Publications

1) M. Roemelt, B. Schille, R. Francke, "The electrochemical reduction of carbon dioxide using molecular electrocatalyts" *Chem. Rev.* **invited review, submitted**

2) O. Koleda, T. Broese, J. Noetzel, M. Roemelt, E. Suna, R. Francke "Synthesis of Benzoxazoles Using Electrochemically Generated Hypervalent Iodine" *J. Org. Chem.* **submitted**

3) A. Sharma, M. Roemelt, M. Reithofer, R. R. Schrock, B. M. Hoffman, F. Neese "EPR/ENDOR and theoretical study of the Jahn-Teller active [HIPTN$_3$N]Mo(V)L complexes (L = N-, NH)" *Inorg. Chem.* **2017**, 56, 6906–6919

4) A. Rosas-Hernández, H. Junge, M. Beller, M. Roemelt, R. Francke "Cyclopentadienone iron complexes as efficient and selective catalysts for the electroreduction of CO_2" *Cat. Sci. Technol.* **2017**, 7, 459-467

5) M. Roemelt, S. Guo, G. K.-L. Chan "A Projected Approximation to Strongly Contracted N-Electron Valence Perturbation Theory for DMRG Wavefunctions" *J. Chem. Phys.* **2016**, 144, 204113

6) M. Roemelt "Spin-Orbit Coupling for ab initio Molecular Density Matrix Renormalization Group Calculations: Application to g-Tensors" *J. Chem. Phys.* **2015**, 143, 044112

7) A. B. Vliegenthart, F. A. L. Welling, M. Roemelt, R. J. M. Klein Gebbink, M. Otte, *Org. Lett*. **2015**, 17, 4172-4175.

8) D. Maganas, M. Roemelt, T. Weyermueller, R. Blume, M. Haevecker, A. Knop-Gericke, S. DeBeer, R. Schlögl, F. Neese "L-Edge X-Ray Absorption Study of Mononuclear Vanadium Complexes and Spectral Predictions Using a Restrictied Open-Shell Configuration Interaction Ansatz" *Phys. Chem. Chem. Phys.* **2014**, 16, 264-276

9) M. Roemelt, D. Maganas, S. DeBeer, F. Neese "A Combined DFT and Restricted Open-Shell Configuration Interaction Method Including Spin-Orbit Coupling: Application to Transition Metal L-Edge X-Ray Absorption Spectroscopy" *J. Chem. Phys.* **2013**, 138, 204101.

10) D. Maganas, M. Roemelt, M. Hävecker, A. Trunschke, A. Knop-Gericke, R. Schlögl, F. Neese "First principles calculations of the structure and V L-edge X-ray absorption spectra of V_2O_5 using local pair natural orbital coupled cluster theory and spin–orbit coupled configuration interaction approaches" *Phys. Chem. Chem. Phys.* **2013**, 15, 7260-7276

11) M. Roemelt, F. Neese "Excited States of Large Open-Shell Molecules: An Efficient, General and Spin-Adapted Approach Based on a Restricted Open-Shell Ground State Wavefunction" *J. Phys. Chem. A* **2013**, 117, 3069–3083.

12) M. Maekawa, M. Roemelt, C. G. Daniliuc, P. G. Jones, P. S. White, F. Neese, M. D. Walter "Reactivity studies on [Cp′MnX(thf)]$_2$: manganese amide and polyhydride synthesis" *Chem. Sci.* **2012**, 3, 2972-2979

13) M. Roemelt, M. A. Beckwith, C. Duboc, M. N. Collomb, F. Neese, S. DeBeer. "Manganese K-Edge Absorption Spectroscopy as a Probe of the Metal-Ligand Interactions in Coordination Compounds" *Inorg. Chem.* **2012**, 51, 680-687.

14) K. M. Lancaster, M. Roemelt, P. Ettenhuber, Y. Hu, M. W. Ribbe, F. Neese, U. Bergmann, S. DeBeer. "X-Ray Emission Spectroscopy evidences a central carbon in the Nitrogenase Iron-Molybdenum Cofactor" *Science* **2011**, 334, 974-977.

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