List of publications: Prof. Dr. Serena DeBeer

2020

- Rengshausen, S., Van Stappen, C., Levin, N., Tricard, S., Luska, K.L., **DeBeer, S.**, Chaudret, B., Bordet, A., Leitner, W. (2020). Organometallic Synthesis of Bimetallic Cobalt-Rhodium Nanoparticles in Supported Ionic Liquid Phases (Co_xRh_{100-x}@SILP) as Catalysts for the Selective Hydrogenation of Multifunctional Aromatic Substrates *Small* https://doi.org/10.1002/smll.202006683
- Van Stappen, C., Decamps, L., **DeBeer, S.** (2020). Preparation and Spectroscopic Characterization of Lyophilized Mo Nitrogenase *Journal of the Biological Inorganic Chemistry* https://doi.org/10.1007/s00775-020-01838-4
- Rodríguez-Maciá, P., Breuer, N., **DeBeer, S.**, Birrell, J.A. (2020). Insight into the Redox Behavior of the [4Fe–4S] Subcluster in [FeFe] Hydrogenases *ACS Catalysis* 10(21), 13084-13095. https://doi.org/10.1021/acscatal.0c02771
- Duan, P.-C., Schulz, R.A., Römer, A., Van Kuiken, B.E., Dechert, S., Demeshko, S., Cutsail III, G.E., **DeBeer, S.**, Mata, R.A., Meyer, F. (2020). Ligand Protonation Triggers H2 Release from a Dinickel Dihydride Complex to Give a Doubly "T"-Shaped Dinickel(I) Metallodiradical *Angewandte Chemie International Edition* https://doi.org/10.1002/anie.202011494
- McCubbin Stepanic, O., Ward, J., Penner-Hahn, J.E., Deb, A., Bergmann, U., **DeBeer, S.** (2020). Probing a silent metal: A Combined X-ray Absorption and Emission Spectroscopic Study of Biologically Relevant Zinc Complexes *Inorganic Chemistry* 59(18), 13551-13560. https://doi.org/10.1021/acs.inorgchem.0c01931
- Jensen, K.M. Ø., **DeBeer, S.**, Koziej, D. (2020). Editorial: Spectroscopy and scattering for chemistry: new possibilities and challenges with large scale facilities *Nanoscale 1*2(35), 17968-17970. https://doi.org/10.1039/D0NR90182B
- Zimmermann, P., Peredkov, S., Abdala P.M., **DeBeer, S.**, Tromp, M., Müller, C., van Bokhoven, J.A. (2020). Modern X-ray spectroscopy: XAS and XES in the laboratory *Coordination Chemistry Reviews* 423, 213466. https://doi.org/10.1016/j.ccr.2020.213466
- Budiyanto, E., Yu, M., Chen, M., **DeBeer, S.**, Rüdiger, O., Tüysüz, H. (2020). Tailoring Morphology and Electronic Structure of Cobalt Iron Oxide Nanowires for Electrochemical Oxygen Evolution Reaction *ACS Applied Energy Materials* 3(9), 8583-8594. https://doi.org/10.1021/acsaem.0c01201
- Beheshti Askari, A., al Samarai, M., Hiraoka, N., Ishii, H., Tillmann, L., Muhler, M., **DeBeer, S.** (2020). In situ X-ray emission and high-resolution X-ray absorption spectroscopy applied to Ni-based Bimetallic Dry Methane Reforming Catalysts *Nanoscale* 20(28), 15185-15192. https://doi.org/10.1039/D0NR01960G
- Yu, M., Moon, G.-H., Castillo, R.G., **DeBeer, S.**, Weidenthaler, C., Tüysüz, H. (2020). Dual Role of Silver Moieties Coupled with Ordered Mesoporous Cobalt Oxide towards Electrocatalytic Oxygen Evolution Reaction *Angewandte Chemie International Edition* 59(38), 16544-16552. https://doi.org/10.1002/anie.202003801
- **DeBeer, S.** (2020). Introduction to X-ray spectroscopy – including X-ray absorption, X-ray emission and resonant inelastic X-ray scattering *Bioorganometallic Chemistry* 407-432. https://doi.org/10.1515/9783110496574-011

- Rodríguez-Maciá, P., Galle, L., Bjornsson, R., Lorent, C., Zebger, I., Yoda, Y., Cramer, S., **DeBeer, S.**, Span, I., Birrell, J.A. (2020). Caught in the H_{inact}: Crystal Structure and Spectroscopy Reveal a Sulfur Bound to the Active Site of an O_2-stable State of [FeFe] Hydrogenase *Angewandte Chemie International Edition* 59(38), 16786-16794. https://doi.org/10.1002/anie.202005208
- Levin, N., Peredkov, S., Weyhermüller, T., Rüdiger, O., Pereira, N.B., Grötzsch, D., Kalinko, A., **DeBeer, S.** (2020). Ruthenium 4d-to-2p X-ray Emission Spectroscopy: A Simultaneous Probe of the Metal and the Bound Ligands *Inorganic Chemistry* 59(12), 8272-8283. https://doi.org/10.1021/acs.inorgchem.0c00663
- Castillo, R.G., Henthorn, J.T., McGale, J., Maganas, D., **DeBeer, S.** (2020). Kβ X-ray Emission Spectroscopic study of a second-row transition metal (Mo) and its application to nitrogenase related model complexes *Angewandte Chemie International Edition* 59(31), 12965-12975. https://doi.org/10.1002/anie.202003621
- Beheshti-Askari. A., al Samarai, M., Morana, B., Tillmann, L., Pfänder, N., Wandzilak, A., Watts, B., Belkhou, R., Muhler, M., **DeBeer, S.** (2020). In-situ X-ray Microscopy reveals particle dynamics in a NiCo dry methane reforming catalyst under operating conditions *ACS Catalysis* 10(11), 6223-6230. https://doi.org/10.1021/acscatal.9b05517
- Van Stappen, C., Decamps, L., Cutsail III, G.E., Bjornsson, R., Henthorn, J.T., Birrell, J.A., **DeBeer, S.** (2020). The Spectroscopy of Nitrogenases *Chemical Reviews* 120(12), 5005-5081. https://doi.org/10.1021/acs.chemrev.9b00650
- 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* 2020(15-16), 1525-1538. 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
- Liu, Y., Resch, S.G., Klawitter, I., Cutsail III, G.E., Demeshko, S., Dechert, S., Kühn, F.E., **DeBeer, S.**, Meyer, F. (2020). An Adaptable N-Heterocyclic Carbene Macrocycle Hosting Copper in three Oxidation States *Angewandte Chemie International Edition* 59(14), 5696-5705. https://doi.org/10.1002/anie.201912745

2019

- Mathe, Z., Pantazis, D.A., Lee, H.B., Gnewkow, R., Van Kuiken, B**.**, Agapie, T., **DeBeer, S.** (2019). Calcium Valence-to-Core X-ray Emission Spectroscopy: A Sensitive Probe of Oxo Protonation in Structural Models of the Oxygen-Evolving Complex *Inorganic Chemistry* 58(23), 16292-16301. https://doi.org/10.1021/acs.inorgchem.9b02866
- 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
- Van Stappen, C., Thorhallsson, A.T., Decamps, L., Bjornsson, R., **DeBeer, S.** (2019). Resolving the structure of the E_1 state of Mo Nitrogenase through Mo and Fe K-edge EXAFS and QM/MM calculations *Chemical Science* 10(42), 9807-9821. https://doi.org/10.1039/c9sc02187f
- Van Stappen, C., Davydov, R., Yang, Z.-Y., Fan, R., Guo, Y., Bill, E., Seefeldt, L.C., Hoffman, B.M., **DeBeer, S.** (2019). A spectroscopic description of the E_1 state of Mo Nitrogenase based on Mo and Fe X-ray absorption and Mössbauer studies *Inorganic Chemistry* 58(18), 12365-12376. https://doi.org/10.1021/acs.inorgchem.9b01951
- Speelman, A.L., Čorić, I., Van Stappen, C., **DeBeer, S.**, Mercado, B.Q., Holland, P.L. (2019). Nitrogenase-Relevant Reactivity of a Synthetic Iron–Sulfur–Carbon Site *Journal of the American Chemical Society* 141(33), 13148-13157. https://doi.org/10.1021/jacs.9b05353
- Chrysina, M., Heyno, E., Kutin Y., Reus, M., Nilsson, H., Nowaczyk. M.N., **DeBeer, S.**, Neese, F., Messinger, J., Lubitz, W., Cox, N. (2019). Five-coordinate Mn^{IV} intermediate in the activation of nature's water splitting cofactor *Proceedings of the National Academy of Sciences of the United States of America* 116(34), 16841-16846. https://doi.org/10.1073/pnas.1817526116
- Henthorn, J.T., Arias, R.J., Koroidov, S., Kroll, T., Sokaras, D., Bergmann, U., Rees, D.C., **DeBeer, S.** (2019). Localized Electronic Structure of Nitrogenase FeMoco Revealed by Selenium K-edge High Resolution X-ray Absorption Spectroscopy *Journal of the American Chemical Society* 141(34), 13676-13688. https://doi.org/10.1021/jacs.9b06988
- Yogendra, S., Weyhermüller, T., Hahn, A.W., **DeBeer, S.** (2019). From Ylides to Doubly Yldiide-Bridged Iron(II) High Spin Dimers via Self-Protolysis *Inorganic Chemistry* 58(14), 9358-9367. https://doi.org/10.1021/acs.inorgchem.9b01086
- Kowalska, J.K., Henthorn, J.T., Van Stappen, C., Trncik, C., Einsle, O., Keavney, D., **DeBeer, S.** (2019). X-ray Magnetic Circular Dichroism Spectroscopy Applied to Nitrogenase and Related Models: Experimental Evidence for a Spin-Coupled Mo(III) *Angewandte Chemie International Edition* 58(28), 9373-9377. https://doi.org/10.1002/anie.201901899
- Cutsail III, G.E., Gagnon, N.L., Spaeth, A.D., Tolman, W.B., **DeBeer, S.** (2019). Valence-to-Core X-ray Emission Spectroscopy as a Probe of O-O Bond Activation in Cu_2O_2 complexes *Angewandte Chemie International Edition* 58(27), 9114-9119. https://doi.org/10.1002/anie.201903749

