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**First-principles calculations of laser-induced spin manipulation in small magnetic clusters with CO** CHUN LI, GEORGIOS LEFKIDIS, WOLFGANG HÜBNER, Kaiserslautern University of Technology — We present a fully *ab initio* controlled ultrafast magneto-optical switch and transfer mechanism in small magnetic clusters exploiting spin-orbit-coupling enabled  $\Lambda$ -processes [1-3]. Two-magnetic-center clusters with CO attached to one of the magnetic atoms are studied to achieve a mapping of the laser-induced spin manipulation to the IR spectrum of CO. The predicted spin-state-dependent CO frequencies can facilitate experimental monitoring of the processes. The lower electronic states of the clusters exhibit a very high degree of spin localization either at the Co or the Ni site. Spin flip on one magnetic atom and transfer from one magnetic center to the other are realized in structurally optimized magnetic clusters with fidelities that reach 99.8%.

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