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List of Publications

Publications

606. Cramer, H. H.; Ye, S; **Neese, F.**; Werlé, C.; Weitner, W., Cobalt-Catalyzed Hydrosilylation of Carbon Dioxide to the Formic Acid, Formaldehyde, and Methanol Level—How to Control the Catalytic Network? *JACS Au* **2021**, (in press) 10.1021/jacsau.1c00350

605. Sharma, B.; Tran, V. A.; Pongratz, T.; Galazzo, L.; Zhurko, I.; Bordignon, E.; Kast, S. M.; **Neese, F.**; Marx, D., A Joint Venture of Ab Initio Molecular Dynamics, Coupled Cluster Electronic Structure Methods, and Liquid-State Theory to Compute Accurate Isotropic Hyperfine Constants of Nitroxide Probes in Water. *J. Chem. Theory Comput.* **2021**, *17*, (10), 6366-6386.

604. Altun, A.; Garcia-Ratés, M.; **Neese, F.**; Bistoni, G., Unveiling the complex pattern of intermolecular interactions responsible for the stability of the DNA duplex. *Chem. Sci.* **2021**, *12*, (38), 12785-12793.

603. Helmich-Paris, B.; De Souza, B.; **Neese, F.**; Izák, R., An improved chain of spheres for exchange algorithm. *J. Chem. Phys*. **2021**, *155*, (10), 104109.

602. Stoychev, G. L.; Auer; A. A.; Gauss, J.; **Neese, F.**, DLPNO-MP2 second derivatives for the computation of polarizabilities and NMR shieldings. *J. Chem. Phys.* **2021**, *154*, (16), 164110.

601. Ásgeirsson, V.; Birgisson, B. O.; Bjornsson, R.; Becker, U.; **Neese, F.**; Riplinger, C.; Jónsson, H., Nudged Elastic Band Method for Molecular Reactions Using Energy-Weighted Springs Combined with Eigenvector Following. *J. Chem. Theory Comput*. **2021**, *17,* (8), 4929-4945.

600. Lechner, M. H.; **Neese, F**.; Izák, R., An excited state coupled-cluster study on indigo dyes. *Mol. Phys*. **2021**, e1965235 (in press), DOI: 10.1080/00268976.2021.1965235

599. Guo, Y.; Sivalingam, K.; Kollmar, C.; **Neese, F.**, Approximations of density matrices in N-electron valence state second-order perturbation theory (NEVPT2). II. The full rank NEVPT2 (FR-NEVPT2) formulation*. J. Chem. Phys*. **2021**, *154*, (21), 2144113.

598. Guo, Y; Sivalingam, K.; **Neese, F**., Approximations of density matrices in N-electron valence state second-order perturbation theory (NEVPT2). I. Revisiting the NEVPT2 construction. *J. Chem. Phys.* **2021**, *154*, (21), 214111.

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597. Garcia-Ratés, M.; Becker, U.; **Neese, F.**, Implicit solvation in domain based pair natural orbital coupled cluster (DLPNO-CCSD) theory. *J. Comput. Chem.* **2021**, *21,* (27), 1959-1973.

596. Haack, A.; Hillenbrand, J.; van Gastel, M.; Fürstner, A.; **Neese, F.**, Spectroscopic and Theoretical Study on Siloxy-Based Molybdenum and Tungsten Alkylidyne Catalysts for Alkyne Metathesis. *ACS Catal*. **2021**, *11* (15), 9086-9101.

595. Lechner, M. H.; Izsák, R.; Mooijen, M.; **Neese, F.**, A perturbative approach to multireference equation-of-motion coupled cluster. *Mol. Phys*. **2021**, e1939185 (in press), DOI: 10.1080/00268976.2021.1939185

594. Ghosh, S.; **Neese, F.**; Izsák, I.; Bistoni, G., Fragment-Based Local Coupled Cluster Embedding Approach for the Quantification and Analysis of Noncovalent Interactions: Exploring the Many-Body Expansion of the Local Coupled Cluster Energy. *J. Chem. Theory Comput.* **2021**, *17*, (6), 3348-3359.

593. Sirohiwal, A.; **Neese, F.**; Pantazis, D.A., Chlorophyll excitation energies and structural stability of the CP47 antenna of photosystem II: a case study in the first-principles simulation of light-harvesting complexes. *Chem. Sci.*, **2021**, *12*, (23), 4463-4476.

592. Tarrago, M.; Römelt, C., Nehrkorn, J.; Schnegg; A.; **Neese, F.**, Bill, E.; Shengfa, Y., Experimental and Theoretical Evidence for an Unusual Almost Triply Degenerate Electronic Ground State of Ferrous Tetraphenylporphyrin. *Inorg. Chem.* **2021**, *60,* (7), 4966-4985.

591. Schulz, C.E.; Van Gastel, M.; Pantazis, D.A.; **Neese, F.**, Converged Structural and Spectroscopic Properties for Refined QM/MM Models of Azurin. *Inorg. Chem.* **2021**, *60*, (10), 7399-7412.

590. Chilkuri, V.G.; **Neese, F.**, Comparison of Many-Particle Representations for Selected Configuration Interaction: II. Numerical Benchmark Calculations. *J. Chem. Theory Comput.* **2021**, *17*, (5), 2868-2855.

589. Schulz, C.E.; Castillo, R.G.; Pantazis; D.A.; DeBeer, S.; **Neese, F.**, Structure–Spectroscopy Correlations for Intermediate Q of Soluble Methane Monooxygenase: Insights from QM/MM Calculations. *J. Am. Chem. Soc.*, **2021**, *143*, (17), 6560-6577

588. Sirohiwal, A.; **Neese, F**.; Pantazis, D.A., How Can We Predict Accurate Electrochromic Shifts for Biochromophores? A Case Study on the Photosynthetic Reaction Center. J*. Chem. Theory Comput.* **2021**, *17*, (3), 1858-1873.

587. Berraud-Pache, R.; Santamaría-Aranda, E.; De Souza, B.; Bistoni, G.; **Neese, F**.; Sampedro, D.; Izsák, R., Redesigning donor–acceptor Stenhouse adduct photoswitches through a joint experimental and computational study. *Chem. Sci.*, **2021**, *12*, (8), 2916-2924.

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586. Stoll, C.; Atanasov, M.; Bandemehr, J.; **Neese, F.**; Pietzonka, C.; Kraus, F.; Karttunen, A.J.; Seibald, M.; Heymann, G.; Huppertz, H., Coexistence of Two Different Distorted Octahedral [MnF6]3− Sites in K3[MnF6]: Manifestation in Spectroscopy and Magnetism. *Chem. Eur. J.*, **2021**, *27*, (38), 9801--9813

585. Haack, A.; Hillenbrand, J.; Leutzsch, M.; Van Gastel, M.; **Neese, F.**; Fürstner, A., Productive Alkyne Metathesis with “Canopy Catalysts” Mandates Pseudorotation. *J. Am. Chem. Soc.* **2021**, *143*, (15), 5643-5648.

584. Chilkuri, V. G.; **Neese, F.**, Comparison of many-particle representations for selected-CI I: A tree based approach. *J. Comp. Chem.*, **2021***, 42*, (14), 982-1005

583. Ravera, E.; Gigli, L.; Czarniecki, B.; Lang, L.; Kummerle, R.; Parigi, G.; Piccioli, M.; **Neese, F.**; Luchinat, C., A Quantum Chemistry View on Two Archetypical Paramagnetic Pentacoordinate Nickel(II) Complexes Offers a Fresh Look on Their NMR Spectra. *Inorg, Chem.* **2021,** *60* (3), 2068-2075.

582. Ni, Z.; Guo, Y.; **Neese, F.**; Li, W.; Li, S., Cluster-in-Molecule Local Correlation Method with an Accurate Distant Pair Correction for Large Systems. *J. Chem. Theory Comput.* **2021**, *17* (2), 756–766

581. Daniel, C.; Gonzalez, L.; **Neese, F.**, Quantum Theory: The Challenge of Transition Metal Complexes. *Phys. Chem. Chem. Phys.* **2021,** *23* (4), 2533-2534.

580. Beck, M. E.; Riplinger, C.; **Neese, F.**; Bistoni, G., Unraveling individual host-guest interactions in molecular recognition from first principles quantum mechanics: Insights into the nature of nicotinic acetylcholine receptor agonist binding. *J. Comp. Chem.,* **2021,** *42* (5), 293-302.

579. Kelai, M.; Cahier, B.; Atanasov, M.; **Neese, F.**; Tong, Y. F.; Zhang, L. Q.; Bellec, A.; Iasco, O.; Riviere, E.; Guillot, R.; Chacon, C.; Girard, Y.; Lagoute, J. M.; Rousset, S.; Repain, V.; Otero, E.; Arrio, M. A.; Sainctavit, P.; Barra, A. L.; Boillot, M. L.; Mallah, T., Robust magnetic anisotropy of a monolayer of hexacoordinate Fe(ii) complexes assembled on Cu(111). *Inorg. Chem. Front.*, **2021**, *8*, 9, 2395-2404

578 Guo, Y.; Riplinger, C.; Lakos, D.G; Becker, U.; Saitow, M.; **Neese, F.**, Linear scaling perturbative triples correction approximations for open-shell domain-based local pair natural orbital coupled cluster singles and doubles theory [DLPNO-CCSD(T_0/T)]. J. Chem. Phys. **2020**, *152*, 024116.

577. Chakarawet, K.; Atanasov, M.; Marbey, J.; Bunting, P. C.; **Neese, F.**; Hill, S.; Long, J. R., Strong Electronic and Magnetic Coupling in M-4 (M = Ni, Cu) Clusters via Direct Orbital Interactions between Low-Coordinate Metal Centers. *J. Am. Chem. Soc.* **2020,** *142* (45), 19161-19169.

576. Datta, D.; Saitow, M.; Sandhofer, B.; **Neese, F.**, Fe-57 Mossbauer parameters from domain based local pair-natural orbital coupled-cluster theory. *J. Chem. Phys.* **2020,** *153* (20), Art. No 204101

575. Lang, L.; Sivalingam, K.; **Neese, F.**, The combination of multipartitioning of the Hamiltonian with canonical Van Vleck perturbation theory leads to a Hermitian variant of quasidegenerate N-electron valence perturbation theory. *J. Chem. Phys.* **2020,** *152* (1), art. No 014109.

574. **Neese, F.**, MQM 2019 Introduction. *Molecular Physics* **2020,** *118* (21-22)

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573. Sirohiwal, A.; **Neese, F.**; Pantazis, D. A., Protein Matrix Control of Reaction Center Excitation in Photosystem II. *J. Am. Chem.Soc.* **2020,** *142* (42), 18174-18190

572. Sirohiwal, A.; Berraud-Pache, R.; **Neese, F.**; Izsak, R.; Pantazis, D.A. Accurate Computation of the Absorption Spectrum of Chlorophyll a with Pair Natural Orbital Coupled Cluster Methods*, J. Phys. Chem. A*, **2020**, *124 (40)*, 8761-8771.

571. Dittmer, A., Stoychev, G.L.; Manganas, D.; Auer, A.A.; **Neese, F.**, Computation of NMR Shielding Constants for Solids Using an Embedded Cluster Approach with DFT, Double Hybrid DFT and MP2, *J. Chem. Theo. Comp.*, **2020**, *16 (11)*, 6950-6967.

570. Altun, A.; **Neese, F.**; Bistoni, G. Extrapolation to the Limit of a Complete Pair Natural Orbital Space in Local Coupled-Cluster Calculations, *J. Chem. Theory Comput.* **2020**, *16 (10)*, 6142-6149

569. Lang, L.; Ravera, E.; Parigi, G.; Luchinat, C.; **Neese, F.** Solution of a Puzzle: High-Level Quantum-Chemical Treatment of Pseudocontact Chemical Shifts Confirms Classic Semiempirical Theory, *J. Phys. Chem. Lett.* **2020**, 11, 8735−8744

568. Hillenbrand, J.; van Gastel, M.; Bill, E.; **Neese, F.**; Fürstner, A. Isolation of a Homoleptic Non-oxo Mo(V) Alkoxide Complex: Synthesis, Structure, and Electronic Properties of Penta-*tert*-Butoxymolybdenum, *J. Am. Chem. Soc.* **2020**, 142, 38, 16392–16402

567. Sanakis, Y; Krzystek, J.; Maganas, D.; Grigoropoulos, A.; Ferentinos, E.; Kostakis, M. G. Petroulea, V.; Pissas, M.; Thirunavukkuarasu, K.; Wernsdorfer, W.; **Neese, F.**; Kyritsis**,** P. Magnetic Properties and Electronic Structure of the *S* = 2 Complex $[Mn^{III}\{(OPPh_2)_2N\}_3]$ Showing Field-Induced Slow Magnetization Relaxation, *Inorg. Chem.* **2020**, 59 (18), 13281–13294

566. **Neese, F.**, Lang, L.; Chilkuri, V.G. Effective Hamiltonians in Chemistry, in Pavarini, E.; Koch, E. (Eds) Topology, Entaglement and Strong Correlations. Modeling and Simulation, Vol. 10, Verlag des Forschungszentrums Jülich, Jülich, Germany, **2020**, 34 pages., ISBN: 978-3-95806-466-9

565. Meyer, F.; **Neese, F.** Impact of Modern Spectroscopy in Inorganic Chemistry*, Inorg. Chem.*, **2020**, *59* (19), 13805-13806.

564. Auer, A. A.; Tran, V. A.; Sharma, B.; Stoychev, G. L.; Marx, D.; **Neese, F.**, A case study of density functional theory and domain-based local pair natural orbital coupled cluster for vibrational effects on EPR hyperfine coupling constants: vibrational perturbation theory versus ab initio molecular dynamics. *Molec. Phys.*, **2020**, 118.

563. Ghosh, S.; Das, S.; De, C. K.; Yepes, D.; **Neese, F.**; Bistoni, G.; Leutzsch, M.; List, B., Strong and Confined Acids Control Five Stereogenic Centers in Catalytic Asymmetric Diels-Alder Reactions of Cyclohexadienones with Cyclopentadiene. *Ang. Chem. Int. Ed.* **2020**, *59* (39), 12347-12351.

562. Ghafarian Shirazi, R.; Pantazis, D. A.; **Neese, F.**, Performance of density functional theory and orbital-optimised second-order perturbation theory methods for geometries and singlet-triplet state splittings of aryl-carbenes. *Molec. Phys.*, **2020**, 12.

561. Flöser, B. M.; Guo, Y.; Riplinger, C.; Tuczek, F.; **Neese, F.**, Detailed Pair Natural Orbital-Based Coupled Cluster Studies of Spin Crossover Energetics. *J. Chem. Theo. Comp.* **2020,** *16* (4), 2224-2235.

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560. Gottschalk, H. C.; Poblotzki, A.; Fatima, M.; Obenchain, D. A.; Perez, C.; Antony, J.; Auer, A. A.; Baptista, L.; Benoit, D. M.; Bistoni, G.; Bohle, F.; Dahmani, R.; Firaha, D.; Grimme, S.; Hansen, A.; Harding, M. E.; Hochlaf, M.; Holzer, C.; Jansen, G.; Klopper, W.; Kopp, W. A.; Kroger, L. C.; Leonhard, K.; Al-Mogren, M. M.; Mouhib, H.; **Neese, F.**; Pereira, X. N.; Prakash, M.; Ulusoy, I. S.; Mata, R. A.; Suhm, M. A.; Schnell, M., The first microsolvation step for furans: New experiments and benchmarking strategies. *J. Chem. Phys.* **2020,** *152* (16), Art. Nr. 164303.

559. Kollmar, C.; Sivalingam, K.; **Neese, F.**, An alternative choice of the zeroth-order Hamiltonian in CASPT2 theory, *J.Chem. Phys.* **2020,** *153*, Art. Nr. 019901.

558. Kumar, A.; **Neese, F.**; Valeev, E. F., Explicitly correlated coupled cluster method for accurate treatment of open-shell molecules with hundreds of atoms. *J. Chem. Phys.* **2020,** *153* (9), Art. Nr. 094105.

557. Lazorski, M. S.; Schapiro, I.; Gaddie, R. S.; Lehnig, A. P.; Atanasov, M.; **Neese, F.**; Steiner, U. E.; Elliott, C. M., Spin-chemical effects on intramolecular photoinduced charge transfer reactions in bisphenanthroline copper(i)-viologen dyad assemblies. *Chem. Sci.,* **2020,** *11* (21), 5511-5525.

556. Maganas, D.; Kowalska, J. K.; Van Stappen, C.; DeBeer, S.; **Neese, F.**, Mechanism of L-2,L-3-edge x-ray magnetic circular dichroism intensity from quantum chemical calculations and experiment-A case study on V-(IV)/V-(III) complexes. *J. Chem. Phys.* **2020,** *152* (11), Art. Nr. 114107.

555. **Neese, F.**; Wennmohs, F.; Becker, U.; Riplinger, C., The ORCA quantum chemistry program package. *J. Chem. Phys.* **2020,** *152*, Art. Nr. L224108.

554. Rolfes, J. D.; **Neese, F.;** Pantazis, D. A., All-electron scalar relativistic basis sets for the elements Rb-Xe. *J. Comp. Chem.* **2020,** *41* (20), 1842-1849.

553. Spiller, N.; Chilkuri, V. G.; DeBeer, S.; **Neese, F.**, Sulfur vs. Selenium as Bridging Ligand in Di-Iron Complexes: A Theoretical Analysis. *Eur. J. Inorg. Chem.* **2020,** *2020* (15-16), 1525-1538.

552. Tran, V. A.; **Neese, F.**, Double-hybrid density functional theory for g-tensor calculations using gauge including atomic orbitals. *J. Chem. Phys.* **2020,** *153*, 054105.

551. Yepes, D.; **Neese, F.**; List, B.; Bistoni, G., Unveiling the Delicate Balance of Steric and Dispersion Interactions in Organocatalysis Using High-Level Computational Methods. *J. Am. Chem. Soc.* **2020**, *142* (7), 3613-3625.

550. Schulz, A. C.; Frielingsdorf, S.; Pommerening, P.; Lauterbach, L.; Bistoni, G.; **Neese, F.**; Oestreich, M.; Lenz, O., Formyltetrahydrofolate Decarbonylase Synthesizes the Active Site CO Ligand of O-2-Tolerant NiFe Hydrogenase. *J. Am. Chem. Soc.* **2020**, 142 (3), 1457-1464.

549. Rolfes, J. D.; van Gastel, M.; **Neese, F.**, Where Is the Fluoro Wall?: A Quantum Chemical Investigation. *Inorg. Chem.* **2020**, *59* (2), 1556-1565.

548. Liakos, D. G.; Guo, Y.; **Neese, F**., Comprehensive Benchmark Results for the Domain Based Local Pair Natural Orbital Coupled Cluster Method (DLPNO-CCSD(T)) for Closed- and Open-Shell Systems. *J. Phys. Chem. A* **2020**, *124* (1), 90-100.

547. Lang, L.; Atanasov, M.; **Neese, F**., Improvement of Ab Initio Ligand Field Theory by Means of Multistate Perturbation Theory. *J. Phys. Chem. A* **2020**, *124* (5), 1025-1037.

546. Jung, J.; Loffler, S. T.; Langmann, J.; Heinemann, F. W.; Bill, E.; Bistoni, G.; Scherer, W.; Atanasov, M.; Meyer, K.; **Neese, F.**, Dispersion Forces Drive the Formation of Uranium-Alkane Adducts. *J. Am. Chem. Soc.* **2020**, *142* (4), 1864-1870.

545. Garcia-Rates, M.; **Neese, F**., Effect of the Solute Cavity on the Solvation Energy and its Derivatives within the Framework of the Gaussian Charge Scheme. *J. Comp. Chem.* **2020**, *41* (9), 922-939.

544. Fürstner, A.; List, B.; Ritter, T.; Schüth, F.; **Neese, F**., Walter Thiel (1949-2019) Obituary. *Angew. Chem., Int. Ed.* **2020**, *59* (4), 1382-1383.

543. Chilkuri, V. G.; DeBeer, S.; **Neese, F**., Ligand Field Theory and Angular Overlap Model Based Analysis of the Electronic Structure of Homovalent Iron-Sulfur Dimers. *Inorg. Chem.* **2020**, *59* (2), 984-995.

542. Berraud-Pache, R.; **Neese, F**.; Bistoni, G.; Izsak, R., Unveiling the Photophysical Properties of Boron-dipyrromethene Dyes Using a New Accurate Excited State Coupled Cluster Method. *J. Chem. Theo. Comput*. **2020**, *16* (1), 564-575.

541. Krewald, V.; **Neese, F**.; Pantazis, D. A., Implications of structural heterogeneity for the electronic structure of the final oxygen-evolving intermediate in photosystem II. *J. Inorg. Biochem.* **2019**, 199.

540. Keilwerth, M.; Hohenberger, J.; Heinemann, F. W.; Sutter, J.; Scheurer, A.; Fang, H. Y.; Bill, E.; **Neese, F**.; Ye, S. F.; Meyer, K., A Series of Iron Nitrosyl Complexes {Fe-NO}(6-9) and a Fleeting {Fe-NO}(10) Intermediate en Route to a Metalacyclic Iron Nitrosoalkane. *J. Am. Chem. Soc.* **2019**, 141 (43), 17217-17235.

539. Dittmer, A.; Izsak, R.; **Neese, F.**; Maganas, D., Accurate Band Gap Predictions of Semiconductors in the Framework of the Similarity Transformed Equation of Motion Coupled Cluster Theory. *Inorg. Chem*. **2019**, 58 (14), 9303-9315.

538. DeRosha, D. E.; Chilkuri, V. G.; Van Stappen, C.; Bill, E.; Mercado, B. Q.; DeBeer, S.; **Neese, F.**; Holland, P. L., Planar three-coordinate iron sulfide in a synthetic 4Fe-3S cluster with biomimetic reactivity*. Nat. Chem.* **2019**, 11 (11), 1019-1025.

537. Chrysina, M.; Heyno, E.; Kutin, Y.; Reus, M.; Nilsson, H.; Nowaczyk, M. M.; DeBeer, S.; **Neese, F**.; Messinger, J.; Lubitz, W.; Cox, N., Five-coordinate Mn-IV intermediate in the activation of nature's water splitting cofactor. *PNAS* **2019**, 116 (34), 16841-16846.

536. Chang, H. C.; Lin, Y. H.; Werle, C.; **Neese, F**.; Lee, W. Z.; Bill, E.; Ye, S. F., Conversion of a Fleeting Open-Shell Iron Nitride into an Iron Nitrosyl. *Angew. Chem., Int. Ed*. **2019**, 58 (49), 17589-17593.

