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Femtosecond functionalization of magnetic 2- and 3-center nanostructures WOLFGANG HÜBNER, Kaiserslautern University of Technology and Research Center OPTIMAS, Box 3049, 67653 Kaiserslautern, Germany, SANDER KERSTEN, Eindhoven University of Technology, Box 513, 5600 MB, Eindhoven, The Netherlands, CHUN LI, Northwestern Polytechnical University, Box 883, Xian 710129, P. R. China, GEORG LEFKIDIS, Kaiserslautern University of Technology and Research Center OPTIMAS, Box 3049, 67653 Kaiserslautern, Germany — We present an *ab initio* theory of ultrafast nanologic elements based on optical Λ-processes [1]. Using high-level quantum chemistry we show that in 2- and 3-magnetic-center structures containing Fe, Co and Ni as active centers both spin flips and spin transfers are possible within a hundred femtoseconds. Spin transfer can be resolved by a sufficiently large shift of the vibrational stretch frequency of a CO marker [2]. From 3-magnetic-center clusters we are able to construct OR, XOR (CNOT), and AND gates [3]. Thus multicenter magnetic clusters allow to exploit spin dynamics for full-fledged logic functionalization.

[1] G. Lefkidis, G. P. Zhang, and W. Hübner, PRL (2009, in press)
[2] C. Li, T. Hartenstein, G. Lefkidis and W. Hübner **79**, 180413(R) (2009)
[3] W. Hübner, S. Kersten and G. Lefkidis PRB **79**, 184431 (2009)

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