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A fast time-dependent density functional theory method for ultrafast magnetic dynamics induced by laser ZHANGHUI CHEN, LIN-WANG WANG, Lawrence Berkeley Natl Lab — Ultrafast demagnetization has attracted a thriving interest, but the fundamental mechanism is still intensively debated. We present a fast real-time time-dependent density functional theory method to investigate the ultrafast spin dynamics induced by laser in nickel bulk and clusters. The Hamiltonian considers non-collinear magnetic moment, spin-orbital coupling, electron-phonon and electron-photon interaction. An accelerated method with leapfrog prediction of charge matrix is used to solve the time-evolving equation. We have observed remarkable energy gain from laser and spin demagnetization that consists of one time-lag stage and one fast demagnetization stage followed by one slow demagnetization stage. The evolution and conservation of angular momentum show that laser induces a large change of electron orbital angular momentum, which supplies part of the spin moment loss by spin-orbital coupling. Another reservoir from ions also plays important role in demagnetization through rapid electron-ion exchange interaction. Finally, further demonstrations are shown for the impact of initial ionic random dynamic and laser parameters, which helps understand the gap between theory and experiment as well as the thermal driving.

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