535. Berraud-Pache, R.; **Neese, F**.; Bistoni, G.; Izsak, R., Computational Design of Near-Infrared Fluorescent Organic Dyes Using an Accurate New Wave Function Approach. *J. Phys. Chem. Let.* **2019**, 10 (17), 4822-4828.

534. Altun, A.; Saitow, M.; **Neese, F.**; Bistoni, G., Local Energy Decomposition of Open-Shell Molecular Systems in the Domain-Based Local Pair Natural Orbital Coupled Cluster Framework. *J. Chem. Theo. Comp.*. **2019**, 15 (3), 1616-1632.

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533. Altun, A.; **Neese, F**.; Bistoni, G., HFLD: A Nonempirical London Dispersion-Corrected Hartree-Fock Method for the Quantification and Analysis of Noncovalent Interaction Energies of Large Molecular Systems. *J. Chem. Theo. Comp.* **2019**, 15 (11), 5894-5907.

532. Shirazi, R. G.; **Neese, F**.; Pantazis, D. A.; Bistoni, G., Physical Nature of Differential Spin-State Stabilization of Carbenes by Hydrogen and Halogen Bonding: A Domain-Based Pair Natural Orbital Coupled Cluster Study. *J. Phys. Chem. A* **2019**, 123 (24), 5081-5090

531. de Souza, B.; Farias, G.; **Neese, F**.; Izsak, R., Efficient simulation of overtones and combination bands in resonant Raman spectra. *J. Chem. Phys.* **2019**, *150* (21) 214102.

530. Garcia-Rates, M.; **Neese, F**., Efficient implementation of the analytical second derivatives of hartree-fock and hybrid DFT energies within the framework of the conductor-like polarizable continuum model. *J. Comp. Chem.* **2019**, 40 (20), 1816-1828.

529. Lu, Q.; **Neese, F**.; Bistoni, G., London dispersion effects in the coordination and activation of alkanes in sigma-complexes: a local energy decomposition study. *Phys. Chem. Chem. Phys.* **2019**, 21 (22), 11569-11577.

528. Salla, C. A. M.; dos Santos, J. T.; Farias, G.; Bortoluzi, A. J.; Curcio, S. F.; Cazati, T.; Izsak, R.; **Neese, F.**; de Souza, B.; Bechtold, I. H., New Boron(III) Blue Emitters for All-Solution Processed OLEDs: Molecular Design Assisted by Theoretical Modeling. *Eur. J. Inorg. Chem*. **2019**, (17), 2247-2257.

527. Thomsen, M. K.; Nyvang, A.; Walsh, J. P. S.; Bunting, P. C.; Long, J. R.; **Neese, F.**; Atanasov, M.; Genoni, A.; Oyergaard, J., Insights into Single-Molecule-Magnet Behavior from the Experimental Electron Density of Linear Two-Coordinate Iron Complexes. *Inorg. Chem.* **2019,** *58* (5), 3211-3218.

526. Sirohiwal, A.; **Neese, F.**; Pantazis, D. A., Microsolvation of the Redox-Active Tyrosine-D in Photosystem II: Correlation of Energetics with EPR Spectroscopy and Oxidation-Induced Proton Transfer. *J. Am. Chem. Soc.* **2019,** *141* (7), 3217-3231.

525. Roy, L.; Al-Afyouni, M. H.; DeRosha, D. E.; Mondal, B.; DiMucci, I. M.; Lancaster, K. M.; Shearer, J.; Bill, E.; Brennessel, W. W.; **Neese, F**.; Ye, S. F.; Holland, P. L., Reduction of CO2 by a masked two-coordinate cobalt(i) complex and characterization of a proposed oxodicobalt(ii) intermediate. *Chem. Sci.* **2019,** *10* (3), 918-929.

524. Pinski, P.; **Neese, F**., Analytical gradient for the domain-based local pair natural orbital second order Moller-Plesset perturbation theory method (DLPNO-MP2). *J. Chem. Phys.* **2019,** *150* (16) 164102.

523. **Neese, F.**; Atanasov, M.; Bistoni, G.; Maganas, D.; Ye, S. F., Chemistry and Quantum Mechanics in 2019: Give Us Insight and Numbers. *J. Am. Chem. Soc.* **2019,** *141* (7), 2814-2824.

522. Maganas, D.; Kowalska, J. K.; Nooijen, M.; DeBeer, S.; **Neese, F.**, Comparison of multireference ab initio wavefunction methodologies for X- ray absorption edges: A case study on Fe(II/III)Cl-4 (2-/1-) molecules. *J. Chem. Phys.* **2019,** *150* (10) 104106.

521. Lang, L.; **Neese, F.**, Spin-dependent properties in the framework of the dynamic correlation dressed complete active space method. *J. Chem. Phys.* **2019,** *150* (10).

520. Lang, J.; Brabec, J.; Saitow, M.; Pittner, J.; **Neese, F.**: Demel, O., Perturbative triples correction to domain-based local pair natural orbital variants of Mukherjee's state specific coupled cluster method. *Phys. Chem. Chem. Phys.* **2019,** *21* (9), 5022-5038.

519. Kollmar, C.; Sivalingam, K.; Helmich-Paris, B.; Angeli, C.; **Neese, F**., A perturbation-based super-CI approach for the orbital optimization of a CASSCF wave function. *J. Comp. Chem.* **2019**, *40* (14), 1463-1470.

518. Kallane, S. I.; Hahn, A. W.; Weyhermuller, T.; Bill, E.; **Neese, F**.; DeBeer, S.; van Gastel, M., Spectroscopic and Quantum Chemical Investigation of Benzene-1,2-dithiolate-Coordinated Diiron Complexes with Relevance to Dinitrogen Activation. *Inorg. Chem.* **2019**, *58* (8), 5111-5125.

517. Haldar, S.; Riplinger, C.; Demoulin, B.; **Neese, F**.; Izsak, R.; Dutta, A. K., Multilayer Approach to the IP-EOM-DLPNO-CCSD Method: Theory, Implementation, and Application. *J. Chem. Theory Comput*. **2019**, *15* (4), 2265-2277.

516. Dutta, A. K.; Saitow, M.; Demoulin, B.; **Neese, F.**; Izsak, R., A domain-based local pair natural orbital implementation of the equation of motion coupled cluster method for electron attached states. *J. Chem. Phys.* **2019**, *150* (16) 164123.

515. de Souza, B.; Farias, G.; **Neese, F**.; Izsak, R., Predicting Phosphorescence Rates of Light Organic Molecules Using Time-Dependent Density Functional Theory and the Path Integral Approach to Dynamics. *J. Chem. Theory Comput*. **2019**, 15 (3), 1896-1904.

514. Chang, H. C.; Mondal, B.; Fang, H. Y.; **Neese, F**.; Bill, E.; Ye, S. F., Electron Paramagnetic Resonance Signature of Tetragonal Low Spin Iron(V)-Nitrido and -Oxo Complexes Derived from the Electronic Structure Analysis of Heme and Non-Heme Archetypes. *J. Am. Chem. Soc.* **2019,** *141* (6), 2421-2434.

513. Altun, A.; **Neese, F**.; Bistoni, G., Effect of Electron Correlation on Intermolecular I nteractions: A Pair Natural Orbitals Coupled Cluster Based Local Energy Decomposition Study. *J. Chem. Theo. Comput.* **2019,** *15* (1), 215-228.

512. Stavretis, S. E.; Cheng, Y.; Daemen, L. L.; Brown, C. M.; Moseley, D. H.; Bill, E.; Atanasov, M.; Ramirez-Cuesta, A. J.; **Neese, F**.; Xue, Z.-L., Probing magnetic excitations in coII single-molecule magnets by inelastic neutron scattering. Eur. *J. Inorg. Chem.* **2019**(08), 1119-1127.

511. Saitow, M.; Dutta, A. K.; **Neese, F**., Accurate ionization potentials, electron affinities and electronegativities of single-walled carbon nanotubes by state-of-the-art local Coupled-Cluster Theory. *Bull. Chem. Soc. Jpn.* **2019,** *92* (1), 170-174.

510. Atanasov, M.; **Neese, F**., Computational studies on vibronic coupling in single molecule magnets: Impact on the mechanism of magnetic relaxation. *J. Phys.: Conf. Ser.* **2018** *1148,* 012006.

509. Ho, L. P.; Nasr, A.; Jones, P. G.; Altun, A.; **Neese, F**.; Bistoni, G.;Tamm, M. London Dispersion Interactions in Pnictogen Cations ECl2 (+) and E=E (2+) (E=P, As, Sb) Supported by Anionic N-Heterocyclic Carbenes, *Chem. Eur. J.*, **2018**, *24* (71), 18922-18932

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508. Dutta, A. K.; **Neese, F.**; Izsak, R. Accelerating the coupled-cluster singles and doubles method using the chain-of-sphere approximation, Mol. Phys. **2018**, *116* (11), 1428-1434

507. Bunting, P. C.; Atanasov, M.; Damgaard-Moller, E.; Perfetti, M.; Crassee, I.; Orlita,M.; Overgaard, J.; van Slageren, J.; **Neese, F.**; Long, J. R. A linear cobalt(II) complex with maximal orbital angular momentum from a non-Aufbau ground state, Science **2018**, 362, eaat7319, DOI:10.1126/science.aat7319

506. David, G.; Wennmohs, F.; **Neese, F**.; Ferre, N. Chemical Tuning of Magnetic Exchange Couplings Using Broken Symmetry Density Functional Theory, *Inorg. Chem.* **2018**, *57* (20), 12769-12776

505. Gatzenmeier, T.; Turberg, M.; Yepes, D.; Xie, Y.W.; **Neese, F**.; Bistoni, G.; List, B. Scalable and highly diastereo- and enantioselective catalytic Diels-Alder reaction of α,β-unsaturated methyl esters, *J. Am. Chem. Soc.* **2018**, *140* (40), 12671-12676

504. Collins, L.; van Gastel, M.; **Neese, F.**; Fürstner, A. Enhanced Electrophilicity of Heterobimetallic Bi-Rh Paddlewheel Carbene Complexes: A Combined Experimental, Spectroscopic, and Computational Study, *J. Am. Chem. Soc.* **2018**, *140* (40), 13042-13055

503. Van Stappen, C.; Maganas, D.; DeBeer, S.; Bill, E.; **Neese, F.** Investigations of the Magnetic and Spectroscopic Properties of V(III) and V(IV) Complexes *Inorg. Chem.* **2018**, *57* (11), 6421-6438

502. Stoychev, G. L.; Auer, A. A.; **Neese, F.** Efficient and Accurate Prediction of Nuclear Magnetic Resonance Shielding Tensors with Double-Hybrid Density Functional Theory *J. Chem. Theory Comp.* **2018**, *14* (9), 4756-4771

501. Singh, S. K.; Atanasov, M.; **Neese, F.**, Challenges in multireference perturbation theory for the calculations of the g-tensor of first-row fransition-metal complexes. *J. Chem. Theory Comp.* **2018,** *14* (9), 4662-4677.

500. Shirazi, R. G.; **Neese, F.**; Pantazis, D. A. Accurate Spin-State Energetics for Aryl Carbenes. *J. Chem. Theory Comput. 2018, 14, 9, 4733–4746*

499. Sen, A.; de Souza, B.; Huntington, L. M. J.; Krupicka, M.; **Neese, F.**; Izsak, R. An efficient pair natural orbital based configuration interaction scheme for the calculation of open-shell ionization potentials *J. Chem. Phys.* **2018**, *149* (11), 114108

498. Saitow, M.; **Neese, F.** Accurate spin-densities based on the domain-based local pair-natural orbital coupled-cluster theory, *J. Chem. Phys.* **2018**, *149* (3), 034104

497. Moseley, D. H.; Stavretis, S. E.; Thirunavukkuarasu, K.; Ozerov, M.; Cheng, Y. Q.; Daemen, L. L.; Ludwig, J.; Lu, Z. G.; Smirnov, D.; Brown, C. M.; Pandey, A.; Ramirez-Cuesta, A. J.; Lamb, A. C.; Atanasov, M.; Bill, E.; **Neese, F**.; Xue, Z. L., Spin-phonon couplings in transition metal complexes with slow magnetic relaxation *Nat. Comm.***2018,** *9,* 2572

496. Mondal, B.; **Neese, F.**; Bill, E.; Ye, S. F. Electronic Structure Contributions of Non-Herne Oxo-Iron(V) Complexes to the Reactivity *J. Am. Chem. Soc.* **2018**, *140* (30), 9531-9544

495. Kubas, A.; Verkamp, M.; Vura-Weis, J.; **Neese, F.**; Maganas, D. Restricted Open-Shell Configuration Interaction Singles Study on M- and L-edge X-ray Absorption Spectroscopy of Solid Chemical Systems *J. Chem. Theo. Comp.* **2018**, *14*, 4320-4334

494. Dutta, A. K.; Saitow, M.; Riplinger, C.; **Neese, F.**; Izsak, R. A near linear scaling equation of motion coupled cluster method for ionized states *J. Chem. Phys.* **2018**, *148* (24), 244101

493. Chantzis, A.; Kowalska, J. K.; Maganas, D.; DeBeer, S.; **Neese, F**. Ab Initio Wave Function-Based Determination of Element Specific Shifts for the Efficient Calculation of X-ray Absorption Spectra of Main Group Elements and First Row Transition Metals *J. Chem. Theo. Comp.* **2018**, *14* (7), 3686-3702.

492. Bistoni, G.; Polyak, I.; Sparta, M.; Thiel, W.; **Neese, F**. Toward Accurate QM/MM Reaction Barriers with Large QM Regions Using Domain Based Pair Natural Orbital Coupled Cluster Theory *J. Chem. Theo. Comp.* **2018**, *14 (7)*, 3524-3531

491. Yamamoto, K.; Li, J. K.; Garber, J. A. O.; Rolfes, J. D.; Boursalian, G. B.; Borghs, J. C.; Genicot, C.; Jacq, J.; van Gastel, M.; **Neese, F.**; Ritter, T., Palladium-catalysed electrophilic aromatic C-H fluorination. *Nature* **2018,** *554* (7693), 511-514.

490. Stoychev, G. L.; Auer, A. A.; Izsak, R.; **Neese, F.**, Self-Consistent Field Calculation of Nuclear Magnetic Resonance Chemical Shielding Constants Using Gauge-Including Atomic Orbitals and Approximate Two-Electron Integrals. *J. Chem. Theo. Comp.* **2018,** *14* (2), 619-637.

489. Scheibe, B.; Pietzonka, C.; Mustonen, O.; Karppinen, M.; Karttunen, A. J.; Atanasov, M.; **Neese, F.**; Conrad, M.; Kraus, F., The U2F12 (2-) Anion of Sr U2F12. *Angew. Chem. Int. Ed.* **2018,** *57* (11), 2914-2918.

488. Römelt, C.; Ye, S. F.; Bill, E.; Weyhermuller, T.; van Gastel, M.; **Neese, F.**, Electronic Structure and Spin Multiplicity of Iron Tetraphenylporphyrins in Their Reduced States as Determined by a Combination of Resonance Raman Spectroscopy and Quantum Chemistry. *Inorg. Chem.* **2018,** *57* (4), 2141-2148.

487. Pinski, P.; **Neese, F.**, Communication: Exact analytical derivatives for the domain-based local pair natural orbital MP2 method (DLPNO-MP2). *J. Chem. Phys.* **148**, 031101.

486. **Neese, F.**, Software update: the ORCA program system, version 4.0. *Wiley Interdiscip Rev Comput Mol Sci.* **2018,** *8* (1).

485. Melo, M. C. R.; Bernardi, R. C.; Rudack, T.; Scheurer, M.; Riplinger, C.; Phillips, J. C.; Maia, J. D. C.; Rocha, G. B.; Ribeiro, J. V.; Stone, J. E.; **Neese, F.**; Schulten, K.; Luthey-Schulten, Z., NAMD goes quantum: an integrative suite for hybrid simulations. *Nat. Meth.* **2018,** *15* (5), 351-354.

484. Maganas, D.; DeBeer, S.; **Neese, F.**, Pair Natural Orbital Restricted Open-Shell Configuration Interaction (PNO-ROCIS) Approach for Calculating X-ray Absorption Spectra of Large Chemical Systems. *J. Phys. Chem. A* **2018,** *122* (5), 1215-1227.

483. Lu, Q.; **Neese, F.**; Bistoni, G., Formation of Agostic Structures Driven by London Dispersion. *Angew. Chem. Int. Ed.* **2018,** *57* (17), 4760-4764.

482. Guo, Y.; Riplinger, C.; Becker, U.; Liakos, D. G.; Minenkov, Y.; Cavallo, L.; **Neese, F.**, Communication: An improved linear scaling perturbative triples correction for the domain based local pair-natural orbital based singles and doubles coupled cluster method DLPNO-CCSD(T). *J. Chem. Phys.* **2018,** *148* (1).

481. Guo, Y.; Becker, U.; **Neese, F.**, Comparison and combination of "direct" and fragment based local correlation methods: Cluster in molecules and domain based local pair natural orbital perturbation and coupled cluster theories. *J. Chem. Phys.* **2018,** *148* (12), 124117.

480. Gottschalk, H. C.; Poblotzki, A.; Suhm, M. A.; Al-Mogren, M. M.; Antony, J.; Auer, A. A.; Baptista, L.; Benoit, D. M.; Bistoni, G.; Bohle, F.; Dahmani, R.; Firaha, D.; Grimme, S.; Hansen, A.; Harding, M. E.; Hochlaf, M.; Holzer, C.; Jansen, G.; Klopper, W.; Kopp, W. A.; Kroger, L. C.; Leonhard, K.; Mouhib, H.; **Neese, F.**; Pereira, M. N.; Ulusoy, I. S.; Wuttke, A.; Mata, R. A., The furan microsolvation blind challenge for quantum chemical methods: First steps. *J. Chem. Phys.* **2018,** *148* (1).

479. Dutta, A. K.; Nooijen, M.; **Neese, F.**; Izsak, R., Exploring the Accuracy of a Low Scaling Similarity Transformed Equation of Motion Method for Vertical Excitation Energies. *J. Chem. Theo. Comp.* **2018,** *14* (1), 72-91.

478. Dutta, A. K.; **Neese, F.**; Izsak, R., Accelerating the coupled-cluster singles and doubles method using the chain-of-sphere approximation. *Mol. Phys.* **2018,** *116* (11), 1428-1434.

477. De Souza, B.; **Neese, F.**; Izsak, R., On the theoretical prediction of fluorescence rates from first principles using the path integral approach. *J. Chem. Phys.* **2018,** *148* (3), 034104.

476. Brabec, J.; Lang, J.; Saitow, M.; Pittner, J.; **Neese, F.**; Demel, O., Domain-Based Local Pair Natural Orbital Version of Mukherjee's State-Specific Coupled Cluster Method. *J. Chem. Theo. Comp.* **2018,** *14* (3), 1370-1382.

475. Altun, A.; **Neese, F.**; Bistoni, G., Local energy decomposition analysis of hydrogen-bonded dimers within a domain-based pair natural orbital coupled cluster study. *Beilstein J. Org. Chem.* **2018,** *14*, 919-929.

474. Pedersen, K. S.; Woodruff, D. N.; Singh, S. K.; Tressaud, A.; Durand, E.; Atanasov, M.; Perlepe, P.; Ollefs, K.; Wilhelm, F.; Mathoniere, C.; **Neese, F.**; Rogalev, A.; Bendix, J.; Clerac, R., OsF6 (x-): Molecular Models for Spin-Orbit Entangled Phenomena. *Chem. Eur. J.* **2017,** *23* (47), 11244-11248.

473. Pathak, S.; Lang, L.; **Neese, F.**, A dynamic correlation dressed complete active space method: Theory, implementation, and preliminary applictions. *J. Chem. Phys.* **2017,** *147* (23), 234109.

472. **Neese, F.**; Suturina, E.; Atanasov, M., How is metal covalency reflected in ligand field parameters? *Abstr. Pap. Am. Chem. Soc.* **2017,** *253*.

471. **Neese, F.**, Coupled cluster theory for hundreds of atoms. *Abstr. Pap. Am. Chem. Soc.* **2017,** *253*.

470. **Neese, F.**, High-Level Spectroscopy, Quantum Chemistry, and Catalysis: Not just a

Passing Fad. *Angew. Chem. Int. Ed.* **2017,** *56* (37), 11003-11010.

469. Matsuoka, H.; Retegan, M.; Schmitt, L.; Hoger, S.; **Neese, F.**; Schiemann, O., Time-Resolved Electron Paramagnetic Resonance and Theoretical Investigations of Metal-Free Room-Temperature Triplet Emitters. *J. Am. Chem. Soc.* **2017,** *139* (37), 12968-12975.

468. Mai, S.; Plasser, F.; Pabst, M.; **Neese, F.**; Kohn, A.; Gonzalez, L., Surface hopping dynamics including intersystem crossing using the algebraic diagrammatic construction method. *J. Chem. Phys.* **2017,** *147* (18).

467. Maganas, D.; DeBeer, S.; **Neese, F.**, A Restricted Open Configuration Interaction with Singles Method To Calculate Valence-to-Core Resonant X-ray Emission Spectra: A Case Study. *Inorg. Chem.* **2017,** *56* (19), 11819-11836.

466. Lubitz, W.; Cox, N.; Pantazis, D.; **Neese, F.**, Multifrequency pulse EPR studies of the water oxidizing complex in photosynthesis. *Abstr. Pap. Am. Chem. Soc.* **2017,** *253*.

465. Lohmiller, T.; Krewald, V.; Sedoud, A.; Rutherford, A. W.; **Neese, F.**; Lubitz, W.; Pantazis, D. A.; Cox, N., The First State in the Catalytic Cycle of the Water-Oxidizing Enzyme: Identification of a Water-Derived mu-Hydroxo Bridge. *J. Am. Chem. Soc.* **2017,** *139* (41), 14412-14424.

464. Kubas, A.; Noak, J.; Trunschke, A.; Schlogl, R.; **Neese, F.**; Maganas, D., A combined experimental and theoretical spectroscopic protocol for determination of the structure of heterogeneous catalysts: developing the information content of the resonance Raman spectra of M1 MoVOx. *Chem. Sci.* **2017,** *8* (9), 6338-6353.

