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TDDFT studies of Spin-Flip and Spin-Current Ultrafast Demagnetization PETER ELLIOTT, KEVIN KRIEGER, J. KAY DEWHURST, SANGEETA SHARMA, E.K.U. GROSS, Max-Planck Institute of Microstructure Physics — We apply the ab-initio simulation method of time dependent density functional theory (TDDFT) to shed light on the underlying physics of ultrafast demagnetization in ferromagnetic materials due to intense laser pulses. A key finding of our previous work is that spin-flips due to the spin-orbit interaction (SOI) can be responsible for ultrafast loss of moment, under the right circumstances. In this work we compare the loss of moment due to 1) spin transport (i.e. transport of the moment from a ferromagnetic layer into a substrate) and 2) spin-flip SOI demagnetization happening in the magnetic layer itself. For the interfaces we study, we find that both processes contribute equally to the demagnetization of the ferromagnet. Furthermore we predict that if the substrate has strong SOI character (e.g. Pt), there can even be SOI type demagnetization of the moment that was transported into the substrate.

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