List of Publications

January 2019

23 peer-reviewed articles, reviews and book contributions, h-index 13 (2019, Web of Science)

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Publications as corresponding author are marked with an asterisk (*).

Peer-reviewed research articles

19. F. Schendzielorz, M. Finger, J. Abbenseth, C. Wurtele, V. Krewald, S. Schneider
* *Metal-Ligand Cooperative Synthesis of Benzonitrile by Electrochemical Reduction and Photolytic Splitting of Dinitrogen*
Angew. Chem. **2019**, 58, 830–834. DOI: 10.1002/anie.201812125

18. W. J. M. Blackaby, S. Sabater, R. C. Poulten, M. J. Page, A. Folli, V. Krewald, M. F. Mahon, D. Murphy, E. Richards, M. K. Whittlesey
* *Mono- and dinuclear Ni(I) products formed upon bromide abstraction from the Ni(I) ring-expanded NHC complex [Ni(6-Mes)(PPh_3)Br]*
Dalton Trans. **2018**, 47, 769–782. DOI: 10.1039/C7DT04187J

17. M. Roemelt, V. Krewald, D. A. Pantazis
* *Exchange coupling interactions from the density matrix renormalization group and N-electron valence perturbation theory: application to a biomimetic mixed valence manganese complex*
J. Chem. Theory Comput. **2018**, 14, 166–179. DOI: 10.1021/acs.jctc.7b01035

16. V. Krewald, L. González *(personal invitation)*
* *A valence-delocalised osmium dimer capable of dinitrogen photocleavage: ab initio insights into its electronic structure*
Chem. Eur. J. **2018**, online. DOI: 10.1002/chem.201704651

15. T. Lohmiller, V. Krewald, A. Sedoud, A. W. Rutherford, F. Neese, W. Lubitz, D. A. Pantazis, N. Cox
The first substrate water of nature's water-oxidizing complex is incorporated as a μ-hydroxo bridge during catalyst regeneration
J. Am. Chem. Soc. **2017**, 139, 14412–14424. DOI: 10.1021/jacs.7b05263

14. P. M. Kusen, G. Wandrey, V. Krewald, M. Holz, S. Meyer zu Berstenhorst, J. Büchs, J. Pietruska
Light-controlled gene expression in yeast using photocaged Cu^{2+}
J. Biotechnol. **2017**, 258, 117–125. DOI: 10.1016/j.jbiotec.2017.04.032

13. V. Krewald, D. A. Pantazis
* *Understanding and tuning the properties of redox-accumulating manganese helicates*
Dalton Trans. **2016**, 45, 18900–18908. DOI: 10.1039/C6DT02800D

12. V. Krewald, F. Neese, D. A. Pantazis
Redox potential tuning by redox-inactive cations in Nature's water oxidizing catalyst and synthetic analogues
Phys. Chem. Chem. Phys. **2016**, 18, 10739–10750. DOI: 10.1039/C5CP07213A

11. M. Retegan, V. Krewald, F. Mamedov, F. Neese, W. Lubitz, N. Cox, D. A. Pantazis
A five-coordinate Mn(IV) intermediate in biological water oxidation: spectroscopic signature and a pivot mechanism for water binding
Chem. Sci. **2016**, 7, 72–84. DOI: 10.1039/C5SC03124A
    - Highly cited paper in Web of Science as of March/April 2016

10. M. A. Beckwith, W. Ames, F. D. Villa, V. Krewald, D. A. Pantazis, C. Mantel, J. Pécaut, M. Gennari, C. Duboc, M.-N. Collomb, J. Yano, J. J. Rehr, F. Neese, S. DeBeer
How accurately can extended X-ray absorption spectra be predicted from first principles? Implications for modelling the oxygen-evolving complex in photosystem II
J. Am. Chem. Soc. **2015**, 137, 12815–12834. DOI: 10.1021/jacs.5b00783

09. V. Krewald, M. Retegan, N. Cox, J. Messinger, W. Lubitz, S. DeBeer, F. Neese, D. A. Pantazis
Metal oxidation states in biological water splitting
Chem. Sci. **2015**, 6, 1676–1695. DOI: 10.1039/c4sc03720k
    - Highly cited paper in Web of Science as of July/August 2015
    - Featured in *chemistryworld* by the Royal Society of Chemistry, in Comp. Chem. Highlights and by Scientific American (scientificamerican.com/article/artificial-photosynthesis-for-energy-takes-a-step-forward/)