463. Jung, J. L.; Atanasov, M.; **Neese, F.**, Ab Initio Ligand-Field Theory Analysis and Covalency Trends in Actinide and Lanthanide Free Ions and Octahedral Complexes. *Inorg. Chem.* **2017,** *56* (15), 8802-8816.

462. Huntington, L. M. J.; Krupicka, M.; **Neese, F.**; Izsak, R., Similarity transformed equation of motion coupled-cluster theory based on an unrestricted Hartree-Fock reference for applications to high-spin open-shell systems. *J. Chem. Phys.* **2017,** *147* (17).

461. Guo, Y.; Sivalingam, K.; Valeev, E. F.; **Neese, F.**, Explicitly correlated N-electron valence state perturbation theory (NEVPT2-F12). *J. Chem. Phys.* **2017,** *147* (6).

460. Grimme, S.; Bannwarth, C.; Dohm, S.; Hansen, A.; Pisarek, J.; Pracht, P.; Seibert, J.; **Neese, F.**, Fully Automated Quantum-Chemistry-Based Computation of Spin-Spin-Coupled Nuclear Magnetic Resonance Spectra. *Angew. Chem. Int. Ed.* **2017,** *56* (46), 14763-14769.

459. Chilkuri, V. G.; DeBeer, S.; **Neese, F.**, Revisiting the Electronic Structure of FeS Monomers Using ab Initio Ligand Field Theory and the Angular Overlap Model. *Inorg. Chem.* **2017,** *56* (17), 10418-10436.

458. Bistoni, G.; Riplinger, C.; Minenkov, Y.; Cavallo, L.; Auer, A. A.; **Neese, F.**, Treating Subvalence Correlation Effects in Domain Based Pair Natural Orbital Coupled Cluster Calculations: An Out-of-the-Box Approach. *J. Chem. Theo. Comp.* **2017**, *13* (7), 3220-3227.

457. Chakraborty, U.; Demeshko, S.; Meyer, F.; Rebreyend, C.; de Bruin, B.; Atanasov, M.; **Neese, F.**; Muhldorf, B.; Wolf, R., Electronic Structure and Magnetic Anisotropy of an Unsaturated Cyclopentadienyl Iron(I) Complex with 15 Valence Electrons. *Angew. Chem. Int. Ed.* **2017**, *56* (27), 7995-7999.

456. Dutta, A. K.; **Neese, F.**; Izsak, R., A simple scheme for calculating approximate transition moments within the equation of motion expectation value formalism. *J. Chem. Phys.* **2017**, *146* (21).

455. Kalinowski, J.; Wennmohs, F.; **Neese, F.**, Arbitrary Angular Momentum Electron Repulsion Integrals with Graphical Processing Units: Application to the Resolution of Identity Hartree-Fock Method. *J. Chem. Theo. Comp.* **2017**, *13* (7), 3160-3170.

454. Krupicka, M.; Sivalingam, K.; Huntington, L.; Auer, A. A.; **Neese, F.**, A toolchain for the automatic generation of computer codes for correlated wavefunction calculations. *J. Comp. Chem.* **2017**, *38* (21), 1853-1868.

453. Kupper, C.; Mondal, B.; Serrano-Plana, J.; Klawitter, I.; **Neese, F.**; Costas, M.; Ye, S. F.; Meyer, F., Nonclassical Single-State Reactivity of an Oxo-Iron(IV) Complex Confined to Triplet Pathways. *J. Am. Chem. Soc.* **2017**, *139* (26), 8939-8949.

452. Paul, S.; **Neese, F.**; Pantazis, D. A., Structural models of the biological oxygen-evolving complex: achievements, insights, and challenges for biomimicry. *Green Chem.* **2017**, *19* (10), 2309-2325.

451. Pavosevic, F.; Peng, C.; Pinski, P.; Riplinger, C.; **Neese, F.**; Valeev, E. F., SparseMaps-A systematic infrastructure for reduced scaling electronic structure methods. V. Linear scaling explicitly correlated coupled-cluster method with pair natural orbitals. *J. Chem. Phys.* **2017**, *146* (17).

450. Roemelt, C.; Song, J. S.; Tarrago, M.; Rees, J. A.; van Gastel, M.; Weyhermuller, T.; DeBeer, S.; Bill, E.; **Neese, F.**; Ye, S. F., Electronic Structure of a Formal Iron(0) Porphyrin Complex Relevant to CO2 Reduction. *Inorg. Chem.* **2017**, *56* (8), 4745-4750.

449. Sabenya, G.; Lazaro, L.; Gamba, I.; Martin-Diaconescu, V.; Andris, E.; Weyhermuller, T.; **Neese, F.**; Roithova, J.; Bill, E.; Lloret-Fillol, J.; Costas, M., Generation, Spectroscopic, and Chemical Characterization of an Octahedral Iron(V)-Nitrido Species with a Neutral Ligand Platform. *J. Am. Chem. Soc.* **2017**, *139* (27), 9168-9177.

448. Saitow, M.; Becker, U.; Riplinger, C.; Valeev, E. F.; **Neese, F.**, A new near-linear scaling, efficient and accurate, open-shell domain-based local pair natural orbital coupled cluster singles and doubles theory. *J. Chem. Phys.* **2017**, *146* (16).

447. Schweinfurth, D.; Krzystek, J.; Atanasov, M.; Klein, J.; Hohloch, S.; Telser, J.; Demeshko, S.; Meyer, F.; **Neese, F.**; Sarkar, B., Tuning Magnetic Anisotropy Through Ligand Substitution in Five-Coordinate Co(II) Complexes. *Inorg. Chem.* **2017**, *56* (9), 5253-5265.

446. Sharma, A.; Roemelt, M.; Reithofer, M.; Schrock, R. R.; Hoffman, B. M.; **Neese, F.**, EPR/ENDOR and Theoretical Study of the Jahn-Teller-Active HIPTN3N (MoL)-L-V Complexes (L = N-, NH). *Inorg. Chem.* **2017**, *56* (12), 6906-6919.

445. Singh, S. K.; Eng, J.; Atanasov, M.; **Neese, F.**, Covalency and chemical bonding in transition metal complexes: An ab initio based ligand field perspective. *Coord. Chem. Rev.* **2017**, *344*, 2-25.

444. Sparta, M.; Retegan, M.; Pinski, P.; Riplinger, C.; Becker, U.; **Neese, F.**, Multilevel Approaches within the Local Pair Natural Orbital Framework. *J. Chem. Theo. Comp.* **2017**, *13* (7), 3198-3207.

443. Veis, L.; Antalik, A.; Brabec, J.; **Neese, F.**; Legeza, O.; Pittner, J., Coupled Cluster Method with Single and Double Excitations Tailored by Matrix Product State Wave Functions (vol 7, pg 4072, 2016). *J. Phys. Chem. Lett.* **2017,** *8* (1), 291-291.

442. Suturina, E. A.; Nehrkorn, J.; Zadrozny, J. M.; Liu, J.; Atanasov, M.; Weyhermuller, T.; Maganas, D.; Hill, S.; Schnegg, A.; Bill, E.; Long, J. R.; **Neese, F.**, Magneto-Structural Correlations in Pseudotetrahedral Forms of the Co(SPh)(4) (2-) Complex Probed by Magnetometry, MCD Spectroscopy, Advanced EPR Techniques, and ab Initio Electronic Structure Calculations. *Inorg. Chem.* **2017,** *56* (5), 3102-3118.

441. Stoychev, G. L.; Auer, A. A.; **Neese, F.**, Automatic Generation of Auxiliary Basis Sets. *J. Chem. Theo. Comp.* **2017,** *13* (2), 554-562.

440. **Neese, F.**, Quantum Chemistry and EPR Parameters. *eMagRes* **2017,** *6* (1), 1-22.

439. Minenkov, Y.; Bistoni, G.; Riplinger, C.; Auer, A. A.; **Neese, F.**; Cavallo, L., Pair natural orbital and canonical coupled cluster reaction enthalpies involving light to heavy alkali and alkaline earth metals: the importance of sub-valence correlation. *Phys. Chem. Chem. Phys.* **2017,** *19* (14), 9374-9391.

438. Dutta, A. K.; Nooijen, M.; **Neese, F.**; Izsak, R., Automatic active space selection for the similarity transformed equations of motion coupled cluster method. *J. Chem. Phys.* **2017,** *146* (7).

437. Caldararu, O.; Olsson, M. A.; Riplinger, C.; **Neese, F.**; Ryde, U., Binding free energies in the SAMPL5 octa-acid host-guest challenge calculated with DFT-D3 and CCSD(T). *J. Comput. Aided Mol. Des.* **2017,** *31* (1), 87-106.

436. Björnsson, R.; **Neese, F.**; DeBeer, S., Revisiting the Mossbauer Isomer Shifts of the FeMoco Cluster of Nitrogenase and the Cofactor Charge. *Inorg. Chem.* **2017,** *56* (3), 1470-1477.

435. Bistoni, G.; Auer, A. A.; **Neese, F.**, Understanding the Role of Dispersion in Frustrated Lewis Pairs and Classical Lewis Adducts: A Domain-Based Local Pair Natural Orbital Coupled Cluster Study. *Chem. Eur. J.* **2017,** *23* (4), 865-873.

434. Bergner, M.; Roy, L.; Dechert, S.; **Neese, F.**; Ye, S. F.; Meyer, F., Ligand Rearrangements at Fe/S Cofactors: Slow Isomerization of a Biomimetic 2Fe-2S Cluster. *Angew. Chem. Int. Ed.* **2017,** *56* (17), 4882-4886.

433. Ye, S. F.; Kupper, C.; Meyer, S.; Andris, E.; Navratil, R.; Krahe, O.; Mondal, B.; Atanasov, M.; Bill, E.; Roithova, 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.

432. Wang, C. C.; Chang, H. C.; Lai, Y. C.; Fang, H. Y.; Li, C. C.; Hsu, H. K.; Li, Z. Y.; Lin, T. S.; Kuo, T. S.; **Neese, F.**; Ye, S. F.; 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.

431. Veis, L.; Antalik, A.; Brabec, J.; **Neese, F.**; Legeza, O.; Pittner, J., Coupled Cluster Method with Single and Double Excitations Tailored by Matrix Product State Wave Functions. *J. Phys. Chem. Lett.* **2016**, 7 (20), 4072-4078.

430. Sivalingam, K.; Krupicka, M.; Auer, A. A.; **Neese, F.**, Comparison of fully internally and strongly contracted multireference configuration interaction procedures. *J. Chem. Phys.* **2016,** *145* (5).

429. Schneider, W. B.; Bistoni, G.; Sparta, M.; Saitow, M.; Riplinger, C.; Auer, A. A.; **Neese, F.**, Decomposition of Intermolecular Interaction Energies within the Local Pair Natural Orbital Coupled Cluster Framework. *J. Chem. Theory Comput.* **2016,** *12* (10), 4778-4792.

428. Ratzke, W.; Schmitt, L.; Matsuoka, H.; Bannwarth, C.; Retegan, M.; Bange, S.; Klemm, P.; **Neese, F.**; Grimme, S.; Schiemann, O.; Lupton, J. M.; Hoger, S., Effect of Conjugation Pathway in Metal-Free Room-Temperature Dual Singlet Triplet Emitters for Organic Light-Emitting Diodes. *J. Phys. Chem. Lett.* **2016,** *7* (22), 4802-4808.

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

426. Kubas, A.; Berger, D.; Oberhofer, H.; Maganas, D.; Reuter, K.; **Neese, F.**, Surface Adsorption Energetics Studied with "Gold Standard" Wave Function-Based Ab Initio Methods: Small-Molecule Binding to TiO2(110). *J. Phys. Chem. Lett.* **2016,** *7* (20), 4207-4212.

425. Datta, D.; Kossmann, S.; **Neese, F.**, Analytic energy derivatives for the calculation of the first-order molecular properties using the domain-based local pair-natural orbital coupled-cluster theory. *J. Chem. Phys.* **2016,** *145* (11).

424. Das, R.; **Neese, F.**; van Gastel, M., Hydrogen evolution in NiFe hydrogenases and related biomimetic systems: similarities and differences. *Phys. Chem. Chem. Phys.* **2016,** *18* (35), 24681-24692.

423. Chu, W. Y.; Gilbert-Wilson, R.; Rauchfuss, T. B.; van Gastel, M.; **Neese, F.**, Cobalt Phosphino-alpha-Iminopyridine-Catalyzed Hydrofunctionalization of Alkenes: Catalyst Development and Mechanistic Analysis. *Organometallics* **2016,** *35* (17), 2900-2914.

422. Tamanaha, E.; Zhang, B.; Guo, Y. S.; Chang, W. C.; Barr, E. W.; Xing, G.; St Clair, J.; Ye, S. F.; **Neese, F.**; Bollinger, J. M.; 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.

421. Rokhsana, D.; Large, T. A. G.; Dienst, M. C.; Retegan, M.; **Neese, F.**, A realistic in silico

model for structure/function studies of molybdenum-copper CO dehydrogenase. *J. Biol. Inorg. Chem.* **2016**, *21* (4), 491-499.

420. Maganas, D.; Trunschke, A.; Schlogl, R.; **Neese, F.**, A unified view on heterogeneous and homogeneous catalysts through a combination of spectroscopy and quantum chemistry. *Faraday Discuss.* **2016**, *188*, 181-197.

419. Dutta, A. K.; **Neese, F.**; Izsak, R., Towards a pair natural orbital coupled cluster method for excited states. *J. Chem. Phys.* **2016**, *145* (3).

418. Perez-Navarro, M.; **Neese, F.**; Lubitz, W.; Pantazis, D. A.; Cox, N., Recent developments in biological water oxidation. *Curr. Opin. Chem. Biol.* **2016,** *31*, 113-9.

417. Pavosevic, F.; Pinski, P.; Riplinger, C.; **Neese, F.**; Valeev, E. F., SparseMaps-A systematic infrastructure for reduced-scaling electronic structure methods. IV. Linear-scaling second-order explicitly correlated energy with pair natural orbitals. *J. Chem. Phys.* **2016,** *144* (14).

416. Mondal, B.; **Neese, F.**; Ye, S., Toward Rational Design of 3d Transition Metal Catalysts for CO2 Hydrogenation Based on Insights into Hydricity-Controlled Rate-Determining Steps. *Inorg. Chem.* **2016,** *55* (11), 5438-44.

415. Krewald, V.; **Neese, F.**; Pantazis, D. A., Redox potential tuning by redox-inactive cations in nature's water oxidizing catalyst and synthetic analogues. *Phys. Chem. Chem. Phys.* **2016,** *18* (16), 10739-10750.

414. Isegawa, M.; **Neese, F.**; Pantazis, D. A., Ionization Energies and Aqueous Redox Potentials of Organic Molecules: Comparison of DFT, Correlated ab Initio Theory and Pair Natural Orbital Approaches. *J. Chem. Theory Comput.* **2016,** *12* (5), 2272-2284.

413. Hugenbruch, S.; Shafaat, H. S.; Kraemer, T.; Delgado-Jaime, M. U.; Weber, K.; **Neese, F.**; Lubitz, W.; DeBeer, S., In search of metal hydrides: an X-ray absorption and emission study of NiFe hydrogenase model complexes. *Phys. Chem. Chem. Phys.* **2016,** *18* (16), 10688-10699.

412. 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.

411. Aravena, D.; Atanasov, M.; **Neese, F.**, Periodic Trends in Lanthanide Compounds through the Eyes of Multireference ab Initio Theory. *Inorg. Chem.* **2016,** *55* (9), 4457-69.

410. Ye, S.; Bill, E.; **Neese, F.**, Electronic Structures of the Fe(N-2)(SiP3iPr) (+1/0/-1) Electron Transfer Series: A Counterintuitive Correlation between Isomer Shifts and Oxidation States. *Inorg. Chem.* **2016,** *55* (7), 3468-3474.

409. Guo, Y.; Sivalingam, K.; Valeev, E. F.; **Neese, F.**, SparseMaps-A systematic infrastructure for reduced-scaling electronic structure methods. III. Linear-scaling multireference domain-based pair natural orbital N-electron valence perturbation theory. *J. Chem. Phys.* **2016,** *144* (9).

408. Aravena, D.; **Neese, F.**; Pantazis, D. A., Improved Segmented All-Electron Relativistically Contracted Basis Sets for the Lanthanides. *J. Chem. Theory Comput.* **2016,** *12* (3), 1148-

1156.

407. Rechkemmer, Y.; Breitgoff, F. D.; van der Meer, M.; Atanasov, M.; Hakl, M.; Orlita, M.; Neugebauer, P.; **Neese, F.**; Sarkar, B.; van Slageren, J., A four-coordinate cobalt(II) single-ion magnet with coercivity and a very high energy barrier. *Nature Communications* **2016,** *7*.

406. Werncke, C. G.; Suturina, E.; Bunting, P. C.; Vendier, L.; Long, J. R.; Atanasov, M.; **Neese, F.**; Sabo-Etienne, S.; Bontemps, S., Homoleptic Two-Coordinate Silylamido Complexes of Chromium(I), Manganese(I), and Cobalt(I). *Chem. Eur. J.* **2016,** *22* (5), 1668-1674.

405. Riplinger, C.; Pinski, P.; Becker, U.; Valeev, E. F.; **Neese, F.**, Sparse maps-A systematic infrastructure for reduced-scaling electronic structure methods. II. Linear scaling domain based pair natural orbital coupled cluster theory. *J. Chem. Phys.* **2016,** *144* (2).

404. Retegan, M.; Krewald, V.; Mamedov, F.; **Neese, F.**; Lubitz, W.; Cox, N.; Pantazis, D. A., A five-coordinate Mn(IV) intermediate in biological water oxidation: spectroscopic signature and a pivot mechanism for water binding. *Chem. Sci.* **2016,** *7* (1), 72-84.

403. Krewald, V.; Retegan, M.; **Neese, F.**; Lubitz, W.; Pantazis, D. A.; Cox, N., Spin State as a Marker for the Structural Evolution of Nature's Water-Splitting Catalyst. *Inorg. Chem.* **2016,** *55* (2), 488-501.

402. Dutta, A. K.; **Neese, F.**; Izsak, R., Speeding up equation of motion coupled cluster theory with the chain of spheres approximation. J. Chem. Phys. **2016**, *144* (3).

401. Krewald, V.; **Neese, F.**; Pantazis, D. A., Resolving the Manganese Oxidation States in the Oxygen-evolving Catalyst of Natural Photosynthesis. *Isr. J. Chem.* **2015,** *55* (11-12), 1219-1232.

400. England, J.; Bill, E.; Weyhermüller, T; **Neese, F**.; Atanasov, M.; Wieghardt, K., Molecular and Electronic Structures of Homoleptic Six-Coordinate Cobalt(I) Complexes of 2,2′:6′,2″-Terpyridine, 2,2′-Bipyridine, and 1,10-Phenanthroline. An Experimental and Computational Study, *Inorg. Chem.* **2015**

399. Meyer, S.; Krahe, O.; Kupper, C.; Klawitter, I.; Demeshko, S.; Bill, E.; **Neese, F.**; Meyer, F., A trans-1,2 End-On Disulfide-Bridged Iron-Tetracarbene Dimer and Its Electronic Structure. *Inorg. Chem.* **2015**, *54* (20), 9770-9776.

398. Bykov, D.; **Neese, F.**, Six-Electron Reduction of Nitrite to Ammonia by Cytochrome c Nitrite Reductase: Insights from Density Functional Theory Studies. *Inorg. Chem.* **2015,** *54* (19), 9303-9316.

397. Suturina, E. A.; Maganas, D.; Bill, E.; Atanasov, M.; **Neese, F.**, Magneto-Structural Correlations in a Series of Pseudotetrahedral Co-II(XR)(4) (2-) Single Molecule Magnets: An ab Initio Ligand Field Study. *Inorg. Chem.* **2015**, *54* (20), 9948-9961.

396. Stavretis, S. E.; Atanasov, M.; Podlesnyak, A. A.; Hunter, S. C.; **Neese, F.**; Xue, Z.-L., Magnetic Transitions in Iron Porphyrin Halides by Inelastic Neutron Scattering and Ab Initio Studies of Zero-Field Splittings. *Inorg. Chem.* **2015,** *54* (20), 9790-9801.

395. Beckwith, M. A.; Ames, W.; Vila, F. D.; Krewald, V.; Pantazis, D. A.; Mantel, C.; Pecaut,

J.; Gennari, M.; Duboc, C.; Collomb, M.-N.; Yano, J.; Rehr, J. J.; **Neese, F.**; DeBeer, S., How Accurately Can Extended X-ray Absorption Spectra Be Predicted from First Principles? Implications for Modeling the Oxygen-Evolving Complex in Photosystem II. *J. Am. Chem. Soc.* **2015,** *137* (40), 12815-12834.

394. Thimm, W.; Gradert, C.; Broda, H.; Wennmohs, F.; **Neese, F.**; Tuczek, F., Free Reaction Enthalpy Profile of the Schrock Cycle Derived from Density Functional Theory Calculations on the Full (MoN3N)-N-HIPT Catalyst. *Inorg. Chem.* **2015,** *54* (19), 9248-9255.

393. Jiang, S.-D.; Maganas, D.; Levesanos, N.; Ferentinos, E.; Haas, S.; Thirunavukkuarasu, K.; Krzystek, J.; Dressel, M.; Bogani, L.; **Neese, F.**; Kyritsis, P., Direct Observation of Very Large Zero-Field Splitting in a Tetrahedral (NiSe4)-Se-II Coordination Complex. *J. Am. Chem. Soc.* **2015,** *137* (40), 12923-12928.

392. Rapatskiy, L.; Ames, W. M.; Perez-Navarro, M.; Savitsky, A.; Griese, J. J.; Weyhermueller, T.; Shafaat, H. S.; Hogbom, M.; **Neese, F.**; Pantazis, D. A.; Cox, N., Characterization of Oxygen Bridged Manganese Model Complexes Using Multifrequency O-17-Hyperfine EPR Spectroscopies and Density Functional Theory. *J. Phys. Chem. B* **2015**, *119* (43), 13904-13921.

391. 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. *Chemical Science* **2015,** *6* (5), 2909-2921.

390. Sundararajan, M.; **Neese, F.**, Distal Histidine Modulates the Unusual O-Binding of Nitrite to Myoglobin: Evidence from the Quantum Chemical Analysis of EPR Parameters. *Inorganic chemistry* **2015,** *54* (15), 7209-17.

