PUBLICATIONS – DR. SHENGFA YE

(1) Wang, C.-C.; Chang, H.-C.; Lai, Y.-C.; Fang, H.; Li, C.-C.; Hsu, H.-K.; Li, Z.-Y.; Lin, T.-S.; Kuo, T.-S.; Neese, F.; Ye, S.; Chiang, Y.-W.; Tsai, M.-L.; Liaw, W.-F.; Lee, W.-Z. A Structurally Characterized Nonheme Cobalt–Hydroperoxo Complex Derived from Its Superoxo Intermediate via Hydrogen Atom Abstraction. *J. Am. Chem. Soc.* **2016**, *138* (43), 14186–14189.

(2) Ye, S.; Kupper, C.; Meyer, S.; Andris, E.; Navrátil, R.; Krahe, O.; Mondal, B.; Atanasov, M.; Bill, E.; Roithová, J.; Meyer, F.; Neese, F. Magnetic Circular Dichroism Evidence for an Unusual Electronic Structure of a Tetracarbene-Oxoiron(IV) Complex. *J. Am. Chem. Soc.* **2016**, *138* (43), 14312–14325.

(3) Mondal, B.; Roy, L.; Neese, F.; Ye, S. High-Valent Iron-Oxo and -Nitrido Complexes: Bonding and Reactivity. *Isr. J. Chem.* **2016**, *56* (9-10), 763–772.

(4) Tamanaha, E.; Zhang, B.; Guo, Y.; Chang, W.-C.; Barr, E. W.; Xing, G.; St Clair, J.; Ye, S.; Neese, F.; Bollinger, J. M., Jr.; Krebs, C. Spectroscopic Evidence for the Two C–H-Cleaving Intermediates of *Aspergillus Nidulans* Isopenicillin *N* Synthase. *J. Am. Chem. Soc.* **2016**, *138* (28), 8862–8874.

(5) Mondal, B.; Neese, F.; Ye, S. Toward Rational Design of 3d Transition Metal Catalysts for CO_2 Hydrogenation Based on Insights into Hydricity-Controlled Rate-Determining Steps. *Inorg. Chem.* **2016**, *55* (11), 5438–5444.

(6) Wang, M.; Weyhermüller, T.; Bill, E.; Ye, S.; Wieghardt, K. Structural and Spectroscopic Characterization of Rhenium Complexes Containing Neutral, Monoanionic, and Dianionic Ligands of 2,2“-Bipyridines and 2,2”:6,2″-Terpyridines: An Experimental and Density Functional Theory (DFT)-Computational Study. *Inorg. Chem.* **2016**, *55* (10), 5019–5036.

(7) Christian, G. J.; Neese, F.; Ye, S. Unravelling the Molecular Origin of the Regiospecificity in Extradiol Catechol Dioxygenases. *Inorg. Chem.*

2016, *55* (8), 3853–3864.

(8) Ye, S.; Bill, E.; Neese, F. Electronic Structures of the $[Fe(N_2)(SiP^iPr_3)]^{+1/0/-1}$ Electron Transfer Series: A Counterintuitive Correlation between Isomer Shifts and Oxidation States. *Inorg. Chem.* **2016**, *55* (7), 3468–3474.

(9) Mondal, B.; Neese, F.; Ye, S. Control in the Rate-Determining Step Provides a Promising Strategy To Develop New Catalysts for CO_2 Hydrogenation: A Local Pair Natural Orbital Coupled Cluster Theory Study. *Inorg. Chem.* **2015**, *54* (15), 7192–7198.

(10) Fang, H.; Jing, H.; Ge, H.; Brothers, P. J.; Fu, X.; Ye, S. The Mechanism of E–H (E = N, O) Bond Activation by a Germanium Corrole Complex: A Combined Experimental and Computational Study. *J. Am. Chem. Soc.* **2015**, *137* (22), 7122–7127.

(11) Paretzki, A.; bner, R. H. X.; Ye, S.; Bubrin, M.; Käper, S. K. X.; Kaim, W. Electronic, Charge and Magnetic Interactions in Three-Centre Systems. *J. Mater. Chem. C* **2015**, *3*, 4801–4809.

