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A fast time-dependent density functional theory method for the simulation of ultrafast demagnetization induced by laser ZHANGHUI CHEN, LIN-WANG WANG, Lawrence Berkeley Natl Lab, MAGNETIC PROJECT TEAM — We present a fast real-time time-dependent density functional theory method to investigate the ultrafast spin dynamics induced by laser. The Hamiltonian considers non-collinear magnetic moment, spin-orbital coupling and electron-laser interaction. An accelerated method with leapfrog prediction of charge matrix is used to solve the time-evolving equation. The investigation of Ni bulk found that the spin demagnetization consists of one time-lag stage and one fast demagnetization stage followed by one slow demagnetization stage. The time-lag and fast stages are mainly affected by the spin-electron interaction and their interactions with photons while the slow stage is affected by phonon-related interaction. Demagnetization appears only when spin-oribital coupling effect is considered. We further demonstrated how to manipulate the spin dynamics by changing laser fluence, duration and wavelength.

Zhanghui Chen
Lawrence Berkeley Natl Lab

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