389. Schweinfurth, D.; Sommer, M. G.; Atanasov, M.; Demeshko, S.; Hohloch, S.; Meyer, F.; **Neese, F.**; Sarkar, B., The Ligand Field of the Azido Ligand: Insights into Bonding Parameters and Magnetic Anisotropy in a Co(II)-Azido Complex. *Journal of the American Chemical Society* **2015,** *137* (5), 1993-2005.

388. Pinski, P.; Riplinger, C.; Valeev, E. F.; **Neese, F.**, Sparse maps-A systematic infrastructure for reduced-scaling electronic structure methods. I. An efficient and simple linear scaling local MP2 method that uses an intermediate basis of pair natural orbitals. *The Journal of chemical physics* **2015,** *143* (3), 034108-034108.

387. Ogata, H.; Kraemer, T.; Wang, H.; Schilter, D.; Pelmenschikov, V.; van Gastel, M.; **Neese, F.**; Rauchfuss, T. B.; Gee, L. B.; Scott, A. D.; Yoda, Y.; Tanaka, Y.; Lubitz, W.; Cramer, S. P., Hydride bridge in NiFe -hydrogenase observed by nuclear resonance vibrational spectroscopy. *Nat. Com.* **2015,** *6*.

386. Nick, T. U.; Lee, W.; Kossmann, S.; **Neese, F.**; Stubbe, J.; Bennati, M., Hydrogen Bond Network between Amino Acid Radical Intermediates on the Proton-Coupled Electron Transfer Pathway of E. coli alpha2 Ribonucleotide Reductase. *Journal of the American Chemical Society* **2015,** *137* (1), 289-98.

385. Mondal, B.; Song, J.; **Neese, F.**; Ye, S., Bio-inspired mechanistic insights into CO2

reduction. *Current Opinion in Chemical Biology* **2015,** *25*, 103-109.

384. Mondal, B.; **Neese, F.**; Ye, S., Control in the Rate-Determining Step Provides a Promising Strategy To Develop New Catalysts for CO2 Hydrogenation: A Local Pair Natural Orbital Coupled Cluster Theory Study. *Inorg. Chem.* **2015,** *54* (15), 7192-8.

383. Liakos, D. G.; Sparta, M.; Kesharwani, M. K.; Martin, J. M. L.; **Neese, F.**, Exploring the Accuracy Limits of Local Pair Natural Orbital Coupled-Cluster Theory. *Journal of Chemical Theory and Computation* **2015,** *11* (4), 1525-1539.

382. Liakos, D. G.; **Neese, F.**, Is It Possible To Obtain Coupled Cluster Quality Energies at near Density Functional Theory Cost? Domain-Based Local Pair Natural Orbital Coupled Cluster vs Modern Density Functional Theory. *Journal of Chemical Theory and Computation* **2015,** *11* (9), 4054-4063.

381. Liakos, D. G.; **Neese, F.**, Domain Based Pair Natural Orbital Coupled Cluster Studies on Linear and Folded Alkane Chains. *Journal of Chemical Theory and Computation* **2015,** *11* (5), 2137-2143.

380. Krewald, V.; Retegan, M.; Cox, N.; Messinger, J.; Lubitz, W.; DeBeer, S.; **Neese, F.**; Pantazis, D. A., Metal oxidation states in biological water splitting. *Chemical Science* **2015,** *6* (3), 1676-1695.

379. Kochem, A.; Weyhermueller,T.; **Neese, F.**; van Gastel, M., EPR and Quantum Chemical Investigation of a Bioinspired Hydrogenase Model with a Redox-Active Ligand in the First Coordination Sphere. *Organometallics* **2015,** *34* (5), 995-1000.

378. Kochem, A.; Bill, E.; **Neese, F.**; van Gastel, M., Mossbauer and computational investigation of a functional NiFe hydrogenase model complex. *Chem. Com.(Cambridge, England)* **2015,** *51* (11), 2099-102.

377. Kirchner, B.; **Neese, F.**, Theoretical chemistry developments: from electronic structure to simulations. *Phys. Chem. Chem. Phys.* **2015,** *17* (22), 14268-14269.

376. Gerey, B.; Gennari, M.; Goure, E.; Pecaut, J.; Blackman, A.; Pantazis, D. A.; **Neese, F.**; Molton, F.; Fortage, J.; Duboc, C.; Collomb, M.-N., Calcium and heterometallic manganese-calcium complexes supported by tripodal pyridine-carboxylate ligands: structural, EPR and theoretical investigations. *Dalton Transactions* **2015,** *44* (28), 12757-12770.

375. Gennari, M.; Brazzolotto, D.; Pecaut, J.; Cherrier, M. V.; Pollock, C. J.; DeBeer, S.; Retegan, M.; Pantazis, D. A.; **Neese, F.**; Rouzieres, M.; Clerac, R.; Duboc, C., 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* **2015,** *137* (26), 8644-8653.

374. Demel, O.; Pittner, J.; **Neese, F.**, A Local Pair Natural Orbital-Based Multireference Mukherjee's Coupled Cluster Method. *Journal of Chemical Theory and Computation* **2015,** *11* (7), 3104-3114.

373. Cox, N.; Pantazis, D. A.; **Neese, F.**; Lubitz, W., Artificial photosynthesis: understanding

water splitting in nature. *Interface Focus* **2015,** *5* (3).

372. Bykov, D.; Petrenko, T.; Izsak, R.; Kossmann, S.; Becker, U.; Valeev, E.; **Neese, F.**, Efficient implementation of the analytic second derivatives of Hartree-Fock and hybrid DFT energies: a detailed analysis of different approximations. *Molecular Physics* **2015,** *113* (13-14), 1961-1977.

371. Bjornsson, R.; **Neese, F.**; Schrock, R. R.; Einsle, O.; DeBeer, S., The discovery of Mo(III) in FeMoco: reuniting enzyme and model chemistry. *Journal of Biological Inorganic Chemistry* **2015,** *20* (2), 447-460.

370. Bjornsson, R.; Delgado-Jaime, M. U.; Lima, F. A.; Sippel, D.; Schlesier, J.; Weyhermueller, T.; Einsle, O.; **Neese, F.**; DeBeer, S., Molybdenum L-Edge XAS Spectra of MoFe Nitrogenase. *Zeitschrift Fur Anorganische Und Allgemeine Chemie* **2015,** *641* (1), 65-71.

369. Barilone, J.; **Neese, F.**; van Gastel, M., Finding the Reactive Electron in Paramagnetic Systems: A Critical Evaluation of Accuracies for EPR Spectroscopy and Density Functional Theory Using 1,3,5-Triphenyl Verdazyl Radical as a Testcase. *Applied Magnetic Resonance* **2015,** *46* (2), 117-139.

368. Atanasov, M.; Aravena, D.; Suturina, E.; Bill, E.; Maganas, D.; **Neese, F.**, First principles approach to the electronic structure, magnetic anisotropy and spin relaxation in mononuclear 3d-transition metal single molecule magnets. *Coordination Chemistry Reviews* **2015,** *289*, 177-214.

367. Al-Afyouni, M. H.; Suturina, E.; Pathak, S.; Atanasov, M.; Bill, E.; DeRosha, D. E.; Brennessel, W. W.; **Neese, F.**; Holland, P. L., Spin Isomers and Ligand Isomerization in a Three-Coordinate Cobalt(I) Carbonyl Complex. *Journal of the American Chemical Society* **2015,** *137* (33), 10689-10699.

366. Zapata-Rivera, J.; Caballol, R.; Calzado, C. J.; Liakos, D. G.; **Neese, F.**, On the Reaction Mechanism of the Complete Intermolecular O-2 Transfer between Mononuclear Nickel and Manganese Complexes with Macrocyclic Ligands. *Chemistry-a European Journal* **2014,** *20* (41), 13296-13304.

365. Sparta, M.; Riplinger, C.; **Neese, F.**, The Mechanism of Olefin Asymmetric Hydrogenation Catalyzed by Iridium Phosphino-Oxazoline: A Pair Natural Orbital Coupled Cluster Study. *J. Chem. Theory Comput.* **2014,** *10* (3), 1099-1108.

364. Sparta, M.; **Neese, F.**, Chemical applications carried out by local pair natural orbital based coupled-cluster methods. *Chem. Soc. Rev.* **2014,** *43* (14), 5032-41.

363. Shafaat, H. S.; Pantazis, D. A.; **Neese, F.;** Lubitz, W.; Cox, N.; Griese, J. J.; Graslund, A.; Hogbom, M.; Roos, K.; Siegbahn, P. E.; Probing the electronic structure of the heterobimetallic Mn/Fe cofactor of the R2lox proteins using advanced EPR techniques. *J. Biol. Inorg. Chem.* **2014** 19, S311-S311.

362. Song, J.; Klein, E. L.; **Neese, F.**; Ye, S., The Mechanism of Homogeneous CO2 Reduction by Ni(cyclam): Product Selectivity, Concerted Proton-Electron Transfer and C-O Bond Cleavage. *Inorganic Chemistry* **2014,** *53* (14), 7500-7507.

361. Sharma, S.; Sivalingam, K.; **Neese, F.**; Chan, G. K.-L., Low-energy spectrum of iron-sulfur clusters directly from many-particle quantum mechanics. *Nature Chemistry* **2014,** *6* (10), 927-933.

360. Shafaat, H. S.; Griese, J. J.; Pantazis, D. A.; Roos, K.; Andersson, C. S.; Popovic-Bijelic, A.; Graslund, A.; Siegbahn, P. E. M.; **Neese, F.**; Lubitz, W.; Hogbom, M.; Cox, N., Electronic Structural Flexibility of Heterobimetallic Mn/Fe Cofactors: R2lox and R2c Proteins. *Journal of the American Chemical Society* **2014,** *136* (38), 13399-13409.

359. Schapiro, I.; **Neese, F.**, SORCI for photochemical and thermal reaction paths: A benchmark study. *Computational and Theoretical Chemistry* **2014,** *1040*, 84-98.

358. Saracini, C.; Liakos, D. G.; Zapata Riviera, J. E.; **Neese, F.**; Meyer, G. J.; Karlin, K. D., Excitation Wavelength Dependent O_2 Release from Copper(II)–Superoxide Compounds: Laser Flash-Photolysis Experiments and Theoretical Studies. *J. Am. Chem. Soc.* **2014,** *136* (4), 1260-1263.

357. Riplinger, C.; Bill, E.; Daiber, A.; Ullrich, V.; Shoun, H.; **Neese, F.**, New Insights into the Nature of Observable Reaction Intermediates in Cytochrome P450 NO Reductase by Using a Combination of Spectroscopy and Quantum Mechanics/Molecular Mechanics Calculations. *Chem. Eur. J.* **2014,** *20* (6), 1602-1614.

356. Retegan, M.; Cox, N.; Pantazis, D. A.; **Neese, F.**, A First-Principles Approach to the Calculation of the on-Site Zero-Field Splitting in Polynuclear Transition Metal Complexes. *Inorganic Chemistry* **2014,** *53* (21), 11785-11793.

355. Retegan, M.; Cox, N.; Lubitz, W.; **Neese, F.**; Pantazis, D. A., The first tyrosyl radical intermediate formed in the S-2-S-3 transition of photosystem II. *Phys. Chem. Chem. Phys.* **2014,** *16* (24), 11901-11910.

354. Pollock, C. J.; Delgado-Jaime, M. U.; Atanasov, M.; **Neese, F.**; DeBeer, S., Kbeta Mainline X-ray Emission Spectroscopy as an Experimental Probe of Metal-Ligand Covalency. *J. Am. Chem. Soc.* **2014,** *136* (26), 9453-63.

353. Pavosevic, F.; **Neese, F.**; Valeev, E. F., Geminal-spanning orbitals make explicitly correlated reduced-scaling coupled-cluster methods robust, yet simple. .J. *Chem. Phys.* **2014,** *141* (5).

352. Pantazis, D. A.; Retegan, M.; Krewald, V.; **Neese, F.**; Cox, N., The diverse functions of calcium in natural water oxidation. *J. Bio. Inorg. Chem.* **2014,** *19*, S762-S763.

351. Pantazis, D. A.; **Neese, F.**, All-electron basis sets for heavy elements. *WIREs Comput. Mol. Sci.* **2014,** *4* (4), 363-374.

350. Pantazis, D. A.; Cox, N.; Lubitz, W.; **Neese, F.**, Oxygen-evolving Photosystem II. In *Encyclopedia of Inorganic and Bioinorganic Chemistry*, John Wiley & Sons, Ltd.: 2014; pp 1-13.

349. Nooijen, M.; Demel, O.; Datta, D.; Kong, L.; Shamasundar, K. R.; Huntington, L. M.; **Neese, F.**, Communication: Multireference equation of motion coupled cluster: A transform and diagonalize approach to electronic structure. *J. Chem. Phys.* **2014,** *140*

(081102).

348. **Neese, F.**, Theoretical Spectroscopy of Open Shell Transition Metals in Enzymes and Model Complexes. *J. Biol. Inorg. Chem.* **2014,** *19*, S108-S108.

347. Maganas, D.; Roemelt, M.; Weyhermüller, T.; Blume, R.; Hävecker, M.; Knop-Gericke, A.; DeBeer, S.; Schlögl, R.; **Neese, F.**, L-edge X-ray absorption study of mononuclear vanadium complexes and spectral predictions using a restricted open shell configuration interaction ansatz. *Phys. Chem. Chem. Phys.* **2014,** *16*, 264-276.

346. Maganas, D.; Kristiansen, P.; Duda, L.-C.; Knop-Gericke, A.; DeBeer, S.; Schloegl, R.; **Neese, F.**, Combined Experimental and Ab Initio Multireference Configuration Interaction Study of the Resonant Inelastic X-ray Scattering Spectrum of CO2. *J. Phys. Chem. C* **2014,** *118* (35), 20163-20175.

345. Maganas, D.; DeBeer, S.; **Neese, F.**, Restricted Open-Shell Configuration Interaction Cluster Calculations of the L-Edge X-ray Absorption Study of TiO_2 and CaF_2 Solids. *Inorg. Chem.* **2014,** *53* (13), 6374-85.

344. Lubitz, W.; Cox, N.; Rapatskiy, L.; Lohmiller, T.; Navarro, M. P.; Ames, W.; Pantazis, D.; **Neese, F.**; Boussac, N.; Messinger, J., Light-induced water oxidation in photosynthesis. *J. Biol. Inorg. Chem.* **2014,** *19*, S350-S350.

343. Lohmiller, T.; Krewald, V.; Navarro, M. P.; Retegan, M.; Rapatskiy, L.; Nowaczyk, M. M.; Boussac, A.; **Neese, F.**; Lubitz, W.; Pantazis, D. A.; Cox, N., 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* (24), 11877-11892.

342. Liu, W.; Christian, J. H.; Al-Oweini, R.; Bassil, B. S.; van Tol, J.; Atanasov, M.; **Neese, F.**; Dalal, N. S.; Kortz, U., Synthesis, Detailed Characterization, and Theoretical Understanding of Mononuclear Chromium(III)-Containing Polyoxotungstates Cr-III((HXW7O28)-W-V)(2) (13-) (X = P, As) with Exceptionally Large Magnetic Anisotropy. *Inorganic Chemistry* **2014,** *53* (17), 9274-9283.

341. Krewald, V.; Retegan, M.; **Neese, F.**; Pantazis, D. A., Spectroscopically consistent Mn oxidation state assignments of the natural water splitting catalyst. *Journal of Biological Inorganic Chemistry* **2014,** *19*, S771-S771.

340. Krewald, V.; **Neese, F.**; Pantazis, D. A., Structural Subunits of Natural and Artificial Water Oxidation Catalysts Investigated in Terms of Their Spectroscopic and Magnetic Properties. *J. Biol. Inorg. Chem.* **2014,** *19*, S499-S499.

339. Krahe, O.; Bill, E.; **Neese, F.**, Decay of Iron(V) Nitride Complexes By a N-N Bond-Coupling Reaction in Solution: A Combined Spectroscopic and Theoretical Analysis. *Angewandte Chemie-International Edition* **2014,** *53* (33), 8727-8731.

338. Kollmar, C.; **Neese, F.**, The static response function in Kohn-Sham theory: An appropriate basis for its matrix representation in case of finite AO basis sets. *Journal of Chemical Physics* **2014,** *141* (13).

337. Klein, E. L.; Hoefer, P.; Frenzen, L.; Song, J.; Ye, S.; van Gastel, M.; **Neese, F.**, Structural

studies of the reduced state of Ni-cyclam in CO_2 activation. *J. Biol. Inorg. Chem.* **2014,** *19*, S529-S529.

336. Kochem, A.; **Neese, F.;** van Gastel, M., Spectroscopic and Quantum Chemical Study of the Ni($P^{Ph}_2N^{C6H4CH2P(O)(OEt)2}_2$)$_2$ Electrocatalyst for Hydrogen Production with Emphasis on the NiI Oxidation State, *J. Phys. Chem. C* **2014** 118, (5), 2350-2360.

335. Klein, E. L.; Belaidi, A. A.; Raitsimring, A. M.; Davis, A. C.; Krämer, T.; Astashkin, A. V.; **Neese, F.**; Schwarz, G.; Enemark, J. H., Pulsed Electron Paramagnetic Resonance Spectroscopy of ^{33}S-Labeled Molybdenum Cofactor in Catalytically Active Bioengineered Sulfite Oxidase. *Inorg. Chem.* **2014,** *53* (2), 961-971.

334. King, A. E.; Nippe, M.; Atanasov, M.; Chantarojsiri, T.; Wray, C. A.; Bill, E.; **Neese, F.**; Long, J. R.; Chang, C. J., A Well-Defined Terminal Vanadium(III) Oxo Complex. *Inorganic Chemistry* **2014,** *53* (21), 11388-11395.

333. Gerey, B.; Gennari, M.; Fortage, J.; Duboc, C.; Collomb, M.; Pecaut, J.; Martin-Diaconescu, V.; **Neese, F.**; DeBeer, S., New homo- and heteronuclear complexes of Manganese/Calcium, as models of the Oxygen-Evolving Center of Photosystem II. *J. Biol. Inorg. Chem.* **2014,** *19*, S504-S504.

332. Gennari, M.; Brazzolotto, D.; Orio, M.; **Neese, F.**; Van Gastel, M.; DeBeer, S.; Pecaut, J.; Duboc, C., Bio-inspired thiolate metal complexes structural, spectroscopic and redox properties, reactivity. *Journal of Biological Inorganic Chemistry* **2014,** *19*, S731-S732.

331. 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 Transactions* **2014,** *43* (16), 6079-6086.

330. Gansaeuer, A.; Karbaum, P.; Schmauch, D.; Einig, M.; Shi, L.; Anoop, A.; **Neese, F.**, Synthetic and Computational Evaluation of Regiodivergent Epoxide Opening for Diol and Polyol Synthesis. *Chemistry-an Asian Journal* **2014,** *9* (8), 2289-2294.

329. Enemark, J. H.; Klein, E. L.; Raitsimring, A. M.; Davis, A. C.; Astashkin, A. V.; Klein, E. L.; Kraemer, T.; **Neese, F.**; Belaidi, A. A.; Schwarz, G., Pulsed EPR Spectroscopy of S-33-Labeled Molybdopterin in Sulfite Oxidase. *J. Biol. Inorg. Chem.* **2014,** *19*, S67-S67.

328. Delgado-Jaime, M. U.; Shaafat, H.; Kramer, T.; Weber, K.; **Neese, F.**; Lubitz, W.; DeBeer, S.; DeBeer, S., Ni Valence-to-Core X-Ray Emission Spectroscopy: An experimental probe of NiFe hydrogenase intermediates. *J. Biol. Inorg. Chem.* **2014,** *19*, S346-S346.

327. DeBeer, S.; Bjornsson, R.; Lima, F. A.; Weyhermueller, T.; **Neese, F.**; Einsle, O., New Insights into the Electronic Structure of the FeMo Cofactor of Nitrogenase. *J. Biol. Inorg. Chem.* **2014,** *19*, S90-S90.

326. Cox, N.; Retegan, M.; **Neese, F.**; Pantazis, D. A.; Boussac, A.; Lubitz, W., Electronic structure of the oxygenevolving complex in photosystem II prior to O-O bond formation. *Science* **2014,** *345* (6198), 804-808.

325. Christian, G. J.; Ye, S.; Neese, F., Probing the Selectivity in Extradiol Dioxygenases. *J. Biol. Inorg. Chem.* **2014,** *19*, S283-S283.

324. Bykov, D.; Plog, M.; **Neese, F.**, Heme-bound nitroxyl, hydroxylamine, and ammonia ligands as intermediates in the reaction cycle of cytochrome c nitrite reductase: a theoretical study. *J. Biol. Inorg. Chem.* **2014,** *19* (1), 97-112.

323. Bjornsson, R.; Lima, F. A.; Weyhermüller, T.; DeBeer, S.; Neese, F.; Einsle, O., Is the molybdenum in FeMoco as innocent as we thought? *J. Biol. Inorg. Chem.* **2014,** *19*, S321-S321.

322. Bjornsson, R.; Lima, F. A.; Spatzal, T.; Weyhermueller, T.; Glatzel, P.; Bill, E.; Einsle, O.; **Neese, F.**; DeBeer, S., Identification of a spin-coupled Mo(III) in the nitrogenase iron-molybdenum cofactor. *Chemical Science* **2014,** *5* (8), 3096-3103.

321. Altun, A.; Breidung, J.; **Neese, F.**; Thiel, W., Correlated Ab Initio and Density Functional Studies on H-2 Activation by FeO+. *Journal of Chemical Theory and Computation* **2014,** *10* (9), 3807-3820.

320. Ali, M. E.; Nair, N. N.; Retegan, M.; **Neese, F.**; Staemmler, V.; Marx, D., The iron-sulfur core in Rieske proteins is not symmetric. *Journal of Biological Inorganic Chemistry* **2014,** *19* (8), 1287-1293.

319. Zadrozny, J. M.; Xiao, D. J.; Long, J. R.; Atanasov, M.; **Neese, F.**; Grandjean, F.; Long, G. J., Mössbauer Spectroscopy as a Probe of Magnetization Dynamics in the Linear Iron(I) and Iron(II) Complexes [Fe(C(SiMe3)3)2]1–/0. *Inorg. Chem.* **2013,** *52* (22), 13123-13131.

318. Zadrozny, J. M.; Xiao, D. J.; Atanasov, M.; Long, G. J.; Grandjean, F.; **Neese, F.**; Long, J. R., Magnetic blocking in a linear iron(I) complex. *Nature Chemistry* **2013,** *5*, 577-581.

