

Ultrafast spin-flip dynamics in transition metal complexes triggered by soft X-ray light

H. Wang¹, S.I. Bokarev^{1*} and O. Kühn¹

¹ *Institute of Physics, University of Rostock, Albert-Einstein-Str. 23-24, 18059 Rostock, Germany*

*Corresponding author: sergey.bokarev@uni-rostock.de

Recent advances in attosecond spectroscopy open the door to understanding the correlated motion of valence and core electrons on their intrinsic timescales. For valence excitations, processes related to the electron spin are usually driven by nuclear motion. When going, however, to the core-excited states where the core hole has a nonzero angular momentum, a strong spin-orbit coupling starts to play a role [1-3]. In this work, we present a theoretical simulation of an ultrafast spin-flip dynamics driven solely by spin-orbit coupling and electron correlation in the L-edge (2p→3d) excited states of a prototypical Fe(II) complex, which occurs faster than the core hole lifetime (about 4 fs) [4]. The non-equilibrium electron dynamics is studied by means of time-dependent restricted active space configuration interaction recast in the form of reduced density matrix propagation. The spin-orbit coupling between electronic states of different multiplicity is considered within the LS-coupling limit employing atomic mean-field integral approximation. Dissipative effects of electronic and vibrational origin are considered as well. A detailed analysis of such phenomena will help to gain a fundamental understanding of spin-crossover processes and build up the basis for their control by light.

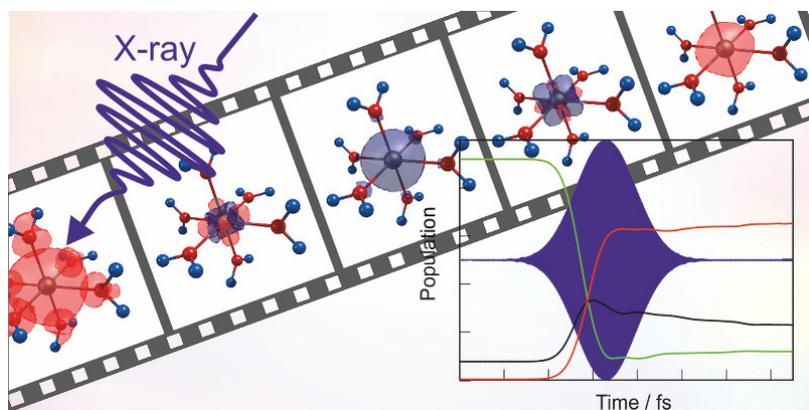


Figure 1: Time-evolution of spin-density and spin-state population for a prototypical Fe(II) complex.

Acknowledgments: We acknowledge financial support by the Deanship of Scientific Research (DSR), King Abdulaziz University, Jeddah, (grant No. D-003-435) and the Deutsche Forschungsgemeinschaft (grant No. KU952/10-1).

References

- [1] S.I. Bokarev, M. Dantz, E. Suljoti, O. Kühn, E.F. Aziz *Phys. Rev. Lett.* 2013, **111**, 083002.
- [2] S.I. Bokarev, M. Khan, M.K. Abdel-Latif, J. Xiao, R. Hilal, S.G. Aziz, E.F. Aziz, O. Kühn *J. Phys. Chem. C* 2015, **119**, 19192-19200.
- [3] R. Golnak, S.I. Bokarev, R. Seidel, J. Xiao, G. Grell, K. Atak, I. Unger, S. Thürmer, S.G. Aziz, O. Kühn, B. Winter, E.F. Aziz *Sci. Rep.* 2016, **6**, 24659.
- [4] H. Wang, S.I. Bokarev, S.G. Aziz, O. Kühn 2016 *submitted*.