List of publications: Prof. Dr. Serena DeBeer

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- Spiller, N., Chilkuri, V.G., **DeBeer, S.**, Neese, F. (2020). Sulfur vs. Selenium as Bridging Ligand in Di-Iron Complexes: A Theoretical Analysis *European Journal of Inorganic Chemistry* https://doi.org/10.1002/ejic.202000033
- Maganas, D., Kowalska, J.K., Van Stappen, C., **DeBeer, S.**, Neese, F. (2020). Mechanism of $L_{2,3}$-edge X-Ray Magnetic Circular Dichroism Intensity from Quantum Chemical Calculations and Experiment - A case study on $V^{(IV)}/V^{(III)}$ complexes *The Journal of Chemical Physics* 152(11), 114107. https://doi.org/10.1063/1.5129029
- Cutsail III, G.E., Blaesi, E.J., Pollock, C.J., Bollinger Jr, J.M., Krebs, C., **DeBeer, S.** (2020). High-resolution iron X-ray absorption spectroscopic and computational studies of non-heme diiron peroxo intermediates *Journal of Inorganic Biochemistry* 203, 110877. https://doi.org/10.1016/j.jinorgbio.2019.110877
- Birrell, J.A., Pelmenschikov, V., Mishra, N., Wang, H., Yoda, Y., Tamasaku, K., Rauchfuss, T.B., Cramer, S.P., Lubitz, W., **DeBeer, S.** (2020). Spectroscopic and Computational Evidence that [FeFe] Hydrogenases Operate Exclusively with CO-bridged Intermediates *Journal of the American Chemical Society* 142(1), 222-232. https://doi.org/10.1021/jacs.9b09745
- Chilkuri, V.G., **DeBeer, S.**, Neese, F. (2020). Ligand Field Theory and Angular Overlap Model Based Analysis of the Electronic Structure of Homovalent Iron–Sulfur Dimers *Inorganic Chemistry* 59(2), 984-995. https://doi.org/10.1021/acs.inorgchem.9b00974
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- DeRosha, D.E., Chilkuri, V.G., Van Stappen, C., Bill, E., Mercado, B.Q., **DeBeer, S.**, Neese, F., Holland, P.L. (2019). Planar three-coordinate iron sulfide in a synthetic [4Fe-3S] cluster with biomimetic reactivity *Nature Chemistry* 11, 1019–1025.
- https://doi.org/10.1038/s41557-019-0341-7
- McGale, J., Cutsail, G.E. III, Joseph, C., Rose, M.J., **DeBeer, S.** (2019). Spectroscopic X-ray and Mössbauer Characterization of M_6 and M_5 Iron(Molybdenum)-Carbonyl Carbide Clusters: High Carbide-Iron Covalency Enhances Local Iron Site Electron Density Despite Cluster Oxidation *Inorganic Chemistry* 58(19), 12918-12932. https://doi.org/10.1021/acs.inorgchem.9b01870
- Al Samarai, M., Hahn, A.W., Askari, A.B., Cui, Y.-T., Yamazoe, K., Miyawaki, J., Harada, Y., Rüdiger, O., **DeBeer, S.** (2019). Elucidation of Structure-Activity Correlations in a Nickel-Manganese Oxide OER Catalyst by Operando Ni L-edge XAS and 2p3d RIXS *ACS Applied Materials and Interfaces* 11(42), 38595-38605. https://doi.org/10.1021/acsami.9b06752

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