317. Zadrozny, J. M.; Atanasov, M.; Bryan, A. M.; Lin, C.-Y.; Rekken, B., D.; **Neese, F.**; Long, J. R., Slow magnetization dynamics in a series of two-coordinate iron(II) complexes. *Chem. Sci.* **2013,** *4* (1), 125-138.

316. 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*, 8017-8030.

315. 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.

314. Schweinfurth, D.; Krzystek, J.; Schapiro, I.; Demeshko, S.; Klein, J.; Telser, J.; Ozarowski, A.; Su, C.-Y.; Meyer, F.; Atanasov, M.; Neese, F.; Sarkar, B., Electronic Structures of Octahedral Ni(II) Complexes with “Click” Derived Triazole Ligands: A Combined Structural, Magnetometric, Spectroscopic, and Theoretical Study. *Inorg. Chem.* **2013,** *52* (12), 6880-6892.

313. Schapiro, I.; Sivalingam, K.; **Neese, F.**, Assessment of n-Electron Valence State Perturbation Theory for Vertical Excitation Energies. *J. Chem. Theory Comput.* **2013,** *9* (8), 3567-3580.

312. Sandhöfer, B.; Kossmann, S.; **Neese, F.**, Derivation and assessment of relativistic hyperfine-coupling tensors on the basis of orbital-optimized second-order Møller–Plesset

perturbation theory and the second-order Douglas–Kroll–Hess transformation. *J. Chem. Phys.* **2013,** *138* (10), 104102.

311. Roemelt, M.; **Neese, F.**, Excited States of Large Open-Shell Molecules: An Efficient, General, and Spin-Adapted Approach Based on a Restricted Open-Shell Ground State Wave function. *J. Phys. Chem. A* **2013,** *117* (4), 3069-3083.

310. Roemelt, M.; Maganas, D.; DeBeer, S.; **Neese, F.**, 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* (20), 204101-22.

309. Riplinger, C.; Sandhöfer, B.; Hansen, A.; **Neese, F.**, Natural triple excitations in local coupled cluster calculations with pair natural orbitals. *J. Chem. Phys.* **2013,** *139*, 134101-12.

308. Riplinger, C.; **Neese, F.**, An efficient and near linear scaling pair natural orbital based local coupled cluster method. *J. Chem. Phys.* **2013,** *138* (3), 034106.

307. Retegan, M.; **Neese, F.**; Pantazis, D. A., Convergence of QM/MM and Cluster Models for the Spectroscopic Properties of the Oxygen-Evolving Complex in Photosystem II. *J. Chem. Theory Comput.* **2013,** *9* (8), 3832-3842.

306. Retegan, M.; Collomb, M.-N.; **Neese, F.**; DuBoc, C., A combined high-field EPR and quantum chemical study on a weakly ferromagnetically coupled dinuclear Mn(III) complex. A complete analysis of the EPR spectrum beyond the strong coupling limit. *Phys. Chem. Chem. Phys.* **2013,** *15* (1), 223-234.

305. Pandelia, M.-E.; Bykov, D.; Izsak, R.; Infossi, P.; Giudici-Orticoni, M.-T.; Bill, E.; **Neese, F.**; Lubitz, W., Electronic structure of the unique [4Fe-3S] cluster in O-2-tolerant hydrogenases characterized by Fe-57 Mössbauer and EPR spectroscopy. *Proc. Natl. Acad. Sci. U.S.A.* **2013,** *110* (2), 483-488.

304. **Neese, F.**, Introduction to Ligand Field Theory. In *Practical Approaches to Biological Inorganic Chemistry*, Crichton, R. R.; Louro, R. O., Eds. Elsevier B. V.: Amsterdam 2013; pp 23-51.

303. Montserrat, P. N.; Ames, W. M.; Hâkan, N.; Lohmiller, T.; Pantazis, D. A.; Rapatskiy, L.; Nowaczyk, M. M.; **Neese, F.**; Boussac, A.; Messinger, J.; Lubitz, W.; Cox, N., Ammonia binding to the oxygen-evolving complex of photosystem II identifies the solvent-exchangeable oxygen bridge (μ-oxo) of the manganese tetramer. *Proc. Natl. Acad. Sci. U.S.A.* **2013,** *110* (39), 15561-6.

302. Maganas, D.; Roemelt, M.; Hävecker, M.; Trunschke, A.; Knop-Gericke, A.; Schlögl, R.; **Neese, F.**, 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.

301. Liakos, D. G.; Izsák, R.; Valeev, E. F.; **Neese, F.**, What is the most efficient way to reach

the canonical MP2 basis set limit? *Mol. Phys.* **2013,** *111* (16-17), 2653-2662.

300. Lassalle-Kaiser, B.; Boron, T. T. I.; Krewald, V.; Kern, J.; Beckwith, M. A.; Delgado-Jaime, M. U.; Schröder, H.; Alonso-Mori; Nordlund, D.; Weng, T.-C.; Sokaras, D.; **Neese, F.**; Bergmann, U.; Yachandra, V. K.; DeBeer, S.; Pecoraro, V. L.; Yano, J., Experimental and Computational X-ray Emission Spectroscopy as a Direct Probe of Protonation States in Oxo-Bridged MnIV Dimers Relevant to Redox-Active Metalloproteins. *Inorg. Chem.* **2013,** *52* (22), 12915-12922.

299. Krewald, V.; **Neese, F.**; Pantazis, D. A., 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* (15), 5726-5739.

298. Krewald, V.; Lassalle-Kaiser, B.; Boron, T. T. I.; Pollock, C. J.; Kern, J.; Beckwith, M. A.; Yachandra, V. K.; Pecoraro, V. L.; Yano, J.; **Neese, F.**; DeBeer, S., The Protonation States of Oxo-Bridged MnIV Dimers Resolved by Experimental and Computational Mn K Pre-Edge X-ray Absorption Spectroscopy. *Inorg. Chem.* **2013,** *52* (22), 12904-12914.

297. Krämer, T.; Kampa, M.; Lubitz, W.; van Gastel, M.; **Neese, F.**, Theoretical Spectroscopy of the Ni^{II} Intermediate States in the Catalytic Cycle and the Activation of [NiFe] Hydrogenases. *ChemBioChem* **2013,** *14*, 1898-1905.

296. Krahe, O.; **Neese, F.**; Engeser, M., Iron Azides with Cyclam-Derived Ligands: Are They Precursors for High-Valent Iron Nitrides in the Gas Phase? *ChemPlusChem* **2013,** *78*, 1053-1057.

295. Kochem, A.; Thomas, F.; Jarjayes, O.; Gellon, G.; Philouze, C.; Weyhermüller, T.; **Neese, F.**; van Gastel, M., Structural and Spectroscopic Investigation of an Anilinosalen Cobalt Complex with Relevance to Hydrogen Production. *Inorg. Chem.* **2013,** *52* (24), 14428-14438.

294. Kampa, M.; Pandelia, M.-E.; Lubitz, W.; van Gastel, M.; **Neese, F.**, A Metal–Metal Bond in the Light-Induced State of [NiFe] Hydrogenases with Relevance to Hydrogen Evolution. *J. Am. Chem. Soc.* **2013,** *135* (10), 3915-3925.

293. Izsák, R.; **Neese, F.**; Klopper, W., Robust fitting techniques in the chain of spheres approximation to the Fock exchange: The role of the complementary space. *J. Chem. Phys.* **2013,** *139*, 094111 (10 pages).

292. Izsák, R.; **Neese, F.**, Speeding up spin-component-scaled third-order pertubation theory with the chain of spheres approximation: the COSX-SCS-MP3 method. *Mol. Phys.* **2013,** *111* (9-11), 1190-1195.

291. Ganyushin, D.; **Neese, F.**, A fully variational spin-orbit coupled complete active space self-consistent field approach: Application to electron paramagnetic resonance g-tensors. *J. Chem. Phys.* **2013,** *138* (10), 104113.

290. Gallo, E.; Bonino, F.; Swarbrick, J. C.; Petrenko, T.; Piovano, A.; Bordiga, S.; Gianolio, D.; Groppo, E.; **Neese, F.**; Lamberti, C.; Glatzel, P., Preference towards Five-Coordination in Ti Silicalite-1 upon Molecular Adsorption. *ChemPhysChem* **2013,** *14* (1), 79-83.

289. Danovich, D.; Shaik, S.; **Neese, F.**; Echeverría, J.; Aullon, G.; Alvarez, S., Understanding the Nature of the CH·HC Interactions in Alkanes. *J. Chem. Theo. Comp.* **2013,** *9* (4), 1977-1991.

288. Cox, N.; Pantazis, D. A.; **Neese, F.**; Lubitz, W., Biological Water Oxidation. *Acc. Chem. Res.* **2013,** *46* (7), 1588-1596.

287. Atanasov, M.; Zadrozny, J. M.; Long, J. R.; **Neese, F.**, A theoretical analysis of chemical bonding, vibronic coupling, and magnetic anisotropy in linear iron(II) complexes with single-molecule magnet behavior. *Chem. Sci.* **2013,** *4* (1), 139-156.

286. Pandelia, ME; Bykov, D; Izsak, R; Infossi, P; Giudici-Orticoni, MT; Bill, E; **Neese, F**; Lubitz, W, Reply to Mouesca et al.: Electronic structure of the proximal [4Fe-3S] cluster of O-2-tolerant [NiFe] hydrogenases, *Proceedings of the National Academy of Sciences of the United States of America (PNAS)* **2013***,* 110 (28), E2539-E2539

285. Lima, F.A.; Bjornsson, R.; Weyhermüller, T.; Chandrasekaran, P.; Glatzel, P.; Neese, F.; DeBeer, S., High-resolution molybdenum K-edge X-ray absorption spectroscopy analyzed with time-dependent density functional theory, *Phys Chem Chem Phys* **2013**, 15 (48), 20911-20920

284. Atanasov, M.; Surawatanawong, P.; Wieghardt, K.; **Neese, F.**, A Theoretical Study of Zero-Field Splitting in Fe(IV)S_6 (S=1) and Fe(III)S_6(S=1/2) Core Complexes, $[Fe^{IV}(Et_2dtc)_{3-n}(mnt)_n]^{(n-1)-}$ and $[Fe^{III}(Et_2dtc)_{3-n}(mnt)_n]^{n-}$ (n=0,1,2,3): The Origin of the Magnetic Anisotropy. *Coord. Chem. Rev.* **2013,** *257* (1), 27-41.

283. 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.

282. 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.

281. Westphal, A.; Broda, H.; Kurz, P.; **Neese, F.**; Tuczek, F., Magnetic Circular Dichroism Spectrum of the Molybdenum(V) Complex [Mo(O)Cl_3dppe]: C-Term Signs and Intensities for Multideterminant Excited Doublet States. *Inorg. Chem.* **2012,** *51* (10), 5748-5763.

280. Weber, K.; Krämer, T.; Shafaat, H. S.; Weyermüller, T.; Bill, E.; van Gastel, M.; **Neese, F.**; Lubitz, W., A Functional [NiFe]-Hydrogenase Model Compound That Undergoes Biologically Relevant Reversible Thiolate Protonation. *J. Am. Chem. Soc.* **2012,** *134* (51), 20745-20755.

279. Vennekate, H.; Schwarzer, D.; Torres-Alacan, J.; Krahe, O.; Filippou, A. C.; **Neese, F.**; Vöhringer, P., Ultrafast primary processes of an iron-(III) azido complex in solution induced with 266 nm light. *Phys. Chem. Chem. Phys.* **2012,** *14* (18), 6165-6172.

278. Torres-Alacan, J.; Krahe, O.; Filippou, A. C.; **Neese, F.**; Schwarzer, D.; Voehringer, P., The Photochemistry of $[Fe^{III}N_3$(cyclam-ac)$]PF_6$ at 266 nm. *Chem. Eur. J.* **2012,** *18* (10),

3043-3055.

277. Thiessen, A.; Wettach, H.; Meerholz, K.; **Neese, F.**; Hoeger, S.; Hertel, D., Control of electronic properties of triphenylene by substitution. *Organic Electronics* **2012,** *13* (1), 71-83.

276. Sundararajan, M.; **Neese, F.**, Detailed QM/MM study of the Electron Paramagnetic Resonance Parameters of Nitrosyl Myoglobin. *J. Chem. Theory Comput.* **2012,** *8* (2), 563-574.

275. Shafaat, H. S.; Weber, K.; Petrenko, T.; **Neese, F.**; Lubitz, W., Key Hydride Vibrational Modes in [NiFe] Hydrogenase Model Compounds Studied by Resonance Raman Spectroscopy and Density Functional Calculations. *Inorg. Chem.* **2012,** *51* (21), 11787-11797.

274. Sandhöfer, B.; **Neese, F.**, One-electron contributions to the g-tensor for second-order Douglas–Kroll–Hess theory. *J. Chem. Phys.* **2012,** *137* (9), 15.

273. Roemelt, M.; Beckwith, M. A.; Duboc, C.; Collomb, M.-N.; **Neese, F.**; DeBeer, S., Manganese K-Edge X-Ray Absorption Spectroscopy as a Probe of the Metal-Ligand Interactions in Coordination Compounds. *Inorg. Chem.* **2012,** *51* (1), 680-687.

272. Rapatskiy, L.; Cox, N.; Savitsky, A.; Ames, W. M.; Sander, J.; Nowaczyk, M. M.; Rögner, M.; Boussac, A.; **Neese, F.**; Messinger, J.; Lubitz, W., Detection of the Water-Binding Sites of the Oxygen-Evolving Complex of Photosystem II Using W-Band ^{17}O Electron–Electron Double Resonance-Detected NMR Spectroscopy. *J. Am. Chem. Soc.* **2012,** *134* (40), 16619-16634.

271. Petrenko, T.; **Neese, F.**, Efficient and automatic calculation of optical band shapes and resonance Raman spectra for larger molecules within the independent mode displaced harmonic oscillator model. *J. Chem. Phys.* **2012,** *137*, 234107.

270. Pantazis, D. A.; **Neese, F.**, All-electron scalar relativistic basis sets for the 6p elements. *Theor. Chem. Acc.* **2012,** *131*, 1292.

269. Pantazis, D. A.; Ames, W.; Cox, N.; Lubitz, W.; **Neese, F.**, Two Interconvertible Structures that Explain the Spectroscopic Properties of the Oxygen-Evolving Complex of Photosystem II in the S2 State**. *Angew. Chem. Int. Ed.* **2012,** *51* (39), 9935-9940.

268. Nesterov, V.; Özbolat-Schön, A.; Schnakenburg, G.; Shi, L.; Cangönül, A.; van Gastel, M.; **Neese, F.**; Streubel, R., An Unusal Case of Facile Non-Degenerate P-C Bond Making and Breaking. *Chem. Asian J.* **2012,** *7* (7), 1708-1712.

267. **Neese, F.**, The ORCA program system. *WIREs Comput. Mol. Sci.* **2012,** *2* (1), 73-78.

266. McLaughlin, M. P.; Retegan, M.; Bill, E.; Payne, T. M.; Shafaat, H. S.; Peña, S.; Sudhamsu, J.; Ensign, A. A.; Crane, B. R.; **Neese, F.**; Holland, P. L., Azurin as a Protein Scaffold for a Low-coordinate Nonheme Iron Site with a Small-molecule Binding Pocket. *J. Am. Chem. Soc.* **2012,** *134* (48), 19746-19757.

265. Maganas, D.; Krzystek, J.; Ferentinos, E.; Whyte, A. M.; Robertson, N.; Psycharis, V.; Terzis, A.; **Neese, F.**; Kyritsis, P., Investigating Magnetostructural Correlations in the

Pseudooctahedral trans-[Ni^{II}{$(OPPh_2)(EPPh_2)N$}$_2(sol)_2$] Complexes (E = S, Se; sol = DMF, THF) by Magnetometry, HFEPR, and ab Initio Quantum Chemistry. *Inorg. Chem.* **2012,** *51* (13), 7218-7231.

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

263. Liakos, D. G.; **Neese, F.**, Improved Correlation Energy Extrapolation Schemes Based on Local Pair Natural Orbital Methods. *J. Phys. Chem. A* **2012,** *116* (19), 4801-4816.

262. Lancaster, K. M.; Zaballa, M.-E.; Sproules, S.; Sundararajan, M.; DeBeer, S.; Richards, J. H.; Vila, A. J.; **Neese, F.**; Gray, H. B., Outer-Sphere Contributions to the Electronic Structure of Type Zero Copper Proteins. *J. Am. Chem. Soc.* **2012,** *134* (19), 8241-8253.

261. Kampa, M.; Lubitz, W.; van Gastel, M.; **Neese, F.**, Computational study of the electronic structure and magnetic properties of the Ni–C state in [NiFe] hydrogenases including the second coordination sphere. *J. Biol. Inorg. Chem.* **2012,** *17*, 1269-1281.

260. Izsák, R.; Hansen, A.; **Neese, F.**, The resolution of identity and chain of spheres approximations for the LPNO-CCSD single Fock term. *Mol. Phys.* **2012,** *110* (19-20), 2413-2417.

259. Huntington, L. M. J.; Hansen, A.; **Neese, F.**; Nooijen, M., Accurate thermochemistry from a parameterized coupled-cluster singles and doubles model and a local pair natural orbital based implementation for applications to larger systems. *J. Chem. Phys.* **2012,** *136* (6), 064101.

258. Gemma, J. C.; Ye, S.; **Neese, F.**, Oxygen activation in extradiol catecholate dioxygenases – a density functional study. *Chem. Sci.* **2012,** *3* (5), 1600-1611.

257. Dugan, T. R.; Bill, E.; MacLeod, K. C.; Gemma, C. 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.

256. Domingo, A.; Carvajal, M. À.; de Graaf, C.; Sivalingam, K.; **Neese, F.**; Angeli, C., Metal-to-metal charge-transfer transitions: reliable excitation energies from ab initio calculations. *Theor. Chem. Acc.* **2012,** *131* (9), 1264.

255. 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.

254. 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*, Schlögl, R., Ed. DeGruyter: 2012; pp 353-378.

253. Cowley, R. E.; Christian, G. J.; Brennessel, W. W.; **Neese, F.**; Holland, P. L., A Reduced (β-Diketiminato)iron Complex with End-On and Side-On Nitriles: Strong Backbonding or Ligand Non-Innocence? *Eur. J. Inorg. Chem.* **2012,** (3), 479-483.

252. Christian, G. J.; Ye, S.; **Neese, F.**, Oxygen activation in extradiol catecholate dioxygenases - a density functional study. *Chem. Sci.* **2012,** *3* (5), 1600-1611.

251. Bykov, D.; **Neese, F.**, Reductive activation of the heme iron–nitrosyl intermediate in the reaction mechanism of cytochrome c nitrite reductase: a theoretical study. *J. Biol. Inorg. Chem.* **2012,** *17* (5), 741-760.

250. Benkhäuser-Schunk, C.; Wezisla, B.; Urbahn, K.; Kiehne, U.; Daniels, J.; Schnakenburg, G.; **Neese, F.**; Lützen, A., Synthesis, Chiral Resolution, and Absolute Configuration of Functionalized Tröger's Base Derivatives: Part II. *ChemPlusChem* **2012,** *77* (5), 396-403.

249. Atanasov, M.; Ganyushin, D.; Sivalingam, K.; **Neese, F.**, A Modern First-Principles View on Ligand Field Theory Through the Eyes of Correlated Multireference Wavefunctions. In *Struct. Bond.*, Springer-Verlag: Berlin Heidelberg, **2012**; Vol. 143, pp 149-220.

248. Atanasov, M.; Comba, P.; Helmle, S.; Müller, D.; **Neese, F.**, Zero-Field Splitting in a Series of Structurally Related Mononuclear NiII–Bispidine Complexes. *Inorg. Chem.* **2012,** *51* (22), 12324-12335.

247. Argirević, T.; Riplinger, C.; Stubbe, J.; Neese, F.; Bennati, M., ENDOR Spectroscopy and DFT Calculations: Evidence for the Hydrogen-Bond Network Within α2 in the PCET of E. coli Ribonucleotide Reductase. *J. Am. Chem. Soc.* **2012,** *134* (42), 17661-17670.

246. Albrecht, C.; Shi, L.; Pérez, J. M.; van Gastel, M.; Schwieger, S.; **Neese, F.**; Streubel, R., Deoxygenation of Coordinated Oxaphosphiranes: A New Route to P=C Double-Bond Systems. *Chem. Eur. J.* **2012,** *18*, 9780-9783.

245. 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.

244. Ye, S.; Christian, G. J.; Geng, C.; **Neese, F.**, Theoretical Spectroscopies of Iron-Containing Enzymes and Biomimetics. In *Iron-Containing Enzymes: Versatile Catalysts of Hydroxylation Reactions in Nature*, de Visser, S. P.; Kumar, D., Eds. Royal Society of Chemistry: **2011**; pp 119-147.

243. Surawatanawong, P.; Sproules, S.; **Neese, F.**; Wieghardt, K., Electronic Structures and Spectroscopy of the Electron Transfer Series $[Fe(NO)L_2]^z$ (z=1+, 0, 1-, 2-,3-; L = Dithiolene). *Inorg. Chem.* **2011,** *50* (23), 12064-12074.

242. Sundararajan, M.; Riplinger, C.; Orio, M.; Wennmohs, F.; **Neese, F.**, Spectroscopic Properties of Protein-Bound Cofactors: Calculation by Combined Quantum Mechanical/Molecular Mechanical (QM/MM) Approaches. *Encyclopedia of Inorganic and Bioinorganic Chemistry* **2011**.

241. Su, J.-H.; Cox, N.; Ames, W.; Pantazis, D. A.; Rapatskiy, L.; Lohmiller, T.; Kulik, L. V.; Dorlet, P.; Rutherford, A. W.; **Neese, F.**; Boussac, A.; Lubitz, W.; Messinger, J., The electronic structures of the S-2 states of the oxygen-evolving complexes of photosystem II in plants and cyanobacteria in the presence and absence of methanol. *Biochim. Biophys. Acta - Bioenergetics* **2011,** *1807* (7), 829-840.

240. Rota, J. B.; Knecht, S.; Fleig, T.; Ganyushin, D.; Saue, T.; **Neese, F.**; Bolvin, H., Zero field splitting of the chalcogen diatomics using relativistic correlated wave-function methods. *J. Chem. Phys.* **2011,** *135* (11), 114106.

239. Riplinger, C.; **Neese, F.**, The Reaction Mechanism of Cytochrome P450 NO Reductase: A Detailed Quantum Mechanics/Molecular Mechanics Study. *ChemPhysChem* **2011,** *12* (17), 3192-3203.