(12) Ye, S.; Xue, G.; Krivokapic, I.; Petrenko, T.; Bill, E.; Que, L., Jr.; Neese, F. Magnetic Circular Dichroism and Computational Study of Mononuclear and Dinuclear Iron(IV) Complexes. *Chem. Sci.* **2015**, *6* (5), 2909–2921.

(13) Mondal, B.; Song, J.; Neese, F.; Ye, S. Bio-inspired Mechanistic Insights into CO_2 Reduction. *Curr. Opin. Chem. Biol.* **2015**, *25C*, 103–109.

(14) Song, J.; Klein, E. L.; Neese, F.; Ye, S. The Mechanism of Homogeneous CO_2 Reduction by Ni(cyclam): Product Selectivity, Concerted Proton-Electron Transfer and C-O Bond Cleavage. *Inorg. Chem.* **2014**, *53* (14), 7500–7507.

(15) Geng, C.; Ye, S.; Neese, F. Does a Higher Metal Oxidation State Necessarily Imply Higher Reactivity toward H-atom Transfer? A Computational Study of C–H Bond Oxidation by High-Valent Iron-Oxo and -Nitrido Complexes. *Dalton Trans.* **2014**, *43* (16), 6079–6086.

(16) Xue, G.; Geng, C.; Ye, S.; Fiedler, A. T.; Neese, F.; Que, L., Jr. Hydrogen-Bonding Effects on the Reactivity of $[X–Fe^{III}–O–Fe^{IV}=O]$ (X = OH, F) Complexes toward C–H Bond Cleavage. *Inorg. Chem.* **2013**,

52 (7), 3976–3984.

(17) Ye, S.; Geng, C.-Y.; Shaik, S.; Neese, F. Electronic Structure Analysis of Multistate Reactivity in Transition Metal Catalyzed Reactions: the Case of C–H Bond Activation by Non-Heme Iron(IV)–Oxo Cores *Phys. Chem. Chem. Phys.*, **2013**, *15* (21), 8017.–8030.

(18) DeBeer, S.; van Gastel, M.; Bill, E.; Ye, S.; Petrenko, T.; Pantazis, D. A.; Neese, F. Challenges in Molecular Energy Research. In *Chemical Energy Storage*, Schlögel, R. Ed., De Gruyter, **2013**, pp. 353–377.

(19) Dugan, T. R.; Bill, E.; MacLeod, K. C.; Christian, G. J.; Cowley, R. E.; Brennessel, W. W.; Ye, S.; Neese, F.; Holland, P. L. Reversible C–C Bond Formation between Redox-Active Pyridine Ligands in Iron Complexes. *J. Am. Chem. Soc.* **2012**, *134* (50), 20352–20364.

(20) Ye, S.; Neese, F. How Do Heavier Halide Ligands Affect the Signs and Magnitudes of the Zero-Field Splittings in Halogenonickel(II) Scorpionate Complexes? A Theoretical Investigation Coupled to Ligand-Field Analysis. *J. Chem. Theory Comput.* **2012**, *8* (7), 2344–2351.

(21) Ye, S.; Riplinger, C.; Hansen, A.; Krebs, C.; Bollinger, J. M., Jr.; Neese, F. Electronic Structure Analysis of the Oxygen-Activation Mechanism by Fe^{II}- and α-Ketoglutarate (αKG)-Dependent Dioxygenases. *Chem. Eur. J.* **2012**, *18* (21), 6555–6567.

(22) Desrochers, P. J.; Sutton, C. A.; Abrams, M. L.; Ye, S.; Neese, F.; Telser, J.; Ozarowski, A.; Krzystek, J. Electronic Structure of Nickel(II) and Zinc(II) Borohydrides from Spectroscopic Measurements and Computational Modeling. *Inorg. Chem.* **2012**, *51* (5), 2793–2805.

(23) Christian, G. J.; Ye, S.; Neese, F. Oxygen Activation in Extradiol Catecholate Dioxygenases – a Density FunctionalSstudy. *Chem. Sci.* **2012**, *3* (5), 1600–1611.

(24) Neese, F.; Liakos, D. G.; Ye, S. Correlated wavefunction methods in bioinorganic chemistry. *J. Biol. Inorg. Chem.* **2011**, *16* (6), 821–829.

