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First-principles dynamical calculation of a pump-probe scenario for the spin flip on NiO GEORGIOS LEFKIDIS, WOLFGANG HÜBNER, University of Kaiserslautern — Using a fully ab-initio approach we calculate in a dynamic way the time-dependent probe signal of a spin flip scenario on the antiferromagnetic NiO surface. We start from a first-principles calculation of the highly correlated, relativistic, electronic states of a doubly embedded NiO_5^{-8} cluster followed by the time-propagation of the system under the influence of the spin-flipping pump pulse *and* the detecting probe pulse. This way we treat both pulses on equal footing and, for the first time, consider the effects of the electronic non-equilibrium due to the concurrent presence of the pulses. Our time-resolved calculations reveal the subtle influence of the probe pulse itself on the detection signal, which cannot be completely treated solely by the time propagation of the pump pulse and the subsequent calculation of the static susceptibility tensor [1,2]. We also analyze the angular-momentum conservation and its distribution among the system and both laser pulses [3].

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