238. Radoul, M.; Bykov, D.; Rinaldo, S.; Cutruzzola, F.; **Neese, F.**; Goldfarb, D., Dynamic Hydrogen-Bonding Network in the Distal Pocket of the Nitrosyl Complex of Pseudomonas aeruginosa cd(1) Nitrite Reductase. *J. Am. Chem. Soc.* **2011,** *133* (9), 3043-3055.

237. Petrenko, T.; Kossmann, S.; **Neese, F.**, Efficient time-dependent density functional theory approximations for hybrid density functionals: Analytical gradients and parallelization. *J. Chem. Phys.* **2011,** *134* (5), 054116.

236. Pantazis, D. A.; **Neese, F.**, All-Electron Scalar Relativistic Basis Sets for the Actinides. *J. Chem. Theory Comput.* **2011,** *7* (3), 677-684.

235. **Neese, F.**; Valeev, E. F., Revisiting the Atomic Natural Orbital Approach for Basis Sets: Robust Systematic Basis Sets for Explicitly Correlated and Conventional Correlated ab initio Methods? *J. Chem. Theory Comput.* **2011,** *7* (1), 33-43.

234. **Neese, F.**; Petrenko, T., Quantum Chemistry and Mo¨ssbauer Spectroscopy. In *Mössbauer Spectroscopy and Transiton Metal Chemistry*, Gütlich, P.; Bill, E.; Trautwein, A. X., Eds. Springer-Verlag: Heidelberg, Germany, **2011**; pp 137-199.

233. **Neese, F.**; Pantazis, D. A., What is not required to make a single molecule magnet. *Faraday Discuss.* **2011,** *148*, 229-238.

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

231. **Neese, F.**, First Principles Approach to Spin-Hamiltonian Parameters. In *Multifrequency Electron Paramagnetic Resonance: Theory and Applications*, Misra, S. K., Ed. Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim, Germany, **2011**; pp 295–326.

230. Maurice, R.; Sivalingam, K.; Ganyushin, D.; Guihery, N.; de Graaf, C.; **Neese, F.**, Theoretical Determination of the Zero-Field Splitting in Copper Acetate Monohydrate. *Inorg. Chem.* **2011,** *50* (13), 6229-6236.

229. Maganas, D.; Sottini, S.; Kyritsis, P.; Groenen, E. J. J.; **Neese, F.**, Theoretical Analysis of the Spin Hamiltonian Parameters in $Co^{(II)}S_4$ Complexes, Using Density Functional Theory and Correlated ab initio Methods. *Inorg. Chem.* **2011,** *50* (18), 8741-8754.

228. Liakos, D. G.; **Neese, F.**, Interplay of Correlation and Relativistic Effects in Correlated Calculations on Transition-Metal Complexes: The $(Cu_2O_2)^{2+}$ Core Revisited. *J. Chem. Theory Comput.* **2011,** *7* (5), 1511-1523.

227. Liakos, D. G.; Hansen, A.; **Neese, F.**, Weak Molecular Interactions Studied with Parallel Implementations of the Local Pair Natural Orbital Coupled Pair and Coupled Cluster Methods. *J. Chem. Theory Comput.* **2011,** *7* (1), 76-87.

226. Lancaster, K. M.; Roemelt, M.; Ettenhuber, P.; Hu, Y.; Ribbe, M. W.; **Neese, F.**; Bergmann, U.; DeBeer, S., X-ray Emission Spectroscopy Evidences a Central Carbon in the Nitrogenase Iron-Molybdenum Cofactor. *Science* **2011,** *334* (6058), 974-977.

225. Kollmar, C.; **Neese, F.**, The relationship between double excitation amplitudes and Z vector components in some post-Hartree-Fock correlation methods. *J. Chem. Phys.* **2011,** *135* (6), 064103.

224. Kollmar, C.; **Neese, F.**, An orbital-invariant and strictly size extensive post-Hartree-Fock correlation functional. *J. Chem. Phys.* **2011,** *135* (8), 084102.

223. Izsak, R.; **Neese, F.**, An overlap fitted chain of spheres exchange method. *J. Chem. Phys.* **2011,** *135* (14), 144105.

222. Hansen, A.; Liakos, D. G.; **Neese, F.**, Efficient and accurate local single reference correlation methods for high-spin open-shell molecules using pair natural orbitals. *J. Chem. Phys.* **2011,** *135* (21).

221. Gennari, M.; Retegan, M.; DeBeer, S.; Pecaut, J.; **Neese, F.**; Collomb, M.-N.; Duboc, C., Experimental and Computational Investigation of Thiolate Alkylation in Ni^{II} and Zn^{II} Complexes: Role of the Metal on the Sulfur Nucleophilicity. *Inorg. Chem.* **2011,** *50* (20), 10047-10055.

220. Gennari, M.; Pecaut, J.; DeBeer, S.; **Neese, F.**; Collomb, M.-N.; Duboc, C., A Fully Delocalized Mixed-Valence Bis-mu(Thiolato) Dicopper Complex: A Structural and Functional Model of the Biological Cu-A Center. *Angew. Chem. Int. Ed./Angew. Chem.* **2011,** *50/123* (25), 5661-5665/5780-5784.

219. Gennari, M.; Orio, M.; Pecaut, J.; Bothe, E.; **Neese, F.**; Collomb, M.-N.; Duboc, C., Influence of Mixed Thiolate/Thioether versus Dithiolate Coordination on the Accessibility of the Uncommon +I and +III Oxidation States for the Nickel Ion: An Experimental and Computational Study. *Inorg. Chem.* **2011,** *50* (8), 3707-3716.

218. Cox, N.; Rapatskiy, L.; Su, J.-H.; Pantazis, D. A.; Sugiura, M.; Kulik, L.; Dorlet, P.; Rutherford, A. W.; Neese, F.; Boussac, A.; Lubitz, W.; Messinger, J., Effect of Ca^{2+}/Sr^{2+} Substitution on the Electronic Structure of the Oxygen-Evolving Complex of Photosystem II: A Combined Multifrequency EPR, ^{55}Mn-ENDOR, and DFT Study of the S_2 State. *J. Am. Chem. Soc.* **2011,** *133* (10), 3635-3648.

217. Cox, N.; Ames, W.; Epel, B.; Kulik, L. V.; Rapatskiy, L.; **Neese, F.**; Messinger, J.; Wieghardt, K.; Lubitz, W., Electronic Structure of a Weakly Antiferromagnetically Coupled $Mn^{II}Mn^{III}$Model Relevant to Manganese Proteins: A Combined EPR, ^{55}Mn-ENDOR, and DFT Study. *Inorg. Chem.* **2011,** *50* (17), 8238-8251.

216. Cimino, P.; **Neese, F.**; Barone, V., Calculation of Magnetic Tensors and EPR Spectra for Free Radicals in Different Environments. In *Computational Spectroscopy: Methods, Experiments and Applications*, Grunenberg, J., Ed. Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim, Germany, **2011**; pp 63–104.

215. Chandrasekaran, P.; Stieber, S. C. E.; Collins, T. J.; Que, L., Jr.; Neese, F.; DeBeer, S.,

Prediction of high-valent iron K-edge absorption spectra by time-dependent Density Functional Theory. *Dalton Trans.* **2011,** *40* (42), 11070-11079.

214. Bykov, D.; **Neese, F.**, Substrate binding and activation in the active site of cytochrome c nitrite reductase: a density functional study. *J. Biol. Inorg. Chem.* **2011,** *16* (3), 417-430.

213. Beckwith, M. A.; Roemelt, M.; Collomb, M.-N.; DuBoc, C.; Weng, T.-C.; Bergmann, U.; Glatzel, P.; **Neese, F.**; DeBeer, S., Manganese Kβ X-ray Emission Spectroscopy As a Probe of Metal-Ligand Interactions. *Inorg. Chem.* **2011,** *50* (17), 8397-8409.

212. Atanasov, M.; Ganyushin, D.; Pantazis, D. A.; Sivalingam, K.; **Neese, F.**, Detailed Ab Initio First-Principles Study of the Magnetic Anisotropy in a Family of Trigonal Pyramidal Iron(II) Pyrrolide Complexes. *Inorg. Chem.* **2011,** *50* (16), 7460-7477.

211. Atanasov, M.; Delley, B.; **Neese, F.**; Tregenna-Piggott, P. L.; Sigrist, M., Theoretical Insights into the Magnetostructural Correlations in Mn-3-Based Single-Molecule Magnets. *Inorg. Chem.* **2011,** *50* (6), 2112-2124.

210. Antony, J.; Grimme, S.; Liakos, D. G.; **Neese, F.**, Protein-Ligand Interaction Energies with Dispersion Corrected Density Functional Theory and High-Level Wave Function Based Methods. *J. Phys. Chem. A* **2011,** *115* (41), 11210-11220.

209. Ames, W.; Pantazis, D. A.; Krewald, V.; Cox, N.; Messinger, J.; Lubitz, W.; **Neese, F.**, 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* (49), 19743-19757.

208. 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.

207. Ye, S.; Neese, F.; Ozarowski, A.; Smirnov, D.; Krzystek, J.; Telser, J.; Liao, J.-H.; Hung, C.-H.; Chu, W.-C.; Tsai, Y.-F.; Wang, R.-C.; Chen, K.-Y.; Hsu, H.-F., 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.

206. 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.

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

204. Woertink, J. S.; Tian, L.; Maiti, D.; Lucas, H. R.; Himes, R. A.; Karlin, K. D.; **Neese, F.**; Würtele, C.; Holthausen, M. C.; Bill, E.; Sundermeyer, J.; Schindler, S.; Solomon, E. I., Spectroscopic and Computational Studies of an End-on Bound Superoxo-Cu(II) Complex: Geometric and Electronic Factors That Determine the Ground State. *Inorg. Chem.* **2010,** *49* (20), 9450-9459.

203. Vancoillie, S.; Chalupsky, J.; Ryde, U.; Solomon, E. I.; Pierloot, K.; **Neese, F.**; Rulisek, L.,

Multireference Ab Initio Calculations of g tensors for Trinuclear Copper Clusters in Multicopper Oxidases. *J. Phys. Chem. B* **2010,** *114* (22), 7692-7702.

202. van Slageren, J.; Piligkos, S.; **Neese, F.**, Magnetic circular dichroism spectroscopy on the Cr_8 antiferromagnetic ring. *Dalton Trans.* **2010,** *39* (20), 4999-5004.

201. Radoul, M.; Sundararajan, M.; Potapov, A.; Riplinger, C.; **Neese, F.**; Goldfarb, D., Revisiting the nitrosyl complex of myoglobin by high-field pulse EPR spectroscopy and quantum mechanical calculations. *Phys. Chem. Chem. Phys.* **2010,** *12* (26), 7276-7289.

200. Pantazis, D. A.; Krewald, V.; Orio, M.; **Neese, F.**, 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* (20), 4959-4967.

199. Özbolat-Schön, A.; Bode, M.; Schnakenburg, G.; Anoop, A.; van Gastel, M.; **Neese, F.**; Streubel, R., Insights into the Chemistry of Transient P-Chlorophosphanyl Complexes. *Angew. Chem. Int. Ed./Angew. Chem.* **2010,** *49/122* (38), 6894-6898/7047-7051.

198. Orio, M.; Philouze, C.; Jarjayes, O.; **Neese, F.**; Thomas, F., Spin Interaction in Octahedral Zinc Complexes of Mono- and Diradical Schiff and Mannich Bases. *Inorg. Chem.* **2010,** *49* (2), 646-658.

197. Orio, M.; Jarjayes, O.; Kanso, H.; Philouze, C.; **Neese, F.**; Thomas, F., X-Ray Structures of Copper(II) and Nickel(II) Radical Salen Complexes: The Preference of Galactose Oxidase for Copper(II). *Angew. Chem. Int. Ed./Angew. Chem.* **2010,** *49/122* (29), 4989-4992/5109-5112.

196. **Neese, F.**; Ames, W.; Christian, G.; Kampa, M.; Liakos, D. G.; Pantazis, D. A.; Roemelt, M.; Surawatanawong, P.; Ye, S., Dealing with Complexity in Open-Shell Transition Metal Chemistry from a Theoretical Perspective: Reaction Pathways, Bonding, Spectroscopy, And Magnetic Properties. In *Advances in Inorganic Chemistry: Theoretical and Computational Inorganic Chemistry*, VanEldik, R. H. J., Ed. **2010**; Vol. 62, pp 301-349.

195. **Neese, F.**, Some Thoughts on the Scope of Linear Scaling Self-Consistent Field Calculations. In *Linear Scaling Methods in Quantum Chemistry*, Papadopoulous, M., Ed. 2010; p in press.

194. McNaughton, R. L.; Roemelt, M.; Chin, J. M.; Schrock, R. R.; Neese, F.; Hoffman, B. M., Experimental and Theoretical EPR Study of Jahn-Teller-Active [HIPTN_3N]MoL Complexes (L) N_2, CO, NH_3). *J. Am. Chem. Soc.* **2010,** *132* (25), 8645-8656.

193. Maganas, D.; Grigoropoulos, A.; Staniland, S. S.; Chatziefthimiou, S. D.; Harrison, A.; Robertson, N.; Kyritsis, P.; **Neese, F.**, Tetrahedral and Square Planar Ni[$(SPR_2)_2N]_2$ complexes, R = Ph & iPr Revisited: Experimental and Theoretical Analysis of Interconversion Pathways, Structural Preferences, and Spin Delocalization. *Inorg. Chem.* **2010,** *49* (11), 5079-5093.

192. Lee, N.; Petrenko, T.; Bergmann, U.; **Neese, F.**; DeBeer, S., Probing Valence Orbital Composition with Iron Kβ X-ray Emission Spectroscopy. *J. Am. Chem. Soc.* **2010,** *132*

(28), 9715-9727.

191. Lassalle-Kaiser, B.; Hureau, C.; Pantazis, D. A.; Pushkar, Y.; Guillot, R.; Yachandra, V. K.; Yano, J.; **Neese, F.**; Anxolabehere-Mallart, E., Activation of a water molecule using a mononuclear Mn complex: from Mn-aquo, to Mn-hydroxo, to Mn-oxyl via charge compensation. *Energy Environ. Sci.* **2010,** *3* (7), 924-938.

190. Kossmann, S.; **Neese, F.**, Efficient Structure Optimization with Second-Order Many-Body Perturbation Theory: The RIJCOSX-MP2 Method. *J. Chem. Theory Comput.* **2010,** *6* (8), 2325-2338.

189. Kossmann, S.; Neese, F., Correlated ab Initio Spin Densities for Larger Molecules: Orbital-Optimized Spin-Component-Scaled MP2 Method. *J. Phys. Chem. A* **2010,** *114* (43), 11768-11781.

188. Kollmar, C.; **Neese, F.**, The coupled electron pair approximation: variational formulation and spin adaptation. *Mol. Phys.* **2010,** *108* (19-20), 2449-2458.

187. Kochem, A.; Orio, M.; Jarjayes, O.; **Neese, F.**; Thomas, F., Unsymmetrical one-electron oxidized Ni(II)-bis(salicylidene) complexes: a protonation-induced shift of the oxidation site. *Chem. Commun.* **2010,** *46* (36), 6765-6767.

186. Hegele, P.; Santhamma, B.; Schnakenburg, G.; Froehlich, R.; Kataeva, O.; Nieger, M.; Kotsis, K.; **Neese, F.**; Doetz, K. H., Hydroquinoid Chromium Complexes Bearing an Acyclic Conjugated Bridge: Chromium-Templated Synthesis, Molecular Structure, and Haptotropic Metal Migration. *Organometallics* **2010,** *29* (23), 6172-6185.

185. Grote, D.; Finke, C.; Kossmann, S.; **Neese, F.**; Sander, W., 3,4,5,6-Tetrafluorophenylnitren-2-yl: A Ground-State Quartet Triradical. *Chem. Eur. J.* **2010,** *16* (15), 4496-4506.

184. George, S. D.; **Neese, F.**, Calibration of Scalar Relativistic Density Functional Theory for the Calculation of Sulfur K-Edge X-ray Absorption Spectra. *Inorg. Chem.* **2010,** *49* (4), 1849-1853.

183. Gennari, M.; Orio, M.; Pecaut, J.; **Neese, F.**; Collomb, M.-N.; Duboc, C., Reversible Apical Coordination of Imidazole between the Ni(III) and Ni(II) Oxidation States of a Dithiolate Complex: A Process Related to the Ni Superoxide Dismutase. *Inorg. Chem.* **2010,** *49* (14), 6399-6401.

182. Geng, C.; Ye, S.; **Neese, F.**, Analysis of Reaction Channels for Alkane Hydroxylation by Nonheme Iron(IV)-Oxo Complexes. *Angew. Chem. Int. Ed./Angew. Chem.* **2010,** *49/112* (33), 5717-5720/5853-5856.

181. Ganyushin, D.; Gilka, N.; Taylor, P. R.; Marian, C. M.; **Neese, F.**, The resolution of the identity approximation for calculations of spin-spin contribution to zero-field splitting parameters. *J. Chem. Phys.* **2010,** *132* (14), 144111.

180. Duboc, C.; Ganyushin, D.; Sivalingam, K.; Collomb, M.-N.; **Neese, F.**, Systematic Theoretical Study of the Zero-Field Splitting in Coordination Complexes of Mn(III). Density Functional Theory versus Multireference Wave Function Approaches. *J. Phys. Chem. A*

2010, *114* (39), 10750-10758.

179. Duboc, C.; Collomb, M.-N.; **Neese, F.**, Understanding the Zero-Field Splitting of Mononuclear Manganese(II) Complexes from Combined EPR Spectroscopy and Quantum Chemistry. *Appl. Magn. Reson.* **2010,** *37* (1-4), 229-245.

178. Anoop, A.; Thiel, W.; **Neese, F.**, A Local Pair Natural Orbital Coupled Cluster Study of Rh Catalyzed Asymmetric Olefin Hydrogenation. *J. Chem. Theory Comput.* **2010,** *6* (10), 3137-3144.

177. 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.

176. Vancoillie, S.; Rulisek, L.; **Neese, F.**; Pierloot, K., Theoretical Description of the Structure and Magnetic Properties of Nitroxide-Cu(II)-Nitroxide Spin Triads by Means of Multiconfigurational Ab Initio Calculations. *J. Phys. Chem. A* **2009,** *113* (21), 6149-6157.

175. Sundararajan, M.; Riplinger, C.; Orio, M.; Wennmohs, F.; **Neese, F.**, Spectroscopic Properties of Protein-Bound Cofactors: Calculation by Combined Quantum Mechanical/Molecular Mechanical (QM/MM) Approaches. *Encyclopedia of Inorganic Chemistry* **2009**.

174. 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,** (30), 6021-6036.

173. Schmitz, C. H.; Rang, C.; Bai, Y.; Kossev, I.; Ikonomov, J.; Su, Y.; Kotsis, K.; Soubatch, S.; Neucheva, O.; Tautz, F. S.; **Neese, F.**; Steinrueck, H.-P.; Gottfried, J. M.; Doetz, K. H.; Sokolowski, M., A Comparative Study of a Triphenylene Tricarbonyl Chromium Complex and Its Uncoordinated Arene Ligand on the Ag(111) Surface: Influence of the Complexation on the Adsorption. *J. Phys. Chem. C* **2009,** *113* (15), 6014-6021.

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

171. Romain, S.; Duboc, C.; **Neese, F.**; Riviere, E.; Hanton, L. R.; Blackman, A. G.; Philouze, C.; Lepretre, J.-C.; Deronzier, A.; Collomb, M.-N., An Unusual Stable Mononuclear Mn^{III} Bis-terpyridine Complex Exhibiting Jahn-Teller Compression: Electrochemical Synthesis, Physical Characterisation and Theoretical Study. *Chem. Eur. J.* **2009,** *15* (4), 980-988.

170. Riplinger, C.; Kao, J. P. Y.; Rosen, G. M.; Kathirvelu, V.; Eaton, G. R.; Eaton, S. S.; Kutateladze, A.; **Neese, F.**, Interaction of Radical Pairs Through-Bond and Through-Space: Scope and Limitations of the Point-Dipole Approximation in Electron Paramagnetic Resonance Spectroscopy. *J. Am. Chem. Soc.* **2009,** *131* (29), 10092-10106.

169. Piligkos, S.; Weihe, H.; Bill, E.; **Neese, F.**; El Mkami, H.; Smith, G. M.; Collison, D.; Rajaraman, G.; Timco, G. A.; Winpenny, R. E. P.; McInnes, E. J. L., EPR Spectroscopy of a Family of $Cr^{III}_7M^{II}$ (M = Cd, Zn, Mn, Ni) "Wheels": Studies of Isostructural Compounds with Different Spin Ground States. *Chem. Eur. J.* **2009,** *15* (13), 3152-3167.

168. Piligkos, S.; Slep, L. D.; Weyhermüller, T.; Chaudhuri, P.; Bill, E.; **Neese, F.**, Magnetic circular dichroism spectroscopy of weakly exchange coupled transition metal dimers: A model study. *Coord. Chem. Rev.* **2009,** *253* (19-20), 2352-2362.

167. Petrenko, T.; Krylova, O.; **Neese, F.**; Sokolowski, M., Optical absorption and emission properties of rubrene: insight from a combined experimental and theoretical study. *New J. Phys.* **2009,** *11*, 015001.

166. Pantazis, D. A.; Orio, M.; Petrenko, T.; Zein, S.; Lubitz, W.; Messinger, J.; **Neese, F.**, Structure of the oxygen-evolving complex of photosystem II: information on the S_2 state through quantum chemical calculation of its magnetic properties. *Phys. Chem. Chem. Phys.* **2009,** *11* (31), 6788-6798.

165. Pantazis, D. A.; Orio, M.; Petrenko, T.; Zein, S.; Bill, E.; Lubitz, W.; Messinger, J.; **Neese, F.**, A New Quantum Chemical Approach to the Magnetic Properties of Oligonuclear Transition-Metal Complexes: Application to a Model for the Tetranuclear Manganese Cluster of Photosystem II. *Chem. Eur. J.* **2009,** *15* (20), 5108-5123.

164. Pantazis, D. A.; **Neese, F.**, All-Electron Scalar Relativistic Basis Sets for the Lanthanides. *J. Chem. Theory Comput.* **2009,** *5* (9), 2229-2238.