- Kalläne, S.I., Hahn, A.W., Weyhermüller, T., Bill, E., Neese, F., **DeBeer, S.**, van Gastel, M. (2019). Spectroscopic and Quantum Chemical Investigation of Benzene-1,2- dithiolate-Coordinated Diiron Complexes with Relevance to Dinitrogen Activation *Inorganic Chemistry* 58(8), 5111-5125. https://doi.org/10.1021/acs.inorgchem.9b00177
- Maganas, D., Kowalska, J.K., Noiijen, M., **DeBeer, S.**, Neese, F. (2019). Comparison of Multireference Ab initio Wavefunction Methodologies for X-Ray Absorption Edges: A Case study on $[Fe(II/III)Cl_4]^{2-/1-}$ molecules *The Journal of Chemical Physics* 150(10), 104106. https://doi.org/10.1063/1.5051613

2018

- Malzer, W., Grötzsch, D., Gnewkow, R., Schlesiger, C., Kowalewski, F., Van Kuiken, B., **DeBeer, S.**, Kanngießer, B. (2018). A laboratory spectrometer for high throughput X-ray emission spectroscopy in catalysis research *Review of Scientific Instruments* 89, 113111. https://doi.org/10.1063/1.5035171
- Cutsail III, G.E., Banerjee, R., Zhou, A., Que, L., Lipscomb, J.D., **DeBeer, S.** (2018). High-Resolution EXAFS Provides Evidence for a Longer Fe•••Fe Distance in the Q Intermediate of Methane Monooxygenase *Journal of American Chemical Society* 140(48) 16807-16820. https://doi.org/10.1021/jacs.8b10313
- Hahn, A.W., Van Kuiken, B.E., Chilkuri, V.G., Levin, N., Bill, E., Weyhermüller, T., Nicolaou, A., Miyawaki, J., Harada, Y., **DeBeer, S.** (2018). Probing the Valence Electronic Structure of Low-Spin Ferrous and Ferric Complexes Using 2p3d Resonant Inelastic X-ray Scattering (RIXS) *Inorganic Chemistry* 57(37), 11918-11923. https://doi.org/10.1021/acs.inorgchem.8b01550
- Rodriguez-Maciá, P., Reijerse, E.J., van Gastel, M., **DeBeer, S.,** Lubitz, W., Rüdiger, O., Birrell, J.A. (2018). Sulfide Protects [FeFe] Hydrogenases From O_2 *Journal of the American Chemical Society* 140(30), 9346-9350. https://doi.org/10.1021/jacs.8b04339
- Chantzis, A., Kowalska, J.K., Maganas, D., **DeBeer, S.,** Neese, F. (2018). Ab initio Wavefunction-based Determination of Element Specific Shifts for the Efficient Calculation of X-Ray Absorption Spectra of Main Group Elements and First Row Transition Metals *Journal of Chemical Theory and Computation* 14(7), 3686-3702. https://doi.org/10.1021/acs.jctc.8b00249
- Galle, L.M., Cutsail, G.E. III, Nischwitz, V., **DeBeer, S.**, Span, I. (2018). Spectroscopic characterization of the Co-substituted C-terminal domain of rubredoxin-2 *Biological Chemistry* 399(7), 787-798. https://doi.org/10.1515/hsz-2018-0142
- Van Kuiken, B.E., Hahn, A.W., Nayyar, B., Schiewer, C.E., Lee, S.C., Meyer, F., Weyhermüller, T., Nicolaou, A., Cui, Y-T., Miyawaki, J., Hatada, Y., **DeBeer, S.** (2018). Electronic Spectra of Iron-Sulfur Complexes Measured by 2p3d RIXS Spectroscopy *Inorganic Chemistry* 57(12), 7355-7361. https://doi.org/10.1021/acs.inorgchem.8b01010
- Van Stappen, C., Maganas, D., **DeBeer, S.**, Bill, E., Neese, F. (2018). Investigation of the Magnetic and Spectroscopic Properties of V(III) and V(IV) Complexes *Inorganic Chemistry* 57(11), 6421-6438. https://doi.org/10.1021/acs.inorgchem.8b00486
- Maganas, D., **DeBeer, S.,** Neese, F. (2018).A Pair Natural Orbitals Restricted Open Shell Configuration Interaction (PNO-ROCIS) Approach for Calculating X-ray Absorption Spectra of Large Chemical Systems *Journal of Physical Chemistry A* 122(5), 1215-1227. https://doi.org/10.1021/acs.jpca.7b10880

- Leipzig, B.K., Rees, J.A., Kowalska, J.K., Theisen, R.M., Kavčič, M., Poon, P.C.Y., Kaminsky, W., **DeBeer, S.,** Bill, E., Kovacs, J.A. (2018). How Do Ring Size and π-Donating Thiolate Ligands Affect Redox-Active, α-Imino-N-heterocycle Ligand Activation? *Inorganic Chemistry* 57(4), 1935-1949. https://doi.org/10.1021/acs.inorgchem.7b02748
- **DeBeer, S.** (2018). Advanced X-ray Spectroscopic Methods for Studying Iron-Sulfur-Containing Proteins and Model Complexes *Methods Enzymology. Fe-S Cluster Enzymes Part B* 599, 427-450. https://doi.org/10.1016/bs.mie.2017.09.008

2017

- Römelt, C., Song, J.S., Tarrago, M., Rees, J.A., van Gastel, M., Weyhermüller, T., **DeBeer, S.**, Bill, E., Neese, F., Ye, S. (2017). Electronic Structure of a Formal Iron(0), Porphyrin Complex Relevant to CO_2 Reduction *Inorganic Chemistry* 56(8), 4745-4750. https://doi.org/10.1021/acs.inorgchem.7b00401
- Rees, J.A., Bjornsson, R., Kowalska, J.K., Lima, F.A., Schlesier, J., Sippel, D., Weyhermüller, T., Einsle, O., Kovacs, J.A., **DeBeer, S.** (2017). Comparative electronic structures of nitrogenase FeMoco and FeVco *Dalton Transactions* 46(8), 2445-2455. https://doi.org/10.1039/c7dt00128b
- Bjornsson, R., Neese, F., **DeBeer, S**. (2017). Revisiting the Mössbauer Isomer Shifts of the FeMoco Cluster of Nitrogenase and the Cofactor Charge *Inorganic Chemistry* 56(3), 1470-1477. https://doi.org/10.1021/acs.inorgchem.6b02540
- Castillo, R.G., Banerjee, R., Allpress, C.J., Rohde, G.T., Bill, E., Que Jr., L., Lipscomb, J.D., **DeBeer, S.** (2017). High-Energy-Resolution Fluorescence-Detected X-ray Absorption of the Q Intermediate of Soluble Methane Monooxygenase *Journal of the American Chemical Society* 139(49), 18024-18033. https://doi.org/10.1021/jacs.7b09560
- Maganas, D., **DeBeer, S.**, Neese, F. (2017). A Restricted Open Configuration Interaction with Singles Method To Calculate Valence-to-Core Resonant X-ray Emission Spectra: A Case Study *Inorganic Chemistry* 56(19), 11819-11836. https://doi.org/10.1021/acs.inorgchem.7b01810
- Koziej, D., **DeBeer, S.** (2017). Application of Modern X-ray Spectroscopy in Chemistry-Beyond Studying the Oxidation State *Chemistry of Materials* 29(17), 7051-7053. https://doi.org/10.1021/acs.chemmater.7b03455
- Chilkuri, V.G., **DeBeer, S.**, Neese, F. (2017). Revisiting the Electronic Structure of FeS Monomers Using ab Initio Ligand Field Theory and the Angular Overlap Model *Inorganic Chemistry* 56(17), 10418-10436. https://doi.org/10.1021/acs.inorgchem.7b01371
- Kowalska, J.K., Nayyar, B., Rees, J.A., Schiewer, C.E., Lee, S.C., Kovacs, J.A., Meyer, F., Weyhermüller, T., Otero, E., **DeBeer, S.** (2017). Iron $L_{2,3}$-edge X-ray Absorption and X-ray Magnetic Circular Dichroism Studies of Molecular Iron Complexes with Relevance to the FeMoco and FeVco Active Sites of Nitrogenase *Inorganic Chemistry* 56(14), 8147-8158. https://doi.org/10.1021/acs.inorgchem.7b00852
- Hahn, A.W., Van Kuiken, B.E., al Samarai, M., Atanasov, M., Weyhermüller, T., Cui, Y.T., Miyawaki, J., Harada, Y., Nicolaou, A., **DeBeer, S.** (2017). Measurement of the Ligand Field Spectra of Ferrous and Ferric Iron Chlorides Using 2p3d RIXS *Inorganic Chemistry* 56(14), 8203-8211. https://doi.org/10.1021/acs.inorgchem.7b00940
- Casitas, A., Rees, J.A., Goddard, R., Bill, E., **DeBeer, S.**, Fürstner, A. (2017). Two Exceptional Homoleptic Iron(IV) Tetraalkyl Complexes *Angewandte Chemie International Edition* 56(34), 10108-10113. https://doi.org/10.1002/anie.201612299