(25) Ye, S.; Neese, F. Nonheme Oxo-iron(IV) Intermediates Form an Oxyl Radical upon Approaching the C-H Bond Activation Transition State. *Proc. Natl. Acad. Sci. U.S.A.* **2011**, *108* (4), 1228–1233.

(26) Ye, S.; Christian, G. J.; Geng, C-Y.; Neese, F. Theoretical

Spectroscopy of Iron Containing Enzymes and Biomimetics In *Iron-containing Enzymes, Versatile Catalysts of Hydroxylation Reaction in Nature* De Visser, S. P.; Kumar, D. Ed. RCS Publishing **2011**, pp. 119–147.

(27) Ye, S.; Price, J. C.; Barr, E. W.; Green, M. T.; Bollinger, J. M., Jr.; Krebs, C.; Neese, F. Cryoreduction of the NO-Adduct of Taurine:alpha-Ketoglutarate Dioxygenase (TauD) Yields an Elusive $\{FeNO\}^8$ Species. *J. Am. Chem. Soc.* **2010**, *132* (13), 4739–4751.

(28) Ye, S.; Neese, F. The Unusual Electronic Structure of Dinitrosyl Iron Complexes. *J. Am. Chem. Soc.* **2010**, *132* (11), 3646–3647.

(29) Ye, S.; Neese, F.; Ozarowski, A.; Smirnov, D.; Krzystek, J.; Telser, J.; Liao, J.-H.; Hung, C.-H.; Chu, W.-C.; Tsai, Y.-F.; et al. Family of V(III)-Tristhiolato Complexes Relevant to Functional Models of Vanadium Nitrogenase: Synthesis and Electronic Structure Investigations by Means of High-Frequency and -Field Electron Paramagnetic Resonance Coupled to Quantum Chemical Computations. *Inorg. Chem.* **2010**, *49* (3), 977–988.

(30) Ye, S.; Neese, F. Accurate Modeling of Spin-State Energetics in Spin-Crossover Systems with Modern Density Functional Theory. *Inorg. Chem.* **2010**, *49* (3), 772–774.

(31) Geng, C.; Ye, S.; Neese, F. Analysis of Reaction Channels for Alkane Hydroxylation by Nonheme Iron(IV)-Oxo Complexes. *Angew. Chem. Int. Ed.* **2010**, *49* (33), 5717–5720.

(32) Roemelt, M.; Ye, S.; Neese, F. Calibration of Modern Density Functional Theory Methods for the Prediction of ^{57}Fe Mossbauer Isomer Shifts: Meta-GGA and Double-Hybrid Functionals. *Inorg. Chem.* **2009**, *48* (3), 784–785.

(33) Ye, S.; Neese, F. Quantum Chemical Studies of C-H Activation Reactions by High-Valent Nonheme Iron Centers. *Curr. Opin. Chem. Biol.* **2009**, *13* (1), 89–98.

(34) Sundararajan, M.; Ganyushin, D.; Ye, S.; Neese, F. Multireference ab initio studies of zero-field splitting and magnetic circular dichroism spectra of tetrahedral Co(II) complexes. *Dalton Trans.* **2009**, No. 30, 6021–6036.

(35) Ye, S.; Tuttle, T.; Bill, E.; Simkhovich, L.; Gross, Z.; Thiel, W.; Neese, F. The Electronic Structure of Iron Corroles: A Combined Experimental and Quantum Chemical Study. *Chem. Eur. J.* **2008**, *14* (34), 10839–10851.

(36) Sinnecker, S.; Svensen, N.; Barr, E. W.; Ye, S.; Bollinger, J. M. J.; Bollinger, J. M.; Neese, F.; Krebs, C. Spectroscopic and Computational Evaluation of the Structure of the High-Spin Fe(IV)-Oxo Intermediates in Taurine: α-Ketoglutarate Dioxygenase from *Escherichia coli* and Its His99Ala Ligand Variant. *J. Am. Chem. Soc.* **2007**, *129* (19), 6168–6179.

(37) Kirchner, B.; Wennmohs, F.; Ye, S.; Neese, F. Theoretical Bioinorganic Chemistry: Electronic Structure Makes a Difference. *Curr. Opin. Chem. Biol.* **2007**, *11* (2), 134–141.

