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Studies of Ultrafast Demagnetization in Ferromagnetic Metal Alloys using TDDFT PETER ELLIOTT, KEVIN KRIEGER, JOHN KAY DE-WHURST, SANGEETA SHARMA, E.K.U. GROSS, Max Planck Institute of Microstructure Physics — Time dependent density functional theory (TDDFT) has recently [1,2] been applied to study magnetization dynamics in periodic systems. In particular it was found for short intense pulses, a significant source of demagnetization is spin-flips mediated by the spin-orbit interaction. In this work, we perform TDDFT simulations for the case of bulk Heusler compounds under the same conditions, and find a similar loss of the global magnetic moment can occur. Furthermore, we also see local loss of moment due to transfer of moment from one sublattice to another during the optical excitation process. This is then followed by the spinorbit mediated demagnetization in certain cases. Additionally we will analyze the spin-current densities to better understand the various processes at work. [1] Laser induced ultrafast demagnetization: an ab-initio perspective, K. Krieger, J.K. Dewhurst, P. Elliott, S. Sharma, E.K.U. Gross, J. Chem. Theory and Comput. 11, 4870 (2015). [2] Demonstration of Optimal Control of Laser Induced Spin-Orbit Mediated Ultrafast Demagnetization, P. Elliott, K. Krieger, J. K. Dewhurst, S. Sharma, E. K. U. Gross, submitted (2015).

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