2016

- Van Kuiken, B.E., Hahn, A.W., Maganas, D., **DeBeer, S.** (2016). Measuring Spin-Allowed and Spin-Forbidden d-d Excitations in Vanadium Complexes with 2p3d Resonant Inelastic X-ray Scattering *Inorganic Chemistry* 55(21), 11497-11501. https://doi.org/10.1021/acs.inorgchem.6b02053
- Kowalska, J.K., Lima, F.A., Pollock, C. J., Rees, J.A., **DeBeer, S.** (2016). A Practical Guide to High-resolution X-ray Spectroscopic Measurements and their Applications in Bioinorganic Chemistry *Israel Journal of Chemistry* 56(9-10), 803-815. https://doi.org/10.1002/ijch.201600037
- Rees, J.A., Wandzilak, A., Maganas, D., Wurster, N.I.C., Hugenbruch, S., Kowalska, J.K., Pollock, C.J., Lima, F.A., Finkelstein, K.D., **DeBeer, S.** (2016). Experimental and theoretical correlations between vanadium K-edge X-ray absorption and Kß emission spectra *Journal of Biological Inorganic Chemistry* 21(5-6), 793-805. https://doi.org/10.1007/s00775-016-1358-7
- Kupper, C., Rees, J.A., Dechert, S., **DeBeer, S.**, Meyer, F. (2016). Complete Series of $\{FeNO\}^8$, $\{FeNO\}^7$, and $\{FeNO\}^6$ Complexes Stabilized by a Tetracarbene Macrocycle *Journal of the American Chemical Society* 138(25), 7888-7898. https://doi.org/10.1021/jacs.6b00584
- Kowalska, J.K., Hahn, A.W., Albers, A., Schiewer, C.E., Bjornsson, R., Lima, F.A., Meyer, F., **DeBeer, S.** (2016). X-ray Absorption and Emission Spectroscopic Studies of $[L_2Fe_2S_2]^n$ Model Complexes: Implications for the Experimental Evaluation of Redox States in Iron-Sulfur Clusters *Inorganic Chemistry* 55(9), 4485-4497. https://doi.org/10.1021/acs.inorgchem.6b00295
- Hugenbruch, S., Shafaat, H.S., Krämer, T., Delgado-Jaime, M.U., Weber, K., Neese, F., Lubitz, W., **DeBeer, S.** (2016). In search of metal hydrides: an X-ray absorption and emission study of [NiFe] hydrogenase model complexes *Physical Chemistry Chemical Physics* 18(16), 10688-10699. https://doi.org/10.1039/c5cp07293j
- Martin-Diaconescu, V., Chacon, K.N., Delgado-Jaime, M.U., Sokaras, D., Weng, T.C., **DeBeer, S.**, Blackburn, N.J. (2016). Kß Valence to Core X-ray Emission Studies of Cu(I) Binding Proteins with Mixed Methionine - Histidine Coordination. Relevance to the Reactivity of the M- and H-sites of Peptidylglycine Monooxygenase *Inorganic Chemistry* 55(7), 3431-3439. https://doi.org/10.1021/acs.inorgchem.5b02842
- **DeBeer, S.**, Bergmann U. (2016). X-ray Emission Spectroscopic Techniques in Bioinorganic Applications *Encyclopedia of Inorganic and Bioinorganic Chemistry* 1-14. https://doi.org/10.1002/9781119951438.eibc2158

2015

- Beckwith M.A., Ames W., Vila F.D., Krewald V., Pantazis D.A., Mantel C., Pécaut J., Gennari M., Duboc C., Collomb M.-N., Yano J., Rehr J.J., Neese F., **DeBeer S.** (2015). How Accurately Can Extended X-ray Absorption Spectra Be Predicted from First Principles? Implications for Modeling the Oxygen-Evolving Complex in Photosystem II *Journal of the American Chemical Society* 137(40), 12815-12834. https://doi.org/10.1021/jacs.5b00783
- Pollock C.J., **DeBeer S.** (2015). Insights into the Geometric and Electronic Structure of Transition Metal Centers from Valence-to-Core X-ray Emission Spectroscopy *Accounts of Chemical Research* 48(11), 2967-2975. https://doi.org/10.1021/acs.accounts.5b00309
- Kowalska J., **DeBeer S.** (2015). The role of X-ray spectroscopy in understanding the geometric and electronic structure of nitrogenase *Biochimica et Biophysica Acta - Molecular Cell Research* 1853(6), 1406-1415. https://doi.org/10.1016/j.bbamcr.2014.11.027

- Yao S.A., Martin-Diaconescu V., Infante I., Lancaster K.M., Götz A.W., **DeBeer S.**, Berry J.F. (2015). Electronic structure of Ni_2E_2 complexes (E = S, Se, Te) and a global analysis of M_2E_2 compounds: A case for quantized E_2^{n-} oxidation levels with n= 2, 3, or 4 *Journal of the American Chemical Society* 137(15), 4993-5011. https://doi.org/10.1021/ja511607j
- Tomson N.C., Williams K.D., Dai X., Sproules S., **DeBeer S.**, Warren T.H., Wieghardt, K. (2015). Re-evaluating the Cu K pre-edge XAS transition in complexes with covalent metal-ligand interactions C*hemical Science* 6(4), 2474-2487. https://doi.org/10.1039/c4sc03294b
- Krewald V., Retegan M., Cox N., Messinger J., Lubitz W., **DeBeer S**., Neese F., Pantazis D.A. (2015). Metal oxidation states in biological water splitting *Chemical Science* 6(3), 1676-1695. https://doi.org/10.1039/c4sc03720k
- Martin-Diaconescu V., Gennari M., Gerey B., Tsui E., Kanady J., Tran R., Pécaut J., Maganas D., Krewald V., Gouré E., Duboc C., Yano J., Agapie T., Collomb M.-N., **DeBeer S.** (2015). Ca K-edge XAS as a probe of calcium centers in complex systems *Inorganic Chemistry* 54 (4), 1283 1292 https://doi.org/10.1021/ic501991e
- Barnett B.R., Moore C.E., Chandrasekaran P., Sproules S., Rheingold A.L., **DeBeer S.**, Figueroa J.S. (2015). Metal-only Lewis pairs between group 10 metals and Tl(I) or Ag(I): Insights into the electronic consequences of Z-type ligand binding *Chemical Science* 6(12), 7169-7178. https://doi.org/10.1039/c5sc03104d
- Rees, J.A., Bjornsson, R., Schlesier, J., Sippel, D., Einsle, O., **DeBeer, S.** (2015). The Fe-V Cofactor of Vanadium Nitrogenase Contains an Interstitial Carbon Atom *Angewandte Chemie International Edition* 54(45), 13249-13252. https://doi.org/10.1002/anie.201505930
- Rees, J.A., Martin-Diaconescu, V., Kovacs, J.A., **DeBeer, S.** (2015). X-ray Absorption and Emission Study of Dioxygen Activation by a Small-Molecule Manganese Complex *Inorganic Chemistry* 54(13), 6410-6422. https://doi.org/10.1021/acs.inorgchem.5b00699
- Bjornsson, R., Neese, F., Schrock, R.R., Einsle, O., **DeBeer, S.** (2015). The discovery of Mo(III) in FeMoco: reuniting enzyme and model chemistry *Journal of Biological Inorganic Chemistry* 20(2), 447-460. https://doi.org/10.1007/s00775-014-1230-6
- van Schooneveld, M.M., DeBeer, S. (2015). A close look at dose: Toward L-edge XAS spectral uniformity, dose quantification and prediction of metal ion photoreduction *Journal of Electron Spectroscopy and Related Phenomena* 198, 31-56. https://doi.org/10.1016/j.elspec.2014.12.001
- Goswami, M., Lyaskovskyy, V., Domingos, S.R., Buma, W.J., Woutersen, S., Troeppner, O., Ivanovic-Burmazovic, I., Lu, H.J., Cui, X., Zhang, X.P., Reijerse, E.J., **DeBeer, S.**, van Schooneveld, M.M., Pfaff, F.F., Ray, K., de Bruin, B. (2015). Characterization of Porphyrin-Co(III)-'Nitrene Radical' Species Relevant in Catalytic Nitrene Transfer Reactions *Journal of the American Chemical Society* 137(16), 5468-5479. https://doi.org/10.1021/jacs.5b01197
- Bjornsson, R., Delgado-Jaime, M.U., Lima, F.A., Sippel, D., Schlesier, J., Weyhermüller, T., Einsle, O., Neese, F., **DeBeer, S.** (2015). Molybdenum L-Edge XAS Spectra of MoFe Nitrogenase *Zeitschrift für Anorganische und Allgemeine Chemie* 641(1), 65-71. https://doi.org/10.1002/zaac.201400446
- Gennari, M., Brazzolotto, D., Pécaut, J., Cherrier, M.V., Pollock, C.J., **DeBeer, S.**, Retegan, M., Pantazis, D.A., Neese, F., Rouziéres, Clérac, R., Duboc, C. (2015). Dioxygen Activation and Catalytic Reduction to Hydrogen Peroxide by a Thiolate-Bridged Dimanganese(II) Complex with a Pendant Thiol *Journal of the American Chemical Society* 137(26), 8644-8653. https://doi.org/10.1021/jacs.5b04917
- **DeBeer, S.** (2015). Biological Catalysts *High-resolution XAS/XES: Analyzing Electronic Structures of Catalysts* 153-167. https://doi.org/10.1201/b17184

