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First-principles laser-driven magnetic switching scenario in NiO GEORGIOS LEFKIDIS, WOLFGANG HÜBNER, Kaiserslautern University of Technology — The dispersionless discrete intragap d-character levels of the (001) surface and the bulk of NiO can be selectively addressed by laser pulses and thus serve as intermediate levels for a Lambda-based all-optical magnetic switching scenario [1]. To this goal the existence of spin-mixing terms in the Hamiltonian of the system is essential, in our case it is the spin-orbit coupling term in combination with a static external magnetic field. We compute from first principles the aforementioned intragap levels with high-level correlated quantum chemistry on a doubly embedded cluster model [2] and we propagate the population in time under the influence of the laser field. The polarization, duration, shape and geometrical dependences on the laser pulse as well as the influence of the static magnetic field are shown, and the importance of going beyond the electric dipole approximation is discussed.

[1] R. Gómez-Abal, O. Ney, K. Satitkovitchai and W. Hübner, Phys. Rev. Lett. 92, 227402 (2004)
[2] G. Lefkidis and W. Hübner, Phys. Rev. Lett. 95, 77401 (2005).

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