08. V. Martin-Diaconescu, M. Gennari, B. Gerey, E. Tsui, J. Kanady, R. Tran, J. Pécaut, D. Maganas, V. Krewald, E. Gouré, C. Duboc, J. Yano, T. Agapie, M.-N. Collomb, S. DeBeer
Ca K-edge XAS as a probe of calcium centers in complex systems
Inorg. Chem. **2015**, 54, 1283–1292. DOI: 10.1021/ic501991e

07. T. Lohmiller, V. Krewald, M. P. Navarro, M. Retegan, L. Rapatskiy, M. M. Nowaczyk, A. Boussac, F. Neese, W. Lubitz, D. A. Pantazis, N. Cox
Structure, ligands and substrate coordination of the oxygen-evolving complex of photosystem II in the S_2 state: a combined EPR and DFT study
Phys. Chem. Chem. Phys. **2014**, 16, 11877–11892. DOI: 10.1039/c3cp55017f

06. V. Krewald, B. Lassalle-Kaiser, T. T. Boron, C. J. Pollock, J. Kern, M. A. Beckwith, V. K. Yachandra, V. L. Pecoraro, J. Yano, F. Neese, S. DeBeer
The protonation states of oxo-bridged Mn^{IV} dimers resolved by experimental and computational Mn K pre-edge X-ray absorption spectroscopy
Inorg. Chem. **2013**, 52, 12904–12914. DOI: 10.1021/ic4008203

05. B. Lassalle-Kaiser, T. T. Boron, V. Krewald, J. Kern, M. A. Beckwith, M. U. Delgado-Jaime, H. Schroeder, R. Alonso-Mori, D. Nordlund, T.-C. Weng, D. Sokaras, F. Neese, U. Bergmann, V. K. Yachandra, S. DeBeer, V. L. Pecoraro, J. Yano
Experimental and computational X-ray emission spectroscopy as a direct probe of protonation states in oxo-bridged Mn^{IV} dimers relevant to redox-active metalloproteins
Inorg. Chem. **2013**, 52, 12915–12922. DOI: 10.1021/ic400821g

04. V. Krewald, F. Neese, D. A. Pantazis
On the magnetic and spectroscopic properties of high-valent Mn_3CaO_4 cubanes as structural units of natural and artificial water-oxidizing catalysts
J. Am. Chem. Soc. **2013**, 135, 5726–5739. DOI: 10.1021/ja312552f

03. A. A. Milischuk, V. Krewald, B. M. Ladanyi
Water dynamics in silica nanopores: The self-intermediate scattering functions
J. Chem. Phys. **2012**, 136, 224704. DOI: 10.1063/1.4724101

02. W. Ames, D. A. Pantazis, V. Krewald, N. Cox, J. Messinger, W. Lubitz, F. Neese
Theoretical evaluation of structural models of the S_2 state in the oxygen evolving complex of photosystem II: Protonation states and magnetic interactions
J. Am. Chem. Soc. **2011**, 133, 19743–19757. DOI: 10.1021/ja2041805

01. D. A. Pantazis, V. Krewald, M. Orio, F. Neese
Theoretical magnetochemistry of dinuclear manganese complexes: Broken symmetry density functional theory investigation on the influence of bridging motifs on structure and magnetism
Dalton Trans. **2010**, 39, 4959–4967. DOI: 10.1039/c001286f

Peer-reviewed overview articles and chapters in collective volumes

–. V. Krewald, D. A. Pantazis *(personal invitation)*
* *Applications of the Density Matrix Renormalization Group to Exchange-Coupled Transition Metal Systems*
Transition metals in coordination environments: computational chemistry and catalysis viewpoints, Eds: E. Broclawik. T. Borowski, M. Radoń; *in press*

04. V.Krewald *(personal invitation)*
* *Dinitrogen Photocleavage: Status Quo and Future Perspectives*
Dalton Trans. **2018**, 47, 10320–10329. DOI: 10.1039/c8dt00418h

03. V. Krewald, M. Retegan, F. Neese, W. Lubitz, D. A. Pantazis, N. Cox
Spin state as a marker for the structural evolution of Nature's water splitting catalyst
Inorg. Chem. **2016**, 55, 488–501. DOI: 10.1021/acs.inorgchem.5b02578

02. V. Krewald, M. Retegan, D. A. Pantazis
Principles of Natural Photosynthesis
in *Top. Curr. Chem.* **2016**, 371, 23–48, Springer Berlin Heidelberg. DOI: 10.1007/128_2015_645
    - Highly cited paper in Web of Science as of March/April 2016

01. V. Krewald, F. Neese, D. A. Pantazis
Resolving the manganese oxidation states in the oxygen evolving catalyst of natural photosynthesis
Isr. J. Chem. **2015**, 55, 1219–1232. DOI: 10.1002/ijch.201500051