2014

- Bjornsson, R., Lima, F. A., Spatzal, T., Weyhermüller, T., Glatzel, T., Bill, E., Einsle, O., Neese, F., **DeBeer, S.** (2014). Identification of a spin-coupled Mo(III) in the nitrogenase iron-molybdenum cofactor *Chemical Science* 5(8), 3096-3103. https://doi.org/10.1039/C4SC00337C
- Blusch, L. K., Mitevski, O., Martin-Diaconescu, V., Pröpper, K., **DeBeer, S.**, Dechert, S., Meyer, F. (2014). Selective Synthesis and Redox Sequence of a Heterobimetallic Nickel/Copper Complex of the Noninnocent Siamese-Twin Porphyrin *Inorganic Chemistry* 53(15), 7876-7885. https://doi.org/10.1021/ic500460n
- Chandrasekaran, P., Greene, A.F., Lillich, K., Capone, S., Mague, J.T., **DeBeer, S.**, Donahue, J.P. (2014). A Structural and Spectroscopic Investigation of Octahedral Platinum Bis(dithiolene)phosphine Complexes: Platinum Dithiolene Internal Redox Chemistry Induced by Phosphine Association *Inorganic Chemistry* 53(17), 9192-9205. https://doi.org/10.1021/ic501273b
- Darmon, J.M., Yu, R.P., Semproni, S.P., Turner, Z.R., Stieber, S.C.E., **DeBeer, S.**, Chirik, P.J. (2014). Electronic Structure Determination of Pyridine N-Heterocyclic Carbene Iron Dinitrogen Complexes and Neutral Ligand Derivatives *Organometallics* 33(19), 5423-5433. https://doi.org/10.1021/om500727t
- Hall, E.R., Pollock, C.J., Bendix, J., Collins, T.J., Glatzel, P., **DeBeer, S.** (2014). Valence-to-Core-Detected X-ray Absorption Spectroscopy: Targeting Ligand Selectivity *Journal of the American Chemical Society* 136(28), 10076-10084. https://doi.org/10.1021/ja504206y
- Jayarathne, U., Chandrasekaran, P., Greene, A.F., Mague, J.T., **DeBeer, S.**, Lancaster, K.M., Sproules, S., Donahue, J.P. (2014). X-ray Absorption Spectroscopy Systematics at the Tungsten L-Edge *Inorganic Chemistry* 53(16), 8230-8241. https://doi.org/10.1021/ic500256a
- Maganas, D., **DeBeer, S.**, Neese, F. (2014). Restricted Open-Shell Configuration Interaction Cluster Calculations of the L-Edge X-ray Absorption Study of TiO_2 and CaF_2 Solids *Inorganic Chemistry* 53(13), 6374-6385. https://doi.org/10.1021/ic500197v
- Maganas, D., Kristiansen, P., Duda, L.C., Knop-Gericke, A., **DeBeer, S.**, Schlögl, R., Neese, F. (2014). Combined Experimental and Ab Initio Multireference Configuration Interaction Study of the Resonant Inelastic X-ray Scattering Spectrum of CO_2 *Journal of Physical Chemistry C* 118(35), 20163-20175. https://doi.org/10.1021/jp505628y
- Maganas, D., Roemelt, M., Weyhermüller, T., Blume, R., Hävecker, M, Knop-Gericke, A., **DeBeer, S.**, Schlögl, R., Neese, F., (2014). L-edge X-ray absorption study of mononuclear vanadium complexes and spectral predictions using a restricted open shell configuration interaction ansatz *Physical Chemistry Chemical Physics* 16(1), 264-276. https://doi.org/10.1039/c3cp52711e
- Neu, H.M., Quesne, M.G., Yang, T.S., Prokop-Prigge, K.A., Lancaster, K.M., Donohoe, J., **DeBeer, S.**, de Visser, S.P., Goldberg, D.P. (2014). Dramatic Influence of an Anionic Donor on the Oxygen-Atom Transfer Reactivity of a Mn^{V}-Oxo Complex *Chemistry-A European Journal* 20(45), 14584-14588. https://doi.org/10.1002/chem.201404349
- Pollock, C. J., Delgado-Jaime, M.U., Atanasov, M., Neese, F., **DeBeer, S.** (2014). Kβ Mainline X-ray Emission Spectroscopy as an Experimental Probe of Metal-Ligand Covalency *Journal of the American Chemical Society* 136(26), 9453-9463. https://doi.org/10.1021/ja504182n
- Pollock, C. J., Lancaster, K.M., Finkelstein, K.D., **DeBeer, S.** (2014). Study of Iron Dimers Reveals Angular Dependence of Valence-to-Core X-ray Emission Spectra *Inorganic Chemistry* 53(19), 10378-10385. https://doi.org/10.1021/ic501462y

- Pollock, C.J., Tan, L.L., Zhang, W., Lancaster, K.M., Lee, S.C., **DeBeer, S.** (2014). Light-Atom Influences on the Electronic Structures of Iron Sulfur Clusters *Inorganic Chemistry* 53(5), 2591-2597. https://doi.org/10.1021/ic402944r
- Russell, S. K., Hoyt, J.M., Bart, S.C., Milsmann, C., Stieber, S.C.E., Semproni, S.P., **DeBeer, S.**, Chirik P.J. (2014). Synthesis, electronic structure and reactivity of bis(imino)pyridine iron carbene complexes: evidence for a carbene radical *Chemical Science* 5(3), 1168-1174. https://doi.org/10.1039/C3SC52450G
- **DeBeer, S.**, Neese, F. (2013) X-ray Spectroscopy *Comprehensive Inorganic Chemistry II* 9(2013), 427-439. https://doi.org/10.1016/B978-0-08-097774-4.00918-9

2013

- Blusch, L.K., Craigo, K.E., Martin-Diaconescu, V., McQuarters, A.B., Bill, E., Dechert, S., **DeBeer, S.**, Lehnert, N., Meyer, F. (2013). Hidden Non-Innocence in an Expanded Porphyrin: Electronic Structure of the Siamese-Twin Porphyrin's Dicopper Complex in Different Oxidation States *Journal of the American Chemical Society* 135(37), 13892-13899. https://doi.org/10.1021/ja406176e
- Chandrasekaran, P., Chiang, K.P., Nordlund, D., Bergmann, U., Holland, P.L., **DeBeer, S.** (2013). Sensitivity of X-ray Core Spectroscopy to Changes in Metal Ligation: A Systematic Study of Low-Coordinate, High-Spin Ferrous Complexes *Inorganic Chemistry* 52(11), 6286-6298. https://doi.org/10.1021/ic3021723
- Coggins, M. K., Martin-Diaconescu, V., **DeBeer, S.**, Kovacs, J. A. (2013). Correlation Between Structural, Spectroscopic, and Reactivity Properties Within a Series of Structurally Analogous Metastable Manganese(III)-Alkylperoxo Complexes *Journal of the American Chemical Society* 135(11), 4260-4272. https://doi.org/10.1021/ja308915x
- Delgado-Jaime, M. U., DeBeer, S., Bauer, M. (2013). Valence-to-Core X-Ray Emission Spectroscopy of Iron-Carbonyl Complexes: Implications for the Examination of Catalytic Intermediates *Chemistry - A European Journal* 19(47) 15888-15897. https://doi.org/10.1002/chem.201301913
- Krewald, V., Lassalle-Kaiser, B., Boron III, T.T., Pollock, C.J., Kern, J., Beckwith, M.A., Yachandra, V.K., Pecoraro, V.L., Yano, J., Neese, F., **DeBeer, S.** (2013). The Protonation States of Oxo-Bridged Mn^{IV} Dimers Resolved by Experimental and Computational Mn K Pre-Edge X-ray Absorption Spectroscopy *Inorganic Chemistry* 52(22), 12904-12914. https://doi.org/10.1021/ic4008203
- Lancaster, K.M., Hu, Y., Bergmann, U., Ribbe, M.W., **DeBeer, S.** (2013). X-ray Spectroscopic Observation of an Interstitial Carbide in NifEN-Bound FeMoco Precursor *Journal of the American Chemical Society* 135(2), 610-612. https://doi.org/10.1021/ja309254g
- Lassalle-Kaiser, B., Boron III, T.T., Krewald, V., Kern, J., Beckwith, M.A., Delgado-Jaime, M.U., Schroeder, H., Alonso-Mori, R., Nordlund, D., Weng, T.-C., Sokaras, D., Neese, F., Bergmann, U., Yachandra, V.K., **DeBeer, S.**, Pecoraro, V.L., Yano, J. (2013). 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 *Inorganic Chemistry* 52(22), 12915-12922. https://doi.org/10.1021/ic400821g
- Lima, F.A., Bjornsson, R., Weyhermüller, T., Chandrasekaran, P., Glatzel, P., Neese, F., **DeBeer, S.** (2013). High-resolution molybdenum K-edge X-ray absorption spectroscopy analyzed with time-dependent density functional theory *Physical Chemistry Chemical Physics* 15(48), 20911-20920. https://doi.org/10.1039/c3cp53133c

