Ab initio study of ultrafast laser-induced demagnetization in elemental ferromagnets and in FePt

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Ultrafast laser-excitation of a ferromagnet leads to a remarkably fast quenching of the equilibrium demagnetization on the femtosecond timescale. The origin of this phenomenon, which was discovered 25 years ago [1], is still being debated. The fast demagnetization offers possible ways to alter the magnetic moments on femtosecond time scales, i.e., much faster than timescales typical for (Landau-Lifshitz-Gilbert) magnetization dynamics.
We investigate the ultrafast demagnetization in elemental ferromagnets (Ni, Fe) as well as in FePt, using state-of-the-art real-time time-dependent density functional theory (TD-DFT), as implemented in the Octopus code [2]. Specifically, we investigate the influence of spin-orbit coupling, which is shown to play a significant role in the demagnetization. We further investigate for FePt how the interplay of inter-site charge transfer and spin-orbit mediated spin-flips causes the demagnetization on the femtosecond timescale. We elucidate how optical excitations can bring about demagnetization and we show that a significant contribution of the demagnetization is due to quenching of the spin angular momentum as compared to the contribution from the orbital angular momentum. To study the transfer of angular momentum to the lattice, we include motions of the atoms through Ehrenfest dynamics and search for evidence for non-equilibrium circular motions of atoms as was proposed in recent experiments [3].

References:

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[3] S. R. Tauchert *et al., Nature* 602, 73 (2022).