European XFEL

THEORY GROUP MEETING

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15:00

AER 19 Seminar Room 3.11

Laser induced ultrafast demagnetization in solids: a time-dependent density functional theory perspective

by

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Light induced demagnetization by intense laser pulses of a few picoseconds was demonstrated already in the 90s and recently these demagnetization times have been measured down to a few femtoseconds, owing to advances made in both the refinement of pump-probe and other experiments and designing of shorter and shorter time laser pulses. However, we are still far from achieving sufficiently controlled and fast manipulation of spins required for the production of useful devices. One main reason for this is that the underlying physical causes of laser induced demagnetization are not well understood and theory lags well behind experiments. Most of the existing theoretical work relies on model calculations and hence can only confirm experiments.

Time dependent density functional theory (TDDFT), which extends density functional theory into the time domain, is a formally exact method for describing the real-time dynamics of electrons under the influence of an external field such as the vector potential of the applied laser pulse. The advantage of such a technique is clear: it does not require any empirical parameters, is fully ab-initio and not only linear, but also includes all non-linear processes naturally as part of the simulation. Recently, using TDDFT, for the first time we predict the physics expected from magnetization dynamics by ultra-short laser experiments: we show that the demagnetization due to light- matter interaction occurs as a two step process where first the electrons make transitions to excited states, followed by spin-orbit-mediated spin-flip transitions which lead to a loss of moment. With future optimal control of spins in mind, we have also explored the effect of intensity, frequency and time of a laser pulse on the process of demagnetization.