- Lundberg, M., Kroll, T., **DeBeer, S.**, Bergmann, U., Wilson, S.A., Glatzel, P., Nordlund, D., Hedman, B., Hodgson, K.O., and Solomon, E.I. (2013). Metal-Ligand Covalency of Iron Complexes from High-Resolution Resonant Inelastic X-ray Scattering *Journal of the American Chemical Society* 135(45), 17121-17134. https://doi.org/10.1021/ja408072q
- Pollock, C.J., Grubel, K., Holland, P.L., **DeBeer, S.** (2013). Experimentally Quantifying Small-Molecule Bond Activation Using Valence-to-Core X-ray Emission Spectroscopy *Journal of the American Chemical Society* 135(82), 11803-11808. https://doi.org/10.1021/ja3116247
- Roemelt, M., Maganas, D., **DeBeer, S.**, Neese, F. (2013). A combined DFT and restricted open-shell configuration interaction method including spin-orbit coupling: Application to transition metal L-edge X-ray absorption spectroscopy *Journal of Chemical Physics* 138(20), 204101. https://doi.org/10.1063/1.4804607
- Wang, M., England, J., Weyhermüller, T., Kokatam, S.-L., Pollock, C.J., **DeBeer, S.**, Shen, J., Yap, G.P.A., Theopold, K.H., Wieghardt, K. (2013). New Complexes of Chromium(III) Containing Organic π-Radical Ligands: An Experimental and Density Functional Theory Study *Inorganic Chemistry* 52(8), 4472-4487. https://doi.org/10.1021/ic302743s
- Yan, Y., Keating, C., Chandrasekaran, P., Jayarathne, U., Mague, J. T., DeBeer, S., Lancaster, K.M., Sproules, S., Rubtsov, I.V., Donahue, J.P. (2013). Ancillary Ligand Effects upon Dithiolene Redox Noninnocence in Tungsten Bis(dithiolene) Complexes *Inorganic Chemistry* 52(11), 6743-6751. https://doi.org/10.1021/ic4009174
- Yu, R.P., Darmon, J.M., Milsmann, C., Margulieux, G.W., Stieber, S.C.E., DeBeer, S., Chirik, P.J. (2013). Catalytic Hydrogenation Activity and Electronic Structure Determination of Bis(arylimidazol-2-ylidene)pyridine Cobalt Alkyl and Hydride Complexes *Journal of the American Chemical Society* 135(35), 13168-13184. https://doi.org/10.1021/ja406608u

2012

- Cho, K., Leeladee, P., McGown, A.J., **DeBeer, S.**, Goldberg, D.P. (2012). A High-Valent Iron-Oxo Corrolazine Activates C-H Bonds via Hydrogen-Atom Transfer *Journal of the American Chemical Society* 134(17), 7392-7399. https://doi.org/10.1021/ja3018658
- Delgado-Jaime, M.U., **DeBeer, S.** (2012). Expedited analysis of DFT outputs: Introducing moanalyzer *Journal of Computational Chemistry* 33(27), 2180-2185. https://doi.org/10.1002/jcc.23028
- Frazier, B.A., Wolczanski, P.T., Keresztes, I., **DeBeer, S.**, Lobkovsky, E.B., Pierpont, A.W., Cundari, T.R. (2012). Synthetic Approaches to $(smif)_2Ti$ (smif=1,3-di-(2-pyridyl)-2-azaallyl) Reveal Redox Non-Innocence and C-C Bond-Formation *Inorganic Chemistry* 51(15), 8177-8186. https://doi.org/10.1021/ic300590t
- Kropp, H., King, A.E., Khusniyarov, M.M., Heinemann, F.W., Lancaster, K.M., **DeBeer, S.**, Bill, E., Meyer, K. (2012). Manganese Nitride Complexes in Oxidation States III, IV, and V: Synthesis and Electronic Structure *Journal of the American Chemical Society* 134(37), 15538-15544. https://doi.org/10.1021/ja306647c
- Lancaster, K.M., Zaballa, M.-E., Sproules, S., Sundararajan, M., **DeBeer, S.**, Richards, J.H., Vila, A.J., Neese, F., Gray, H.B. (2012). Outer-Sphere Contributions to the Electronic Structure of Type Zero Copper Proteins *Journal of the American Chemical Society* 134(19), 8241-8253. https://doi.org/10.1021/ja302190r

- Roemelt, M., Beckwith, M.A., Duboc, C., Collomb, M.-N., Neese, F., **DeBeer, S.** (2012). Manganese K-Edge X-Ray Absorption Spectroscopy as a Probe of the Metal-Ligand Interactions in Coordination Compounds *Inorganic Chemistry* 51(1), 680-687. https://doi.org/10.1021/ic202229b
- Scarborough, C.C., Lancaster, K.M., **DeBeer, S.**, Weyhermüller, T., Sproules, S., Wieghardt, K. (2012). Experimental Fingerprints for Redox-Active Terpyridine in $Cr(tpy)_2(PF6)_n$ (*n*=3-0), and the Remarkable Electronic Structure of $[Cr(tpy)_2]^{1-}$ *Inorganic Chemistry* 51(6), 3718-3732. https://doi.org/10.1021/ic2027219
- Stieber, S.C.E., Milsmann, C., Hoyt, J.M., Turner, Z.R., Finkelstein, K.D., Wieghardt, K., **DeBeer, S.**, Chirik, P.J. (2012). Bis(imino)pyridine Iron Dinitrogen Compounds Revisited: Differences in Electronic Structure Between Four- and Five-Coordinate Derivatives *Inorganic Chemistry* 51(6), 3770-3785. https://doi.org/10.1021/ic202750n
- Yan, Y., Chandrasekaran, P., Mague, J.T., **DeBeer, S.**, Sproules, S., Donahue, J.P. (2012). Redox-Controlled Interconversion between Trigonal Prismatic and Octahedral Geometries in a Monodithiolene Tetracarbonyl Complex of Tungsten *Inorganic Chemistry* 51(1), 346-361. https://doi.org/10.1021/ic201748v
- Yao, S.A., Lancaster, K.M., Götz, A.W., **DeBeer, S.**, Berry, J.F. (2012). X-ray Absorption Spectroscopic, Crystallographic, Theoretical (DFT) and Chemical Evidence for a Chalcogen-Chalcogen Two-Center/Three-Electron Half Bond in an Unprecedented "Subselenide" Se_2^{3-} Ligand *Chemistry – A European Journal* 18(30), 9179-9183. https://doi.org/10.1002/chem.201201291
- **DeBeer, S.,** van Gastel, M., Bill, E., Ye, S., Petrenko, T., Pantazis, D.A., Neese, F. (2012). Challenges in Molecular Energy Research *Chemical Energy* Storage 4.5, 353-377. https://doi.org/10.1515/9783110266320.353

2011

- Beckwith, M.A., Roemelt, M., Collomb, M.-N., DuBoc, C., Weng, T.-C., Bergmann, U., Glatzel, P., Neese, F., DeBeer, S. (2011). Manganese Kβ X-ray Emission Spectroscopy As a Probe of Metal-Ligand Interactions *Inorganic Chemistry* 50(17), 8397-8409. https://doi.org/10.1021/ic200970t
- Bowman, A.C., Milsmann, C., Bill, E., Turner, Z.R., Lobkovsky, E., DeBeer, S., Wieghardt, K., Chirik, P.J. (2011). Synthesis and Electronic Structure Determination of *N*-Alkyl-Substituted Bis(imino)pyridine Iron Imides Exhibiting Spin Crossover Behavior *Journal of the American Chemical Society* 133(43), 17353-17369. https://doi.org/10.1021/ja205736m
- Chandrasekaran, P., Stieber, S.C.E., Collins, T.J., Que Jr., L., Neese, F., DeBeer, S. (2011). Prediction of high-valent iron K-edge absorption spectra by time-dependent Density Functional Theory *Dalton Transactions* 40(42), 11070-11079. https://doi.org/10.1039/c1dt11331c
- Delgado-Jaime, M.U., Dible, B.R., Chiang, K.P., Brennessel, W.W., Bergmann, U., Holland, P.L., **DeBeer, S.** (2011). Identification of a Single Light Atom within a Multinuclear Metal Cluster Using Valence-to-Core X-ray Emission Spectroscopy *Inorganic Chemistry* 50(21), 10709-10717. https://doi.org/10.1021/ic201173j
- Frazier, B.A., Bartholomew, E.R., Wolczanski, P.T., **DeBeer, S.**, Santiago-Berrios, M.E., Abruna, H.D., Lobkovsky, E.B., Bart, S.C., Mossin, S., Meyer, K., Cundari, T.R. (2011). Synthesis and Characterization of $(smif)_2M^n$ (*n*=0, M = V, Cr, Mn, Fe, Co, Ni, Ru; *n* =+1, M = Cr, Mn, Co, Rh, Ir; smif=1,3-di-(2-pyridyl)-2-azaallyl) *Inorganic Chemistry* 50(24), 12414-12436. https://doi.org/10.1021/ic200376f

