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Ab initio calculation of magnetic interactions and time-dependent density functional theory simulation for ultrafast magnetic dynamics ZHANGHUI CHEN, LIN-WANG WANG, Lawrence Berkeley Natl Lab — The competition between exchange interaction and spin-orbital coupling, especially in the presence of the symmetry-breaking of interfaces, provides a path to magnetic interactions which can cause novel magnetic structures like skyrmions. We will use a noncollinear spin ab initio calculation to predict the spin-spin interactions near such interfaces. A new algorithm is developed for such calculations. Similarly, a newly developed fast time-dependent density functional theory algorithm will be used to study femtosecond spin relaxation after an initial excitation by a fast laser pulse. Such simulation is mean to reveal the underlying mechanism which causes fast magnetic decays.

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