

Ultrafast laser-induced demagnetization of solids: Understanding the mechanism with real-time TDDFT

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In the past two decades several experiments have demonstrated the laser-induced demagnetization of ferromagnetic solids in less than 100 femto-seconds. This is orders of magnitude faster than magnetic switching in present-day magnetic-field-based technology. To shed light on the underlying microscopic mechanism, we have performed an ab-initio study of Fe, Co, Ni and Cr in short laser pulses, using real-time non-collinear time-dependent spin density functional theory (TDDFT). We show [1] that the demagnetization proceeds in two distinct steps: First, a fraction of the electrons is excited without much change in the total spin polarization. In a second step, the spin magnetic moment of the remaining localized d-electrons decreases through spin-flip transitions induced by spin-orbit coupling. For pulse lengths of a few femto-seconds, the whole process of demagnetization happens in less than 50 femto-seconds. For antiferromagnetic Heusler compounds, such as Mn_3Ga and Ni_2MnGa , an even faster process is found [2] where magnetic moment is transferred from one sublattice to the other. Employing a combination [3] of TDDFT with Optimal Control Theory, we furthermore demonstrate how the demagnetization process can be controlled with suitably shaped laser pulses. Finally, we assess the influence of the approximation used for the exchange-correlation (xc) functional by comparing non-collinear LSDA results with a novel xc functional [4] that exerts a local exchange-correlation torque.

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[2] P. Elliott, T. Mueller, J. K. Dewhurst, S. Sharma, and E. K.U. Gross. arXiv 1603.05603 (2016).

[3] A. Castro, J. Werschnik, and E. K.U. Gross. *Controlling the dynamics of many-electron systems from first principles: A combination of Optimal Control and Time-Dependent Density-Functional Theory*, Phys. Rev. Lett. **109**, 153603 (2012).

[4] F. G. Eich and E. K. U. Gross. *Transverse spin-gradient functional for noncollinear spin-density-functional theory*, Phys. Rev. Lett. **111**, 156401 (2013).