- Gennari, M., Pecaut, J., **DeBeer, S.**, Neese, F., Collomb, M.-N., Duboc, C. (2011). A Fully Delocalized Mixed-Valence Bis-μ(Thiolato) Dicopper Complex: A Structural and Functional Model of the Biological Cu_A Center *Angewandte Chemie International Edition* 50(25), 5661-5665. https://doi.org/10.1002/anie.201100605
- Gennari, M., Retegan, M., **DeBeer, S.**, Pecaut, J., Neese, F., Collomb, M.-N., Duboc, C. (2011). Experimental and Computational Investigation of Thiolate Alkylation in Ni^{II} and Zn^{II} Complexes: Role of the Metal on the Sulfur Nucleophilicity *Inorganic Chemistry* 50(20), 10047-10055. https://doi.org/10.1021/ic200899w
- Lancaster, K.M., Finkelstein, K.D., **DeBeer, S.** (2011). Kβ X-ray Emission Spectroscopy offers Unique Chemical Bonding Insights: Revisiting the Electronic Structure of Ferrocene *Inorganic Chemistry* 50(14), 6767-6774. https://doi.org/10.1021/ic200822b
- Lancaster, K.M., Roemelt, M., Ettenhuber, P., Hu, Y., Ribbe, M.W., Neese, F., Bergmann, U., **DeBeer, S.** (2011). X-ray Emission Spectroscopy Evidences a Central Carbon in the Nitrogenase Iron-Molybdenum Cofactor *Science* 334(6058), 974-977. https://doi.org/10.1126/science.1206445
- Pollock, C.J., **DeBeer, S.** (2011). Valence-to-Core X-ray Emission Spectroscopy: A Sensitive Probe of the Nature of a Bound Ligand *Journal of the American Chemical Society* 133(14), 5594-5601. https://doi.org/10.1021/ja200560z
- Scarborough, C.C., Sproules, S., Weyhermüller, T., **DeBeer, S.**, Wieghardt, K. (2011). Electronic and Molecular Structures of the Members of the Electron Transfer Series $[Cr(^tbpy)_3]^n$ (n=3+, 2+, 1+, 0): An X-ray Absorption Spectroscopic and Density Functional Theoretical Study *Inorganic Chemistry* 50(24), 12446-12462. https://doi.org/10.1021/ic201123x
- Strautmann, J.B.H., von Richthofen, C.-G.F., Heinze-Brückner, G., **DeBeer, S.**, Bothe, E., Bill, E., Weyhermüller, T., Stammler, A., Bögge, H., Glaser, T. (2011). Molecular and Electronic Structures of Dinuclear Iron Complexes Incorporating Strongly Electron-Donating Ligands: Implications for the Generation of the One- and Two-Electron Oxidized Forms *Inorganic Chemistry* 50(1), 155-171. https://doi.org/10.1021/ic101535y
- Tomson, N.C., Crimmin, M.R., Petrenko, T., Rosebrugh, L.E., Sproules, S., Boyd, W.C., Bergman, R.G., **DeBeer, S.**, Toste, F.D., Wieghardt, K. (2011). A Step beyond the Feltham-Enennark Notation: Spectroscopic and Correlated *ab Initio* Computational Support for an Antiferromagnetically Coupled $M(II)^{-}$–$(NO)^{-}$ Description of Tp*M(NO) (M = Co, Ni) *Journal of the American Chemical Society* 133(46), 18785-18801. https://doi.org/10.1021/ja206042k
- McGown, A.J., Badiei, Y.M., Leeladee, P., Prokop, K.A., **DeBeer, S.**, Goldberg, D.P. (2011). Synthesis and Reactivity of High-Valent Transition Metal Corroles and Corrolazines *Handbook of Porphyrin Science with Applications to Chemistry, Physics, Materials Science, Engineering, Biology and Medicine:* Theoretical, Electron Transfer and Physical Studies 14, 525-599. https://doi.org/10.1142/9789814322386_0018
- **DeBeer, S.** (2011). X-ray Spectroscopy *Nitrogen Fixation. Methods in Molecular Biology (Methods and Protocols)* 766, 165-176. https://doi.org/10.1007/978-1-61779-194-9_11

2010

- Cowley, R.E., DeYonker, N.J., Eckert, N.A., Cundari, T.R., **DeBeer, S.**, Bill, E., Ottenwaelder, X., Flaschenriem, C., Holland, P.L. (2010). Three-Coordinate Terminal Imidoiron(III) Complexes: Structure, Spectroscopy, and Mechanism of Formation *Inorganic Chemistry* 49(13), 6172-6187. https://doi.org/10.1021/ic100846b

- **DeBeer George, S.**, Neese, F. (2010). Calibration of Scalar Relativistic Density Functional Theory for the Calculation of Sulfur K-Edge X-ray Absorption Spectra *Inorganic Chemistry* 49(4), 1849-1853. https://doi.org/10.1021/ic902202s
- Hassanin, H.A., El-Shahat, M.F., **DeBeer, S.**, Smith, C.A., Brasch, N.E. (2010). Redetermination of the X-ray structure of nitroxylcobalamin: base-on nitroxylcobalamin exhibits a remarkably long Co-N(dimethylbenzimidazole) bond distance *Dalton Transactions* 39(44), 10626-10630. https://doi.org/10.1039/c0dt00628a
- Hocking, R. K., **DeBeer George, S.**, Raymond, K.N., Hodgson, K.O., Hedman, B., Solomon, E.I. (2010). Fe L-Edge X-ray Absorption Spectroscopy Determination of Differential Orbital Covalency of Siderophore Model Compounds: Electronic Structure Contributions to High Stability Constants *Journal of the American Chemical Society* 132(11), 4006-4015. https://doi.org/10.1021/ja9090098
- Lee, N., Petrenko, T., Bergmann, U., Neese, F., **DeBeer, S.** (2010). Probing Valence Orbital Composition with Iron Kβ X-ray Emission Spectroscopy *Journal of the American Chemical Society* 132(28), 9715-9727. https://doi.org/10.1021/ja101281e
- Lucas, H. R., **DeBeer, S.**, Hong, M.-S., Lee, J. C. (2010). Evidence for Copper-dioxygen Reactivity during α-Synuclein Fibril Formation *Journal of the American Chemical Society* 132(19), 6636-6637. https://doi.org/10.1021/ja101756m
- Milsmann, C., Sproules, S., Bill, E., Weyhermüller, T., **DeBeer George, S.**, Wieghardt, K. (2010). Stabilization of High-Valent $Fe^{IV}S_6$-Cores by Dithiocarbamate(1-) and 1,2-Dithiolate(2-) Ligands in Octahedral $[Fe^{IV}(Et_2dtc)_{3-n}(mnt)_n]^{(n-1)-}$ Complexes (n=0, 1, 2, 3): A Spectroscopic and Density Functional Theory Computational Study *Chemistry - A European Journal* 16(12), 3628-3645. https://doi.org/10.1002/chem.200903381
- Siluvai, G.S., Mayfield, M., Nilges, M.J., **DeBeer George, S.**, Blackburn, N.J. (2010). Anatomy of a Red Copper Center: Spectroscopic Identification and Reactivity of the Copper Centers of *Bacillus subtilis* Sco and Its Cys-to-Ala Variants *Journal of the American Chemical Society* 132(14), 5215-5226. https://doi.org/10.1021/ja910759v
- Sproules, S., Weyhermüller, T., **DeBeer, S.**, Wieghardt, K. (2010). Six-Membered Electron Transfer Series $[V(dithiolene)_3]^z$ (z=1+, 0, 1-, 2-, 3-, 4-). An X-ray Absorption Spectroscopic and Density Functional Theoretical Study *Inorganic Chemistry* 49(11), 5241-5261. https://doi.org/10.1021/ic100344f

2009

- Aliaga-Alcalde, N., **DeBeer George, S.**, Alfaro-Fuentes, I., Cooper, G.J.T., Barba-Behrens, N., Bernès, S., Reedijk, J. (2009). Physical characterization and biological studies of a (streptidine)($Pt^{II}Cl_4$) compound *Polyhedron* 28(16), 3459-3466. https://doi.org/10.1016/j.poly.2009.07.022
- Banerjee, P., Sproules, S., Weyhermüller, T., **DeBeer George, S.**, Wieghardt, K. (2009). Electronic Structure of the [Tris(dithiolene)chromium]^z (z=0, 1-, 2-, 3-) Electron Transfer Series and their Manganese(IV) Analogues. An X-ray Absorption Spectroscopic and Density Functional Theoretical Study *Inorganic Chemistry* 48(13), 5829-5847. https://doi.org/10.1021/ic900154v
- Hocking, R.K., **DeBeer George, S.**, Gross, Z., Walker, F.A., Hodgson, K.O., Hedman, B., Solomon, E.I. (2009). Fe L- and K-edge XAS of Low-Spin Ferric Corrole: Bonding and Reactivity Relative to Low-Spin Ferric Porphyrin *Inorganic Chemistry* 48(4), 1678-1688. https://doi.org/10.1021/ic802248t