163. Orio, M.; Pantazis, D. A.; Petrenko, T.; **Neese, F.**, Magnetic and Spectroscopic Properties of Mixed Valence Manganese(III,IV) Dimers: A Systematic Study Using Broken Symmetry Density Functional Theory. *Inorg. Chem.* **2009,** *48* (15), 7251-7260.

162. Orio, M.; Pantazis, D. A.; **Neese, F.**, Density functional theory. *Photosynth. Res.* **2009,** *102* (2-3), 443-453.

161. **Neese, F.**; Wennmohs, F.; Hansen, A.; Becker, U., Efficient, approximate and parallel Hartree-Fock and hybrid DFT calculations. A 'chain-of-spheres' algorithm for the Hartree-Fock exchange. *Chem. Phys.* **2009,** *356* (1-3), 98-109.

160. **Neese, F.**; Wennmohs, F.; Hansen, A., Efficient and accurate local approximations to coupled-electron pair approaches: An attempt to revive the pair natural orbital method. *J. Chem. Phys.* **2009,** *130* (11), 114108.

159. **Neese, F.**; Schwabe, T.; Kossmann, S.; Schirmer, B.; Grimme, S., Assessment of Orbital-Optimized, Spin-Component Scaled Second-Order Many-Body Perturbation Theory for Thermochemistry and Kinetics. *J. Chem. Theory Comput.* **2009,** *5* (11), 3060-3073.

158. **Neese, F.**; Hansen, A.; Wennmohs, F.; Grimme, S., Accurate Theoretical Chemistry with Coupled Pair Models. *Acc. Chem. Res.* **2009,** *42* (5), 641-648.

157. **Neese, F.**; Hansen, A.; Liakos, D. G., Efficient and accurate approximations to the local coupled cluster singles doubles method using a truncated pair natural orbital basis. *J. Chem. Phys.* **2009,** *131* (6), 064103.

156. **Neese, F.**, Density Functional Theory and EPR Spectroscopy: a guided tour. *EPR Newsletter* **2009,** *18* (4), Pro & Contra section.

155. **Neese, F.**, Mit der Quantenchemie „ins Auge“ von Proteinen **2009,** *Labor & More* (3).

154. **Neese, F.**, Spin-Hamiltonian Parameters from first Principle Calculations: Theory and Application. In *High Resolution EPR: Applications to Metalloenzymes and Metals in Medicine*, Hanson, G. B. L., Ed. 2009; Vol. 28, pp 175-229.

153. **Neese, F.**, Prediction of molecular properties and molecular spectroscopy with density functional theory: From fundamental theory to exchange-coupling. *Coord. Chem. Rev.* **2009,** *253* (5-6), 526-563.

152. Liakos, D. G.; Ganyushin, D.; **Neese, F.**, A Multiconfigurational ab Initio Study of the Zero-Field Splitting in the Di- and Trivalent Hexaquo-Chromium Complexes. *Inorg. Chem.* **2009,** *48* (22), 10572-10580.

151. Krahe, O.; **Neese, F.**; Streubel, R., The Quest for Ring Opening of Oxaphosphirane Complexes: A Coupled-Cluster and Density Functional Study of CH_3PO Isomers and Their $Cr(CO)_5$ Complexes. *Chem. Eur. J.* **2009,** *15* (11), 2594-2601.

150. Kossmann, S.; **Neese, F.**, Comparison of two efficient approximate Hartee-Fock approaches. *Chem. Phys. Lett.* **2009,** *481* (4-6), 240-243.

149. Klein, E. L.; Astashkin, A. V.; Ganyushin, D.; Riplinger, C.; Johnson-Winters, K.; Neese, F.; Enemark, J. H., Direct Detection and Characterization of Chloride in the Active Site of the Low-pH Form of Sulfite Oxidase Using Electron Spin Echo Envelope Modulation Spectroscopy, Isotopic Labeling, and Density Functional Theory Calculations. *Inorg. Chem.* **2009,** *48* (11), 4743-4752.

148. Gauss, J.; Kallay, M.; **Neese, F.**, Calculation of Electronic g-Tensors using Coupled Cluster Theory. *J. Phys. Chem. A* **2009,** *113* (43), 11541-11549.

147. Gansäuer, A.; Fleckhaus, A.; Lafont, M. A.; Okkel, A.; Kotsis, K.; Anoop, A.; **Neese, F.**, Catalysis via Homolytic Substitutions with C-O and Ti-O Bonds: Oxidative Additions and Reductive Eliminations in Single Electron Steps. *J. Am. Chem. Soc.* **2009,** *131* (46), 16989-16999.

146. Cowley, R. E.; Bill, E.; **Neese, F.**; Brennessel, W. W.; Holland, P. L., Iron(II) Complexes with Redox-Active Tetrazene (RNNNNR) Ligands. *Inorg. Chem.* **2009,** *48* (11), 4828-4836.

145. Cirera, J.; Ruiz, E.; Alvarez, S.; **Neese, F.**; Kortus, J., How to Build Molecules with Large Magnetic Anisotropy. *Chem. Eur. J.* **2009,** *15* (16), 4078-4087.

144. Baffert, C.; Orio, M.; Pantazis, D. A.; Duboc, C.; Blackman, A. G.; Blondin, G.; **Neese, F.**; Deronzier, A.; Collomb, M.-N., Trinuclear Terpyridine Frustrated Spin System with a $Mn^{IV}_3O_4$ Core: Synthesis, Physical Characterization, and Quantum Chemical Modeling of Its Magnetic Properties. *Inorg. Chem.* **2009,** *48* (21), 10281-10288.

143. Astashkin, A. V.; Klein, E. L.; Ganyushin, D.; Johnson-Winters, K.; **Neese, F.**; Kappler, U.; Enemark, J. H., Exchangeable oxygens in the vicinity of the molybdenum center of the high-pH form of sulfite oxidase and sulfite dehydrogenase. *Phys. Chem. Chem. Phys.* **2009,** *11* (31), 6733-6742.

142. Zein, S.; **Neese, F.**, Ab initio and coupled-perturbed density functional theory estimation

of zero-field splittings in Mn-II transition metal complexes. *J. Phys. Chem. A* **2008,** *112* (34), 7976-7983.

141. Zein, S.; Kulik, L. V.; Yano, J.; Kern, J.; Pushkar, Y.; Zouni, A.; Yachandra, V. K.; Lubitz, W.; **Neese, F.**; Messinger, J., Focusing the view on nature's water-splitting catalyst. *Philosophical Transactions of the Royal Society B-Biological Sciences* **2008,** *363* (1494), 1167-1177.

140. Zein, S.; Duboc, C.; Lubitz, W.; **Neese, F.**, A systematic density functional study of the zero-field splitting in Mn(II) coordination compounds. *Inorg. Chem.* **2008,** *47* (1), 134-142.

139. 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.

138. Wennmohs, F.; **Neese, F.**, A comparative study of single reference correlation methods of the coupled-pair type. *Chem. Phys.* **2008,** *343* (2-3), 217-230.

137. Scheifele, Q.; Riplinger, C.; **Neese, F.**; Weihe, H.; Barra, A.-L.; Juranyi, F.; Podlesnyak, A.; Tregenna-Piggott, P. L. W., Spectroscopic and theoretical study of a mononuclear manganese(III) complex exhibiting a tetragonally compressed geometry. *Inorg. Chem.* **2008,** *47* (2), 439-447.

136. Sander, W.; Grote, D.; Kossmann, S.; **Neese, F.**, 2,3,5,6-tetrafluorophenyinitren-4-yl: Electron paramagnetic resonance spectroscopic characterization of a quartet-ground-state nitreno radical. *J. Am. Chem. Soc.* **2008,** *130* (13), 4396-4403.

135. Pantazis, D. A.; Chen, X.-Y.; Landis, C. R.; **Neese, F.**, All-electron scalar relativistic basis sets for third-row transition metal atoms. *J. Chem. Theory Comput.* **2008,** *4* (6), 908-919.

134. Marian, C. M.; **Neese, F.**; Engels, B.; Grimme, S.; Peric, M., Theoretical spectroscopy and its impact on experiment - in honour of Sigrid D. Peyerimhoff. *Chemical Physics* **2008,** *343* (2-3), VII-IX.

133. Guihery, N.; Robert, V.; **Neese, F.**, Ab Initio Study of Intriguing Coordination Complexes: A Metal Field Theory Picture. *J. Phys. Chem. A* **2008,** *112* (50), 12975-12979.

132. George, S. D.; Petrenko, T.; **Neese, F.**, Time-dependent density functional calculations of ligand K-edge X-ray absorption spectra. *Inorg. Chim. Acta* **2008,** *361* (4), 965-972.

131. George, S. D.; Petrenko, T.; **Neese, F.**, Prediction of Iron K-Edge Absorption Spectra Using Time-Dependent Density Functional Theory. *J. Phys. Chem. A* **2008,** *112* (50), 12936-12943.

130. Ganyushin, D.; **Neese, F.**, First-principles calculations of magnetic circular dichroism spectra. *J. Chem. Phys.* **2008,** *128* (11), 114117.

129. Duboc, C.; Collomb, M.-N.; Pecaut, J.; Deronzier, A.; **Neese, F.**, Definition of magneto-structural correlations for the Mn^{II} ion. *Chem. Eur. J.* **2008,** *14* (21), 6498-6509.

128. Bühl, M.; Reimann, C.; Pantazis, D. A.; Bredow, T.; **Neese, F.**, Geometries of third-row transition-metal complexes from density-functional theory. *J. Chem. Theory Comput.*

2008, *4* (9), 1449-1459.

127. Berry, J. F.; George, S. D.; **Neese, F.**, Electronic structure and spectroscopy of "superoxidized" iron centers in model systems: theoretical and experimental trends. *Phys. Chem. Chem. Phys.* **2008,** *10* (30), 4361-4374.

126. Atanasov, M.; Comba, P.; Daul, C. A.; **Neese, F.**, The Ligand-Field Paradigm: Insight into Electronic Properties of Transition-metal Complexes Based on Calculations of Electronic Structure. In *Models, Mysteries and Magic of Molecules*, Boeyens, J. C. A.; Ogilvie, J. F., Eds. Springer: Dordrecht, The Netherlands, **2008**; p 411.

125. Altun, A.; Kumar, D.; **Neese, F.**; Thiel, W., Multireference Ab Initio Quantum Mechanics/Molecular Mechanics Study on Intermediates in the Catalytic Cycle of Cytochrome $P450_{cam}$. *J. Phys. Chem. A* **2008,** *112* (50), 12904-12910.

124. Sinnecker, S.; Svensen, N.; Barr, E. W.; Ye, S.; Bollinger, J. M., Jr.; **Neese, F.**; Krebs, C., Spectroscopic and computational evaluation of the structure of the high-spin Fe(IV)-oxo intermediates in taurine: alpha-Ketoglutarate dioxygenase from Escherichia coli and its His99Ala ligand variant. *J. Am. Chem. Soc.* **2007,** *129* (19), 6168-6179.

123. Sinnecker, S.; **Neese, F.**, Theoretical bioinorganic spectroscopy. In *Atomistic Approaches in Modern Biology: From Quantum Chemistry to Molecular Simulations*, Reiher, M., Ed. Springer-Verlag: Heidelberg, **2007**; Vol. 268, pp 47-83.

122. Schröder, D.; Schwarz, H.; Aliaga-Alcalde, N.; **Neese, F.**, Fragmentation of the (cyclam-acetato)iron azide cation in the gas phase. *Eur. J. Inorg. Chem.* **2007,** (6), 816-821.

121. Ray, K.; Petrenko, T.; Wieghardt, K.; **Neese, F.**, Joint spectroscopic and theoretical investigations of transition metal complexes involving non-innocent ligands. *Dalton Trans.* **2007,** (16), 1552-1566.

120. Ray, K.; George, S. D.; Solomon, E. I.; Wieghardt, K.; **Neese, F.**, Description of the ground-state covalencies of the bis(dithiolato) transition-metal complexes from X-ray absorption spectroscopy and time-dependent density-functional calculations. *Chem. Eur. J.* **2007,** *13* (10), 2783-2797.

119. Piligkos, S.; Bill, E.; Collison, D.; McInnes, E. J. L.; Timco, G. A.; Weihe, H.; Winpenny, R. E. P.; **Neese, F.**, Importance of the anisotropic exchange interaction for the magnetic anisotropy of polymetallic systems. *J. Am. Chem. Soc.* **2007,** *129* (4), 760-761.

118. Petrenko, T.; Sturhahn, W.; **Neese, F.**, First-principles calculation of nuclear resonance vibrational spectra. *Hyperfine Interact.* **2007,** *175* (1-3), 165-174.

117. Petrenko, T.; **Neese, F.**, Analysis and prediction of absorption band shapes, fluorescence band shapes, resonance Raman intensities, and excitation profiles using the time-dependent theory of electronic spectroscopy. *J. Chem. Phys.* **2007,** *127* (16), 164319.

116. Petrenko, T.; George, S. D.; Aliaga-Alcalde, N.; Bill, E.; Mienert, B.; Xiao, Y.; Guo, Y.; Sturhahn, W.; Cramer, S. P.; Wieghardt, K.; **Neese, F.**, Characterization of a genuine Iron(V)-nitrido species by nuclear resonant vibrational spectroscopy coupled to density functional calculations. *J. Am. Chem. Soc.* **2007,** *129* (36), 11053-11060.

115. **Neese, F.**; Schwabe, T.; Grimme, S., Analytic derivatives for perturbatively corrected "double hybrid" density functionals: Theory, implementation, and applications. *J. Chem. Phys.* **2007,** *126* (12), 124115.

114. **Neese, F.**; Petrenko, T.; Ganyushin, D.; Olbrich, G., Advanced aspects of ab initio theoretical optical spectroscopy of transition metal complexes: Multiplets, spin-orbit coupling and resonance Raman intensities. *Coord. Chem. Rev.* **2007,** *251* (3-4), 288-327.

113. **Neese, F.**, Quantum Chemical Approaches to Spin-Hamiltonian Parameters. In *Electron Paramag. Reson.*, Gilbert, B. C.; Davies, M. B.; Murphy, D. M., Eds. Royal Society of Chemistry: **2007**; Vol. 20, pp 73-95.

112. **Neese, F.**, Analytic derivative calculation of electronic g-tensors based on multireference configuration interaction wavefunctions. *Mol. Phys.* **2007,** *105* (19-22), 2507-2514.

111. **Neese, F.**, Calculation of the zero-field splitting tensor on the basis of hybrid density functional and Hartree-Fock theory. *J. Chem. Phys.* **2007,** *127* (16), 164112.

110. Muresan, N.; Chlopek, K.; Weyhermuller, T.; **Neese, F.**; Wieghardt, K., Bis(r-diimine)nickel Complexes: Molecular and Electronic Structure of Three Members of the Electron-Transfer Series $[Ni(L)_2]^z$ (z) 0, 1+, 2+) (L) 2-Phenyl-1,4-bis(isopropyl)-1,4-diazabutadiene). A Combined Experimental and Theoretical Study. *Inorg. Chem.* **2007,** *46* (13), 5327-5337.

109. Lehnert, N.; Cornelissen, U.; **Neese, F.**; Ono, T.; Noguchi, Y.; Okamoto, K.-I.; Fujisawa, K., Synthesis and spectroscopic characterization of copper(II)-nitrito complexes with hydrotris(pyrazolyl)borate and related coligands. *Inorg. Chem.* **2007,** *46* (10), 3916-3933.

108. Kossmann, S.; Kirchner, B.; **Neese, F.**, Performance of modern density functional theory for the prediction of hyperfine structure: meta-GGA and double hybrid functionals. *Mol. Phys.* **2007,** *105* (15-16), 2049-2071.

107. Kokatam, S.; Ray, K.; Pap, J.; Bill, E.; Geiger, W. E.; LeSuer, R. J.; Rieger, P. H.; Weyhermuller, T.; **Neese, F.**; Wieghardt, K., Molecular and Electronic Structure of Square-Planar Gold Complexes Containing Two 1,2-Di(4-tert-butylphenyl)ethylene-1,2-dithiolato Ligands: $[Au(^2L)_2]^{1+/0/1-/2-}$. A Combined Experimental and Computational Study. *Inorg. Chem.* **2007,** *46* (4), 1100-1111.

106. Kirchner, B.; Wennmohs, F.; Ye, S.; **Neese, F.**, Theoretical bioinorganic chemistry: the electronic structure makes a difference. *Curr. Opin. Chem. Biol.* **2007,** *11* (2), 134-141.

105. Grimme, S.; **Neese, F.**, Double-hybrid density functional theory for excited electronic states of molecules. *J. Chem. Phys.* **2007,** *127* (15), 154116.

104. Duboc, C.; Phoeung, T.; Zein, S.; Pecaut, J.; Collomb, M.-N.; **Neese, F.**, Origin of the zero-field splitting in mononuclear octahedral dihalide Mn-II complexes: An investigation by multifrequency high-field electron paramagnetic resonance and density functional theory. *Inorg. Chem.* **2007,** *46* (12), 4905-4916.

103. Chlopek, K.; Muresan, N.; **Neese, F.**; Wieghardt, K., Electronic structures of five-coordinate complexes of iron containing zero, one, or two π-radical ligands: A broken-

symmetry density functional theoretical study. *Chem. Eur. J.* **2007,** *13* (30), 8391-8403.

102. Carmieli, R.; Larsen, T. M.; Reed, G. H.; Zein, S.; **Neese, F.**; Goldfarb, D., The catalytic Mn^{2+} sites in the enolase-inhibitor complex: Crystallography, single-crystal EPR, and DFT calculations. *J. Am. Chem. Soc.* **2007,** *129* (14), 4240-4252.

101. Benisvy, L.; Hammond, D.; Parker, D. J.; Davies, E. S.; Garner, C. D.; McMaster, J.; Wilson, C.; **Neese, F.**; Bothe, E.; Bittl, R.; Teutloff, C., Insights into the nature of the hydrogen bonding of Tyr_{272} in apo-galactose oxidase. *J. Inorg. Biochem.* **2007,** *101* (11-12), 1859-1864.

100. Ye, S.; **Neese, F.**, Spectroscopic and Quantum Chemical Studies on the Electronic Structures of Transition-Metal Complexes With Coordinated Radicals. *ChemTracts* **2006,** *19* (2), 77-86.

99. Sinnecker, S.; Rajendran, A.; Klamt, A.; Diedenhofen, M.; **Neese, F.**, Calculation of solvent shifts on electronic g-tensors with the conductor-like screening model (COSMO) and its self-consistent generalization to real solvents (Direct COSMO-RS). *J. Phys. Chem. A* **2006,** *110* (6), 2235-2245.

98. Sinnecker, S.; **Neese, F.**, QM/MM calculations with DFT for taking into account protein effects on the EPR and optical spectra of metalloproteins. Plastocyanin as a case study. *J. Comput. Chem.* **2006,** *27* (12), 1463-1475.

97. Sinnecker, S.; **Neese, F.**, Spin-spin contributions to the zero-field splitting tensor in organic triplets, carbenes and biradicalss - A density functional and ab initio study. *J. Phys. Chem. A* **2006,** *110* (44), 12267-12275.

96. Petrenko, T.; Ray, K.; Wieghardt, K. E.; **Neese, F.**, Vibrational markers for the open-shell character of transition metal bis-dithiolenes: An infrared, resonance Raman, and quantum chemical study. *J. Am. Chem. Soc.* **2006,** *128* (13), 4422-4436.

95. Patra, A. K.; Bill, E.; Bothe, E.; Chlopek, K.; **Neese, F.**; Weyhermueller, T.; Stobie, K.; Ward, M. D.; McCleverty, J. A.; Wieghardt, K., Electronic structure of mononuclear bis(1,2-diaryl-1,2-ethylenedithiolato)iron complexes containing a fifth cyanide or phosphite ligand: A combined experimental and computational study. *Inorg. Chem.* **2006,** *45* (19), 7877-7890.

94. **Neese, F.**; Schmatz, S.; Hättig, C., Theoretische Chemie 2005. *Nachr. Chem.* **2006,** *54* (3), 276-281.

93. **Neese, F.**, The Yandulov/Schrock cycle and the nitrogenase reaction: Pathways of nitrogen fixation studied by density functional theory. *Angew. Chem. Int. Ed./Angew. Chem.* **2006,** *45/118* (2), 196-199/202-205.

92. **Neese, F.**, Theoretical spectroscopy of model-nonheme $[Fe(IV)OL_5]^{2+}$ complexes in their lowest triplet and quintet states using multireference ab initio and density functional theory methods. *J. Inorg. Biochem.* **2006,** *100* (4), 716-726.

91. **Neese, F.**, Importance of direct spin-spin coupling and spin-flip excitations for the zero-field splittings of transition metal complexes: A case study. *J. Am. Chem. Soc.* **2006,** *128*

(31), 10213-10222.

90. **Neese, F.**, A critical evaluation of DFT, including time-dependent DFT, applied to bioinorganic chemistry. *J. Biol. Inorg. Chem.* **2006,** *11* (6), 702-711.

89. Kapre, R.; Ray, K.; Sylvestre, I.; Weyhermueller, T.; George, S. D.; **Neese, F.**; Wieghardt, K., Molecular and electronic structures of oxo-bis(benzene-1,2-dithiolato)chromate(V) monoanions. A combined experimental and density functional study. *Inorg. Chem.* **2006,** *45* (9), 3499-3509.

88. Kababya, S.; Nelson, J.; Calle, C.; **Neese, F.**; Goldfarb, D., Electronic structure of binuclear mixed valence copper azacryptates derived from integrated advanced EPR and DFT calculations. *J. Am. Chem. Soc.* **2006,** *128* (6), 2017-2029.

87. Ganyushin, D.; **Neese, F.**, First-principles calculations of zero-field splitting parameters. *J. Chem. Phys.* **2006,** *125* (2), 024103.

86. Chlopek, K.; Bothe, E.; **Neese, F.**; Weyhermuller, T.; Wieghardt, K., Molecular and electronic structures of tetrahedral complexes of nickel and cobalt containing N,N '-disubstituted, bulky o-diiminobenzosemiquinonate(1-) pi-radical ligands. *Inorg. Chem.* **2006,** *45* (16), 6298-6307.

85. Chalupsky, J.; **Neese, F.**; Solomon, E. I.; Ryde, U.; Rulisek, L., Multireference ab initio calculations on reaction intermediates of the multicopper oxidases. *Inorg. Chem.* **2006,** *45* (26), 11051-11059.

84. Berry, J. F.; Bill, E.; Garcia-Serres, R.; **Neese, F.**; Weyhermuller, T.; Wieghardt, K., Effect of N-methylation of macrocyclic amine ligands on the spin state of iron(III): A tale of two fluoro complexes. *Inorg. Chem.* **2006,** *45* (5), 2027-2037.