(38) Ye, S.; Neese, F. Combined Quantum Chemical and Spectroscopic Studies on Transition Metal Complexes with Coordinating Radicals. *Chemtracts (Special Volume on Computational Inorganic Chemistry)*, **2006**, *19* (6), 77–86.

(39) Ye, S.; Sarkar, B.; Niemeyer, M.; Kaim, W. Mixed-ligand copper complexes with 8-methylthioquinoline and triphenylphosphane or the o-semiquinone/catecholate redox system. *Eur. J. Inorg. Chem.* **2005**, No. 23, 4735–4738.

(40) Ye, S.; Kaim, W.; Niemeyer, M.; Hosmane, N. S. Intramolecular S→Pt Transmethylation from 8-Methylthioquinoline to Coordinated $PtMe_2$: Formation of *syn*-[*fac*-$Pt^{IV}Me_3$(μ-8-quinolinethiolato)]$_2$ with Stacked Quinoline Rings. *Organometallics* **2005**, *24*, 794–796.

(41) Ye, S.; Sarkar, B.; Duboc, C.; Fiedler, J.; Kaim, W. The Redox Series [M(bpy)2(Q)]n+, M = Ru or Os, Q = 3,5-Di-tert-butyl-N-phenyl-1,2-benzoquinonemonoimine. Isolation and a Complete X and W Band EPR Study of the Semiquinone States (n = 1). *Inorg. Chem.* **2005**, *44*, 2843–2847.

(42) Ye, S.; Sarkar, B.; Lissner, F.; Schleid, T.; van Slageren, J.; Fiedler, J.; Kaim, W. Three-Spin System with a Twist: A Bis(semiquinonato)copper Complex with Non-Planar Copper(II). *Angew. Chem. Int. Ed.* **2005**, *44* (14), 2103–2106.

(43) Ye, S.; Kaim, W.; Albrecht, M.; Lissner, F.; Schleid, T. Complexes of the Imine/Thioether Mixed-donor Ligand 8-Methylthioquinoline with d^6-Configurated Transition Metal Centers: Synthesis, Structures and Comparison with Complexes of 1-Methyl-2-(Methylthiomethyl)-*1H*-Benzimidazole. *Inorg. Chim. Acta* **2004**, *357* (11), 3325–3330.

(44) Ye, S.; Kaim, W.; Sarkar, B.; Schwederski, B.; Lissner, F.; Schleid, T.; Duboc-Toia, C.; Fiedler, J. First Crystal Structure Determination and High-Frequency EPR Study of an Organoarsanecopper Radical Complex. *Inorg. Chem. Commun.* **2003**, *6* (9), 1196–1200.

(45) Lu, X.; Tao, S.; Hu, H.; Cao, J.; Ye, S. Comparison of Koc Prediction Models Based on Fragment Constants and Molecular Indices *Chinese Journal of Soil Science* (in Chinese), **2000**, *31*, 166.

(46) Lu, X.; Tao, S.; Hu, H.; Ye, S. Prediction of Bioconcentration Factor of Organic Compounds in Fish by Molecular Connectivity Indices and Function Correction Factors *Chinese Journal of Applied Ecology* (in Chinese), **2000,** *11*, 277.

(47) Piao, H.; Tao, S.; Hu, H.; Lu, X.; Ye, S. Estimation of Sorption Coefficients of Organic Compounds Based on Fragment Constants *Chinese Journal of Soil Science* (in Chinese), **2000,** *37*, 209.

(48) Tao, S.; Ye, S.; Hu, H. Modeling of Complex Dissociation within Diffusion Layer during Free Metal Determination Using ASV Technique. *Environmental Chemistry* (in Chinese), **1999**, *18*, 103.

(49) Lu, X.; Tao, S.; Hu, H.; Ye, S. Prediction of Bioconcentration Factor of Non-polar Organic Compounds by Molecular Connectivity Indices *Environmental Science* (in Chinese), **1999**, *20*, 9.

(50) Piao, H.; Tao, S.; Hu, H.; Lu, X.; Ye, S. Estimation of Sorption Coefficients of Organic Compounds with Kow *Environmental Science and Technology* (in Chinese), **1999**, *87*, 8.