- Kennepohl, P., Wasinger, E.C., **DeBeer George, S.** (2009). X-ray spectroscopic approaches to the investigation and characterization of photochemical processes *Journal of Synchrotron Radiation* 16, 484-488. https://doi.org/10.1107/S0909049509021384
- Lancaster, K.M., **DeBeer George, S.**, Yokoyama, K., Richards, J.H., Gray, H.B. (2009). Type-zero copper proteins *Nature Chemistry* 1, 711-715. https://doi.org/10.1038/nchem.412
- Milsmann, C., Bill, E., Weyhermüller, T., **DeBeer George, S.**, Wieghardt, K. (2009). Electronic Structures of $[Ru^{II}(cyclam)(Et_2dtc)]^+$, $[Ru(cyclam)(tdt)]^+$, and $[Ru(cyclam)(tdt)]^{2+}$: An X-ray Absorption Spectroscopic and Computational Study (tdt = toluene-3,4-dithiolate; Et_2dtc = *N,N*-diethyldithiocarbamate(1-)) *Inorganic Chemistry* 48(20), 9754-9766. https://doi.org/10.1021/ic9011845
- Milsmann, C., Patra, G.K., Bill, E., Weyhermüller, T., **DeBeer George, S.**, Wieghardt, K. (2009). Octahedral Monodithiolene Complexes of Iron: Characterization of *S,S'*-Coordinated Dithiolate(1-) π Radical Monoanions: A Spectroscopic and Density Functional Theoretical Investigation *Inorganic Chemistry* 48(15), 7430-7445. https://doi.org/10.1021/ic900936p
- Mooibroek, T.J., Aromi, G., Quesada, M., Roubeau, O., Gamez, P., **DeBeer George, S.**, van Slageren, J., Yasin, S., Ruiz, E., Reedijk, J. (2009). A Mixed-Valent Pentanuclear $Cu^{II}_4Cu^{I}$ Compound Containing a Radical-Anion Ligand *Inorganic Chemistry* 48(22), 10643-10651. https://doi.org/10.1021/ic901337r
- Schöffel, J., Rogachev, A.Y., **DeBeer George, S.**, Burger, P. (2009). Isolation and Hydrogenation of a Complex with a Terminal Iridium-Nitrido Bond *Angewandte Chemie International Edition* 48(26), 4734-4738. https://doi.org/10.1002/anie.200901494
- Sproules, S., Benedito, F.L., Bill, E., Weyhermüller, T., **DeBeer George, S.**, Wieghardt, K. (2009). Characterization and Electronic Structures of Five Members of the Electron Transfer Series $[Re(benzene\text{-}1,2\text{-}dithiolato)_3]^z$ (z=1+,0,1-,2-,3-): A Spectroscopic and Density Functional Theoretical Study *Inorganic Chemistry* 48(23), 10926-10941. https://doi.org/10.1021/ic9010532
- Strautmann, J.B. H., von Richthofen, C.-G.F., **DeBeer George, S.**, Bothe, E., Bill, E., Glaser, T. (2009). Highly oxidized diiron complexes: generation, spectroscopy, and stabilities *Chemical Communications* 2009(19), 2637-2639. https://doi.org/10.1039/b903500a

2008

- Berry, J.F., **DeBeer George, S.**, Neese, F. (2008). Electronic structure and spectroscopy of "superoxidized" iron centers in model systems: theoretical and experimental trends *Physical Chemistry Chemical Physics* 10(30), 4361-4374. https://doi.org/10.1039/b801803k
- **DeBeer George, S.**, Karlin, K.D. (2008) Protagonists in chemistry *Inorganica Chimica Acta* 361(4), 807-808. https://doi.org/10.1016/j.ica.2007.09.001
- **DeBeer George, S.**, Petrenko, T., Neese, F. (2008). Prediction of Iron K-Edge Absorption Spectra Using Time-Dependent Density Functional Theory *Journal of Physical Chemistry A* 112(50), 12936-12943. https://doi.org/10.1021/jp803174m
- **DeBeer George, S.**, Petrenko, T., Neese, F. (2008). Time-dependent density functional calculations of ligand K-edge X-ray absorption spectra *Inorganica Chimica Acta* 361(4), 965-972. https://doi.org/10.1016/j.ica.2007.05.046
- Lu, C.C., **DeBeer George, S.**, Weyhermüller, T., Bill, E., Bothe, E., Wieghardt, K. (2008). An electron-transfer series of high-valent chromium complexes with redox non-innocent, non-heme ligands *Angewandte Chemie International Edition* 47(34), 6384-6387. https://doi.org/10.1002/anie.200800669

- Pap, J.S., **DeBeer George, S.**, Berry, J.F. (2008). Delocalized Metal−Metal and Metal−Ligand Multiple Bonding in a Linear Ru−Ru≡N Unit: Elongation of a Traditionally Short Ru≡N Bond *Angewandte Chemie International Edition* 47(52), 10102-10105. https://doi.org/10.1002/anie.200804397
- Paulat, F., Berto, T.C., **DeBeer George, S.**, Goodrich, L., Praneeth, V.K.K., Sulok, C.D., Lehnert, N. (2008). Vibrational Assignments of Six-Coordinate Ferrous Heme Nitrosyls: New Insight from Nuclear Resonance Vibrational Spectroscopy *Inorganic Chemistry* 47(24), 11449-11451. https://doi.org/10.1021/ic801626w
- Praneeth, V.K.K., Paulat, F., Berto, T.C., **DeBeer George, S.**, Näther, C., Sulok, C.D., Lehnert, N. (2008). Electronic Structure of Six-Coordinate Iron(III)−Porphyrin NO Adducts: The Elusive Iron(III)-NO(radical) State and Its Influence on the Properties of These Complexes *Journal of the American Chemical Society* 130(46), 15288-15303. https://doi.org/10.1021/ja801860u
- Strautmann, J.B.H., **DeBeer George, S.**, Bothe, E., Bill, E., Weyhermüller, T., Stammler, A., Bögge, H., Glaser, T. (2008). Molecular and electronic structures of mononuclear iron complexes using strongly electron-donating ligands and their oxidized forms *Inorganic Chemistry* 47(15), 6804-6824. https://doi.org/10.1021/ic800335t

2007

- Ghosh, S., Gorelsky, S.I., **DeBeer George, S.**, Chan, J.M., Cabrito, I., Dooley, D.M., Moura, J.J.G., Moura, I., Solomon, E.I. (2007). Spectroscopic, computational, and kinetic studies of the μ_4-sulfide-bridged tetranuclear Cu_Z cluster in N_2O reductase: pH effect on the edge ligand and its contribution to reactivity *Journal of the American Chemical Society* 129(13), 3955-3965. https://doi.org/10.1021/ja068059e
- Kapre, R.R., Bothe, E., Weyhermüller, T., **DeBeer George, S.**, Muresan, N., Wieghard, K. (2007). Electronic structures of tris(dioxolene)chromium and tris(dithiolene)chroimium complexes of the electron-transfer series $[Cr(dioxolene)_3]^z$ and $[Cr(dithiolene)_3]^z$ (z=0, 1-, 2-, 3-). A combined experimental and density functional theoretical study *Inorganic Chemistry* 46(19), 7827-7839. https://doi.org/10.1021/ic7008607
- Kapre, R.R., Bothe, E., Weyhermüller, T., **DeBeer George, S.**, Wieghardt, K. (2007). Electronic structure of neutral and monoanionic tris(benzene-1,2-dithiolato) metal complexes of molybdenum and tungsten *Inorganic Chemistry* 46(14), 5642-5650. https://doi.org/10.1021/ic700600r
- Pap, J.S., Benedito, F.L., Bothe, E., Bill, E., **DeBeer George, S.**, Weyhermüller, T., Wieghardt, K. (2007). Dimerization processes of square planar $[Pt^{II}(^tbpy)(dithiolato\cdot)]^+$ radicals *Inorganic Chemistry* 46(10), 4187-4196. https://doi.org/10.1021/ic070130+
- Petrenko, T., **DeBeer George, S.**, Aliaga-Alcalde, N., Bill, E., Mienert, B., Xiao, Y., Guo, Y., Sturhahn, W., Cramer, S.P., Wieghardt, K., Neese, F. (2007). Characterization of a genuine Iron(V)-nitrido species by nuclear resonant vibrational spectroscopy coupled to density functional calculations *Journal of the American Chemical Society* 129(36), 11053-11060. https://doi.org/10.1021/ja070792y
- Ray, K., **DeBeer George, S.**, Solomon, E.I., Wieghardt, K., Neese, F. (2007). Description of the ground-state covalencies of the bis(dithiolato) transition-metal complexes from X-ray absorption spectroscopy and time-dependent density-functional calculations *Chemistry – A European Journal* 13(10), 2783-2797. https://doi.org/10.1002/chem.200601425

- Sarangi, R., **DeBeer George, S.**, Rudd, D.J., Szilagyi, R.K., Ribas, X., Rovira, C., Almeida, M., Hodgson, K.O., Hedman, B., Solomon, E.I. (2007). Sulfur K-edge X-ray absorption spectroscopy as a probe of ligand-metal bond covalency: Metal vs ligand oxidation in copper and nickel dithiolene complexes *Journal of the American Chemical Society* 129(8), 2316-2326. https://doi.org/10.1021/ja0665949
- Song, W. J., Seo, M. S., **DeBeer George, S.**, Ohta, T., Song, R., Kang, M.-J., Tosha, T., Kitagawa, T., Solomon, E.I., and Nam, W. (2007). Synthesis, characterization, and reactivities of manganese(V)-oxo porphyrin complexes *Journal of the American Chemical Society* 129(5), 1268-1277. https://doi.org/10.1021/ja066460v
- Yano, J., Robblee, J., Pushkar, Y., Marcus, M.A., Bendix, J., Workman, J.M., Collins, T.J., Solomon, E.I., **DeBeer George, S.**, Yachandra, V.K. (2007). Polarized X-ray absorption spectroscopy of single-crystal Mn(V) complexes relevant to the oxygen-evolving complex of photosystem II *Journal of the American Chemical Society* 129(43), 12989-13000. https://doi.org/10.1021/ja071286b

