O.21 Ultrafast magnetic phase transition in DyFeO₃

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Nowadays, ultrashort laser pulses (in femtosecond time scale) are being used to either excite materials and study its time resolved behaviour or to study intrinsic material properties and their dynamics in ultrafast time scales. Here we will present a combined experimental + DFT simulations work of a magnetic phase transition in DyFeO₃ from an non-collinear antiferromagnetic phase (AFM) to a non-collinear weak ferromagnetic phase (wFM) using ultrashort laser pulses.

In the experiment, the laser frequency is such that it excites the highest frequency polar mode of DyFeO₃. After this initial excitation, it is observed that oscillations responses at lower frequencies are present in the material and that is linked with the magnetic phase transition. To understad the underneath microscopic mechanism, we have done DFT simulations with the ABINIT code to study this phenomenon through non-linear phonon-phonon and spin-phonon couplings. The phonon-phonon coupling analysis shows that the highest frequency polar mode has a strong non-linear coupling to two of the lowest frequency invariant modes (Γ_1^+ label in the Pnma sapce group), also explaining the second low frequency regime observed experimentally. The spin-phonon coupling analysis shows that the non-linear phononic coupling can be seen as to quasistatically freezes the invariant mode in the structure at a picosecond time scale, which alter the exchange interaction between Dy and Fe magnetic sublattices. Together with a Heisenberg magnetic model including both Fe and Dy spins, we show that the Dy and Fe interactions modification through the non-linear phonon couplings is responsible for tuning the AFM to wFM phase transition.

This phase transition last longer compared to the initial laser pulse frequency and it is also happens orders of magnitude faster than phase transition driven by heat. This mechanism can have potential applications in spintronic devices if playing with time scale.

