov, Phys. Rev. B 54, 1019 (1996).