2006

- Berry, J.F., Bill, E., Bothe, E., **DeBeer George, S.**, Mienert, B., Neese, F., Wieghardt, K. (2006). An octahedral coordination complex of iron(VI) *Science* 312(5782), 1937-1941. https://doi.org/10.1126/science.1128506
- Frank, P., **DeBeer George, S.**, Anxolabehere-Mallart, E., Hedman, B., Hodgson, K.O. (2006). A systematic resolution of sulfur in reticulated vitreous carbon using X-ray absorption spectroscopy *Inorganic Chemistry* 45(24), 9864-9876. https://doi.org/10.1021/ic0610637
- **DeBeer George, S.**, Huang, K.W., Waymouth, R.M., Solomon, E.I. (2006). Metal and ligand K-edge XAS of titanium-TEMPO complexes: Determination of oxidation states and insights into Ti-O bond homolysis *Inorganic Chemistry* 45(11), 4468-4477. https://doi.org/10.1021/ic060402t
- Kapre, R., Ray, K., Sylvestre, I., Weyhermüller, T., **DeBeer George, S.**, Neese, F., Wieghardt, K. (2006). Molecular and electronic structures of oxo-bis(benzene-1,2-dithiolato)chromate(V) monoanions. A combined experimental and density functional study *Inorganic Chemistry* 45(9), 3499-3509. https://doi.org/10.1021/ic051844s

2005

- Aliaga-Alcalde, N., **DeBeer George, S.**, Mienert, B., Bill, E., Wieghardt, K., Neese, F. (2005) The geometric and electronic structure of $[(\text{cyclam-acetato})\text{Fe}(\text{N})]^{+}$: A genuine iron(V) species with a ground-state spin S=1/2 *Angewandte Chemie International Edition* 44(19), 2908-2912. https://doi.org/10.1002/anie.200462368
- Basumallick, L., Sarangi, R., **DeBeer George, S.**, Elmore, B., Hooper, A. B., Hedman, B., Hodgson, K.O., Solomon, E.I. (2005). Spectroscopic and density functional studies of the red copper site in nitrosocyanin: Role of the protein in determining active site geometric and electronic structure *Journal of the American Chemical Society* 127(10), 3531-3544. https://doi.org/10.1021/ja044412+
- **DeBeer George, S.**, Brant, P., Solomon, E.I. (2005). Metal and ligand K-Edge XAS of organotitanium complexes: Metal 4p and 3d contributions to pre-edge intensity and their contributions to bonding *Journal of the American Chemical Society* 127(2), 667-674. https://doi.org/10.1021/ja044827v

- Hart, P.J., Nersissian, A.M., **DeBeer George, S.** (2005) Copper Proteins with Type 1 Sites *Encyclopedia of Inorganic Chemistry* 1173-1201. https://doi.org/10.1002/9781119951438.eibc0054

2004

- Solomon, E.I., Szilagyi, R.K., **DeBeer George, S.**, Basumallick, L. (2004). Electronic structures of metal sites in proteins and models: Contributions to function in blue copper proteins *Chemical Reviews* 104(2), 419-458. https://doi.org/10.1021/cr0206317
- Szilagyi, R.K., Frank, P., **DeBeer George, S.**, Hedman, B., Hodgson, K.O. (2004). High covalence in $CuSO_4$ and the radicalization of sulfate: An X-ray absorption and density functional study *Inorganic Chemistry* 43(26), 8318-8329. https://doi.org/10.1021/ic030311l

2003

- **DeBeer George, S.**, Basumallick, L., Szilagyi, R.K., Randall, D.W., Hill, M.G., Nersissian, A.M., Valentine, J.S., Hedman, B., Hodgson, K.O., Solomon, E.I. (2003). Spectroscopic investigation of stellacyanin mutants: Axial ligand interactions at the blue copper site, *Journal of the American Chemical Society* 125(37), 11314-11328. https://doi.org/10.1021/ja035802j

2002

- Basumallick, L., **DeBeer George, S.**, Randall, D.W., Hedman, B., Hodgson, K.O., Fujisawa, K., Solomon, E.I. (2002). Spectroscopic comparison of the five-coordinate [Cu(SMeIm)(HB(3,5-$iPr_2pz)_3$)] with the four-coordinate [$Cu(SCPh_3)$(HB(3,5-$iPr_2pz)_3$)]: effect of coordination number increase on a blue cop per type site *Inorganica Chimica Acta* 337, 357-365. https://doi.org/10.1016/S0020-1693(02)01104-0
- Chen, P., **DeBeer George, S.**, Cabrito, I., Antholine, W.E., Moura, J.J. G., Moura, I., Hedman, B., Hodgson, K.O., Solomon, E.I. (2002). Electronic structure description of the μ_4-sulfide bridged tetranuclear Cu_Z center in N_2O reductase *Journal of the American Chemical Society* 124(5), 744-745. https://doi.org/10.1021/ja0169623
- Lee, S.K., **DeBeer George, S.**, Antholine, W.E., Hedman, B., Hodgson, K.O., Solomon, E.I. (2002). Nature of the intermediate formed in the reduction of O_2 to H_2O at the trinuclear copper cluster active site in native laccase *Journal of the American Chemical Society* 124(21), 6180-6193. https://doi.org/10.1021/ja0114052

2001

- **DeBeer George, S.**, Metz, M., Szilagyi, R.K., Wang, H.X., Cramer, S.P., Lu, Y., Tolman, W.B., Hedman, B., Hodgson, K.O., Solomon, E.I. (2001). A quantitative description of the ground-state wave function of Cu_A by X-ray absorption spectroscopy: Comparison to plastocyanin and relevance to electron transfer *Journal of the American Chemical Society* 123(24), 5757-5767. https://doi.org/10.1021/ja004109i

- Hirsch, J., **DeBeer George, S.**, Solomon, E.I., Hedman, B., Hodgson, K.O., Burstyn, J.N. (2001). Raman and extended X-ray absorption fine structure characterization of a sulfur-ligated Cu(I) ethylene complex: Modeling the proposed ethylene binding site of *Arabidopsisthaliana* ETR1 *Inorganic Chemistry* 40(10), 2439. https://doi.org/10.1021/ic000671y
- Lehnert, N., **DeBeer George, S.**, Solomon, E.I. (2001). Recent advances in bioinorganic spectroscopy *Current Opinion in Chemical Biology* 5(2), 176-187. https://doi.org/10.1016/S1367-5931(00)00188-5

2000

- **DeBeer, S.**, Randall, D.W., Nersissian, A.M., Valentine, J.S., Hedman, B., Hodgson, K.O., Solomon, E. I. (2000). X-ray absorption edge and EXAFS studies of the blue copper site in stellacyanin: Effects of axial amide coordination *Journal of Physical Chemistry B* 104(46), 10814-10819. https://doi.org/10.1021/jp001334d
- **DeBeer, S.**, Wittung-Stafshede, P., Leckner, J., Karlsson, G., Winkler, J.R., Gray, H.B., Malmström, B.G., Solomon, E.I., Hedman, B., Hodgson, K.O. (2000). X-ray absorption spectroscopy of folded and unfolded copper(I) azurin *Inorganica Chimica Acta* 297(1-2), 278-282. https://doi.org/10.1016/S0020-1693(99)00315-1
- Randall, D.W., **DeBeer George, S.**, Hedman, B., Hodgson, K.O., Fujisawa, K., Solomon, E.I. (2000). Spectroscopic and electronic structural studies of blue copper model complexes. 1. Perturbation of the thiolate−Cu bond *Journal of the American Chemical Society* 122(47), 11620-11631. https://doi.org/10.1021/ja001591w
- Randall, D. W., , **DeBeer George, S.**Holland, P.L., Hedman, B., Hodgson, K.O., Tolman, W.B., Solomon, E.I. (2000). Spectroscopic and electronic structural studies of blue copper model complexes. 2. Comparison of three- and four-coordinate Cu(II)−thiolate complexes and fungal laccase *Journal of the American Chemical Society* 122(47), 11632-11648. https://doi.org/10.1021/ja001592o

1999

- **DeBeer, S.**, Kiser, C.N., Mines, G.A., Richards, J.H., Gray, H.B., Solomon, E.I., Hedman, B., Hodgson, K.O. (1999). X-ray absorption spectra of the oxidized and reduced forms of C112D azurin from *Pseudomonas aeruginosa Inorganic Chemistry* 38(30), 433-438. https://doi.org/10.1021/ic9804622
- Pidcock, E., **DeBeer, S.**, Obias, H.V., Hedman, B., Hodgson, K.O., Karlin, K.D., Solomon, E.I. (1999). A study of solid $[\{Cu(MePY2)\}_2O_2]^{2+}$ using resonance Raman and X-ray absorption spectroscopies: An intermediate Cu_2O_2 core structure or a solid solution? *Journal of the American Chemical Society* 121(9), 1870-1878. https://doi.org/10.1021/ja983444s