83. Berry, J. F.; Bill, E.; Bothe, E.; **Neese, F.**; Wieghardt, K., Octahedral non-heme oxo and non-oxo Fe(IV) complexes: An experimental/theoretical comparison. *J. Am. Chem. Soc.* **2006,** *128* (41), 13515-13528.

82. Berry, J. F.; Bill, E.; Bothe, E.; George, S. D.; Mienert, B.; **Neese, F.**; Wieghardt, K., An octahedral coordination complex of iron(VI). *Science* **2006,** *312* (5782), 1937-1941.

81. Bart, S. C.; Chlopek, K.; Bill, E.; Bouwkamp, M. W.; Lobkovsky, E.; **Neese, F.**; Wieghardt, K.; Chirik, P. J., Electronic structure of bis(imino)pyridine iron dichloride, monochloride, and neutral ligand complexes: A combined structural, spectroscopic, and computational study. *J. Am. Chem. Soc.* **2006,** *128* (42), 13901-13912.

80. Zhu, W. F.; Marr, A. C.; Wang, Q.; **Neese, F.**; Spencer, D. J. E.; Blake, A. J.; Cooke, P. A.; Wilson, C.; Schroder, M., Modulation of the electronic structure and the Ni-Fe distance in heterobimetallic models for the active site in NiFe hydrogenase. *Proceedings of the National Academy of Sciences of the United States of America* **2005,** *102* (51), 18280-18285.

79. Wunsch, P.; Korner, H.; **Neese, F.**; van Spanning, R. J. M.; Kroneck, P. M. H.; Zumft, W. G., NosX function connects to nitrous oxide (N_2O) reduction by affecting the Cu_Z center of NosZ and its activity in vivo. *FEBS Letters* **2005,** *579* (21), 4605-4609.

78. Wanko, M.; Hoffmann, M.; Strodel, P.; Koslowski, A.; Thiel, W.; **Neese, F.**; Frauenheim, T.; Elstner, M., Calculating absorption shifts for retinal proteins: Computational challenges. *Journal of Physical Chemistry B* **2005,** *109* (8), 3606-3615.

77. van Gastel, M.; Fichtner, C.; **Neese, F.**; Lubitz, W., EPR experiments to elucidate the structure of the ready and unready states of the NiFe hydrogenase of Desulfolvibrio vulgaris Miyazaki F. *Biochemical Society Transactions* **2005,** *33*, 7-11.

76. Sinnecker, S.; Slep, L. D.; Bill, E.; **Neese, F.**, Performance of nonrelativistic and quasi-relativistic hybrid DFT for the prediction of electric and magnetic hyperfine parameters in Fe-57 Mossbauer spectra. *Inorg. Chem.* **2005,** *44* (7), 2245-2254.

75. Sinnecker, S.; **Neese, F.**; Lubitz, W., Dimanganese catalase-spectroscopic parameters from broken-symmetry density functional theory of the superoxidized Mn-III/Mn-IV state. *Journal of Biological Inorganic Chemistry* **2005,** *10* (3), 231-238.

74. Schöneboom, J. C.; **Neese, F.**; Thiel, W., Toward identification of the Compound I reactive intermediate in cytochrome P450 chemistry: A QM/MM study of its EPR and Mossbauer parameters. *J. Am. Chem. Soc.* **2005,** *127* (16), 5840-5853.

73. Ray, K.; Weyhermuller, T.; **Neese, F.**; Wieghardt, K., Electronic Structure of Square Planar Bis(benzene-1,2-dithiolato)metal Complexes $[M(L)_2]^z$ (z = 2−, 1−, 0; M = Ni, Pd, Pt, Cu, Au): An Experimental, Density Functional, and Correlated ab Initio Study. *Inorg. Chem.* **2005,** *44* (15), 5345-5360.

72. Ray, K.; Begum, A.; Weyhermuller, T.; Piligkos, S.; van Slageren, J.; **Neese, F.**; Wieghardt, K., The Electronic Structure of the Isoelectronic, Square-Planar Complexes [FeII(L)2]2- and [CoIII(LBu)2]- (L2- and (LBu)2- = Benzene-1,2-dithiolates): An Experimental and Density Functional Theoretical Study. *J. Am. Chem. Soc.* **2005,** *127* (12), 4403-4415.

71. Praneeth, V. K. K.; **Neese, F.**; Lehnert, N., Spin density distribution in five- and six-coordinate iron(II)-porphyrin NO complexes evidenced by magnetic circular dichroism spectroscopy. *Inorg. Chem.* **2005,** *44* (8), 2570-2572.

70. **Neese, F.**; Wolf, A.; Fleig, T.; Reiher, M.; Hess, B. A., Calculation of electric-field gradients based on higher-order generalized Douglas-Kroll transformations. *J. Chem. Phys.* **2005,** *122* (20), 204107.

69. **Neese, F.**, Efficient and accurate approximations to the molecular spin-orbit coupling operator and their use in molecular g-tensor calculations. *J. Chem. Phys.* **2005,** *122* (3), 034107.

68. Lin, P. C.; Puhar, A.; Turk, K.; Piligkos, S.; Bill, E.; **Neese, F.**; Steuber, J., A vertebrate-type ferredoxin domain in the Na^+-translocating NADH dehydrogenase from *Vibrio cholerae*. *J. Biol. Chem.* **2005,** *280* (24), 22560-22563.

67. Kennepohl, P.; **Neese, F.**; Schweitzer, D.; Jackson, H. L.; Kovacs, J. A.; Solomon, E. I., Spectroscopy of non-heme iron thiolate complexes: Insight into the electronic structure of the low-spin active site of nitrile hydratase. *Inorg. Chem.* **2005,** *44* (6), 1826-1836.

66. Fouqueau, A.; Casida, M. E.; Daku, L. M. L.; Hauser, A.; **Neese, F.**, Comparison of density functionals for energy and structural differences between the high- T-5(2g):(t(2g))(4)(e(g))(2) and low- (1)A(1g):(t(2g))(6)(e(g))(0) spin states of iron(II) coordination compounds. II. More functionals and the hexaminoferrous cation, Fe(NH3)(6)(2+). *J. Chem. Phys.* **2005,** *122* (4), 044110.

65. Cosper, M. M.; **Neese, F.**; Astashkin, A. V.; Carducci, M. D.; Raitsimring, A. M.; Enemark, J. H., Determination of the g-Tensors and Their Orientations for *cis,trans*-(L-N_2S_2)$Mo^{V}OX$ (X=Cl, SCH_2Ph) by Single-Crystal EPR Spectroscopy and Molecular Orbital Calculations. *Inorg. Chem.* **2005,** *44* (5), 1290-1301.

64. Blanchard, S.; **Neese, F.**; Bothe, E.; Bill, E.; Weyhermuller, T.; Wieghardt, K., Square planar vs tetrahedral coordination in diamagnetic complexes of nickel(II) containing two bidentate pi-radical monoanions. *Inorg. Chem.* **2005,** *44* (10), 3636-3656.

63. Benisvy, L.; Bittl, R.; Bothe, E.; Garner, C. D.; McMaster, J.; Ross, S.; Teutloff, C.; **Neese, F.**, Phenoxyl radicals hydrogen-bonded to imidazolium: Analogues of tyrosyl D of photosystem II: High-field EPR and DFT studies. *Angew. Chem. Int. Ed./Angew. Chem.* **2005,** *447/117* (33), 5314-5317/5448-5451.

62. Astashkin, A. V.; **Neese, F.**; Raitsimring, A. M.; Cooney, J. J. A.; Bultman, E.; Enemark, J. H., Pulsed EPR Investigations of Systems Modeling Molybdenum Enzymes: Hyperfine and Quadrupole Parameters of Oxo-^{17}O in $[Mo^{17}O(SPh)_4]^-$. *J. Am. Chem. Soc.* **2005,** *127* (47), 16713-16722.

61. Aliaga-Alcalde, M.; George, S. D.; Mienert, B.; Bill, E.; Wieghardt, K.; **Neese, F.**, The Geometric and Electronic Structure of $[(cyclam\text{-}acetato)Fe(N)]^+$: A Genuine Iron(v) Species with a Ground-State Spin S = 1/2. *Angew. Chem. Int. Ed./Angew. Chem.* **2005,** *44/117* (19), 2908-2912/2968-2972.

60. van Gastel, M.; Lubitz, W.; Lassmann, G.; **Neese, F.**, Electronic structure of the cysteine thiyl radical: A DFT and correlated ab initio study. *J. Am. Chem. Soc.* **2004,** *126* (7), 2237-2246.

59. Türk, K.; Puhar, A.; **Neese, F.**; Bill, E.; Fritz, G.; Steuber, J., NADH oxidation by the Na^+-translocating NADH:quinone oxidoreductase from *Vibrio cholerae* - Functional role of the NqrF subunit. *J. Biol. Chem.* **2004,** *279* (20), 21349-21355.

58. Sinnecker, S.; Reijerse, E.; **Neese, F.**; Lubitz, W., Hydrogen bond geometries from electron paramagnetic resonance and electron-nuclear double resonance parameters: Density functional study of quinone radical anion-solvent interactions. *J. Am. Chem. Soc.* **2004,** *126* (10), 3280-3290.

57. Sinnecker, S.; **Neese, F.**; Noodleman, L.; Lubitz, W., Calculating the electron paramagnetic resonance parameters of exchange coupled transition metal complexes using broken symmetry density functional theory: Application to a Mn(III)/Mn(IV) model compound. *J. Am. Chem. Soc.* **2004,** *126* (8), 2613-2622.

56. Serres, R. G.; Grapperhaus, C. A.; Bothe, E.; Bill, E.; Weyhermuller, T.; **Neese, F.**; Wieghardt, K., Structural, spectroscopic, and computational study of an octahedral, non-

heme {Fe-NO}(6-8) series: Fe(NO)(cyclam-ac) (2+/+/O). *J. Am. Chem. Soc.* **2004,** *126* (16), 5138-5153.

55. Paine, T. K.; Weyhermuller, T.; Slep, L. D.; **Neese, F.**; Bill, E.; Bothe, E.; Wieghardt, K.; Chaudhuri, P., Nonoxovanadium(IV) and oxovanadium(V) complexes with mixed O, X, O-donor ligands (X = S, Se, P, or PO). *Inorg. Chem.* **2004,** *43* (23), 7324-7338.

54. **Neese, F.**; Munzarová, M. L., Historical Aspects of EPR Parameter Calculations. In *Calculation of NMR and EPR Parameters: Theory and Applications*, Kaupp, M.; Bühl, M.; Malkin, V. G., Eds. Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim, FRG, **2004**; pp 21-32.

53. **Neese, F.**, Applications to EPR in Bioinorganic Chemistry. In *Calculation of NMR and EPR Parameters: Theory and Applications*, Kaupp, M.; Bühl, M.; Malkin, V. G., Eds. Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim, FRG, **2004**; pp 581-591.

52. **Neese, F.**, Zero-Field Splitting. In *Calculation of NMR and EPR Parameters: Theory and Applications*, Kaupp, M.; Bühl, M.; Malkin, V. G., Eds. Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim, FRG, **2004**; pp 541-564.

51. **Neese, F.**, Definition of corresponding orbitals and the diradical character in broken symmetry DFT calculations on spin coupled systems. *J. Phys. Chem. Solids* **2004,** *65* (4), 781-785.

50. **Neese, F.**, Sum-over-states based multireference ab initio calculation of EPR spin Hamiltonian parameters for transition metal complexes. A case study. *Magn. Reson. Chem.* **2004,** *42*, S187-S198.

49. Fouqueau, A.; Mer, S.; Casida, M. E.; Daku, L. M. L.; Hauser, A.; Mineva, T.; **Neese, F.**, Comparison of density functionals for energy and structural differences between the high-T-5(2g):(t(2g))(4)(e(g))(2) and low- (1)A(1g):(t(2g))(6)(e(g))(0) spin states of iron(II) coordination compounds. *J. Chem. Phys.* **2004,** *120* (20), 9473-9486.

48. Bill, E.; Bothe, E.; Chaudhuri, P.; Chlopek, K.; Herebian, D.; Kokatam, S.; Ray, K.; Weyhermuller, T.; **Neese, F.**; Wieghardt, K., Molecular and electronic structure of four- and five-coordinate cobalt complexes containing two o-phenylenediamine- or two o-aminophenol-type ligands at various oxidation levels: An experimental, density functional, and correlated ab initio study. *Chem. Eur. J.* **2004,** *11* (1), 204-224.

47. Baute, D.; Arieli, D.; Neese, F.; Zimmermann, H.; Weckhuysen, B. M.; Goldfarb, D., Carboxylate binding in copper histidine complexes in solution and in zeolite Y: X- and W-band pulsed EPR/ENDOR combined with DFT calculations. *J. Am. Chem. Soc.* **2004,** *126* (37), 11733-11745.

46. Solomon, E. I.; Davis, M. I.; **Neese, F.**; Pau, M. Y. M., Variable-Temperature Variable-Field Magnetic Circular Dichroism Combined with Electron Paramagnetic Resonance: Polarizations of Electronic Transitions in Solution. In *Paramagnetic Resonance of Metallobiomolecules*, Telser, J., Ed. ACS Symposium Series; American Chemical Society: Washington, D. C., **2003**; Vol. 858, pp 328-339.

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45. Slep, L. D.; **Neese, F.**, Bioinorganic reaction mechanisms: From high-valent iron to bioorganometallic chemistry. *Angew. Chem. Int. Ed./Angew. Chem.* **2003,** *42/115* (26), 2942-2945/3048-3051.

44. Slep, L. D.; Mijovilovich, A.; Meyer-Klaucke, W.; Weyhermuller, T.; Bill, E.; Bothe, E.; **Neese, F.**; Wieghardt, K., Mixed-Valent $\{Fe^{IV}(\mu\text{-}O)(\mu\text{-carboxylato})_2Fe^{III}\}^{3+}$ Core. *J. Am. Chem. Soc.* **2003,** *125* (50), 15554-15570.

43. **Neese, F.**; Solomon, E. I., Interpretation and Calculation of Spin-Hamiltonian Parameters in Transition Metal Complexes. In *Magnetism: Molecules to Materials IV: Nanosized Magnetic Materials*, MIller, J. S.; Drillon, M., Eds. Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim, FRG, **2003**; pp 345-466.

42. **Neese, F.**, Quantum chemical calculations of spectroscopic properties of metalloproteins and model compounds: EPR and Mossbauer properties. *Curr. Opin. Chem. Biol.* **2003,** *7* (1), 125-135.

41. **Neese, F.**, Metal and ligand hyperfine couplings in transition metal complexes: The effect of spin-orbit coupling as studied by coupled perturbed Kohn-Sham theory. *J. Chem. Phys.* **2003,** *118* (9), 3939-3948.

40. **Neese, F.**, Correlated ab initio calculation of electronic g-tensors using a sum over states formulation. *Chem. Phys. Lett.* **2003,** *380* (5-6), 721-728.

39. **Neese, F.**, A spectroscopy oriented configuration interaction procedure. *J. Chem. Phys.* **2003,** *119* (18), 9428-9443.

38. **Neese, F.**, An improvement of the resolution of the identity approximation for the formation of the Coulomb matrix. *J. Comput. Chem.* **2003,** *24* (14), 1740-1747.

37. Herebian, D.; Wieghardt, K. E.; **Neese, F.**, Analysis and Interpretation of Metal-Radical Coupling in a Series of Square Planar Nickel Complexes: Correlated Ab Initio and Density Functional Investigation of $[Ni(L^{ISQ})_2]$ (L^{ISQ}=3,5-di-tert-butyl-o-diiminobenzosemiquinonate(1-)). *J. Am. Chem. Soc.* **2003,** *125* (36), 10997-11005.

36. Herebian, D.; Bothe, E.; **Neese, F.**; Weyhermuller, T.; Wieghardt, K., Molecular and electronic structures of bis-(o-diiminobenzosemiquinonato)metal(II) complexes (Ni, Pd, Pt), their monocations and -anions, and of dimeric dications containing weak metal-metal bonds. *J. Am. Chem. Soc.* **2003,** *125* (30), 9116-9128.

35. Ghosh, P.; Bill, E.; Weyhermuller, T.; **Neese, F.**; Wieghardt, K., Noninnocence of the ligand glyoxal-bis(2-mercaptoanil). The electronic structures of Fe(gma) (2), Fe(gma)(py) center dot py, Fe(gma)(CN) (1-/0), Fe(gma)l , and Fe(gma)(PR3)n (n = 1, 2). Experimental and theoretical evidence for "excited state" coordination. *J. Am. Chem. Soc.* **2003,** *125* (5), 1293-1308.

34. Sun, X. R.; Chun, H.; Hildenbrand, K.; Bothe, E.; Weyhermuller, T.; **Neese, F.**; Wieghardt, K., *o*-Iminobenzosemiquinonato(1−) and *o*-Amidophenolato(2−) Complexes of Palladium(II) and Platinum(II): A Combined Experimental and Density Functional Theoretical Study. *Inorg. Chem.* **2002,** *41* (16), 4295-4303.

33. Steuber, J.; Rufibach, M.; Fritz, G.; **Neese, F.**; Dimroth, P., Inactivation of the Na^+-translocating NADH : ubiquinone oxidoreductase from *Vibrio alginolyticus* by reactive oxygen species. *Eur. J. Biochem.* **2002,** *269* (4), 1287-1292.

32. Rudolf, M.; Einsle, O.; **Neese, F.**; Kroneck, P. M. H., Pentahaem cytochrome c nitrite reductase: reaction with hydroxylamine, a potential reaction intermediate and substrate. *Biochem. Soc. Trans.* **2002,** *30*, 649-653.

31. **Neese, F.**; Olbrich, G., Efficient use of the resolution of the identity approximation in time-dependent density functional calculations with hybrid density functionals. *Chem. Phys. Lett.* **2002,** *362* (1-2), 170-178.

30. **Neese, F.**, Prediction and interpretation of the ^{57}Fe isomer shift in Mossbauer spectra by density functional theory. *Inorg. Chim. Acta* **2002,** *337*, 181-192.

29. Li, M.; Bonnet, D.; Bill, E.; **Neese, F.**; Weyhermuller, T.; Blum, N.; Sellman, D.; Wieghardt, K., Tuning the electronic structure of octahedral iron complexes FeL(X) (L=1-alkyl-4,7-bis(4-tert-butyl-2-mercaptobenzyl)-1,4,7-triazacyclononan e, X = Cl, CH3O, CN, NO). The S=1/2 reversible arrow S=3/2 spin equilibrium of FeLPr(NO). *Inorg. Chem.* **2002,** *41* (13), 3444-3456.

28. Lehnert, N.; **Neese, F.**; Ho, R. Y. N.; Que, L.; Solomon, E. I., Electronic structure and reactivity of low-spin Fe(III)-hydroperoxo complexes: Comparison to activated bleomycin. *J. Am. Chem. Soc.* **2002,** *124* (36), 10810-10822.

27. Epel, B.; Slutter, C. S.; **Neese, F.**; Kroneck, P. M. H.; Zumft, W. G.; Pecht, I.; Farver, O.; Lu, Y.; Goldfarb, D., Electron-mediating Cu-A Centers in proteins: A comparative high field H-1 ENDOR study. *J. Am. Chem. Soc.* **2002,** *124* (27), 8152-8162.

26. Einsle, O.; Messerschmidt, A.; Huber, R.; Kroneck, P. M. H.; **Neese, F.**, Mechanism of the six-electron reduction of nitrite to ammonia by cytochrome c nitrite reductase. *J. Am. Chem. Soc.* **2002,** *124* (39), 11737-11745.

25. Davis, M. I.; Orville, A. M.; **Neese, F.**; Zaleski, J. M.; Lipscomb, J. D.; Solomon, E. I., Spectroscopic and electronic structure studies of protocatechuate 3,4-dioxygenase: Nature of tyrosinate-Fe(III) bonds and their contribution to reactivity. *J. Am. Chem. Soc.* **2002,** *124* (4), 602-614.

24. Bachler, V.; Olbrich, G.; **Neese, F.**; Wieghardt, K., Theoretical evidence for the singlet diradical character of square planar nickel complexes containing two omicron-semiquinonato type ligands. *Inorg. Chem.* **2002,** *41* (16), 4179-4193.

23. **Neese, F.**, Theoretical study of ligand superhyperfine structure. Application to Cu(II) complexes. *J. Phys. Chem. A* **2001,** *105* (17), 4290-4299.

22. **Neese, F.**, Configuration interaction calculation of electronic g tensors in transition metal complexes. *Int. J. Quantum Chem.* **2001,** *83* (3-4), 104-114.

21. **Neese, F.**, Prediction of electron paramagnetic resonance g values using coupled perturbed Hartree-Fock and Kohn-Sham theory. *J. Chem. Phys.* **2001,** *115* (24), 11080-11096.

20. Grapperhaus, C. A.; Bill, E.; Weyhermuller, T.; **Neese, F.**; Wieghardt, K., Molecular and electronic structure of (MnN)-N-V(cyclam-acetato) PF6. A combined experimental and DFT study. *Inorg. Chem.* **2001,** *40* (17), 4191-4198.

19. Solomon, E. I.; Brunold, T. C.; Davis, M. I.; Kemsley, J. N.; Lee, S. K.; Lehnert, N.; **Neese, F.**; Skulan, A. J.; Yang, Y. S.; Zhou, J., Geometric and electronic structure/function correlations in non-heme iron enzymes. *Chem. Rev.* **2000,** *100* (1), 235-349.

18. **Neese, F.**; Zaleski, J. M.; Zaleski, K. L.; Solomon, E. I., Electronic structure of activated bleomycin: Oxygen intermediates in heme versus non-heme iron. *J. Am. Chem. Soc.* **2000,** *122* (47), 11703-11724.

17. **Neese, F.**, Approximate second-order SCF convergence for spin unrestricted wavefunctions. *Chem. Phys. Lett.* **2000,** *325* (1-3), 93-98.

16. Charnock, J. M.; Dreusch, A.; Korner, H.; **Neese, F.**; Nelson, J.; Kannt, A.; Michel, H.; Garner, C. D.; Kroneck, P. M. H.; Zumft, W. G., Structural investigations of the Cu_A centre of nitrous oxide reductase from *Pseudomonas stutzeri* by site-directed mutagenesis and X-ray absorption spectroscopy. *Eur. J. Biochem.* **2000,** *267* (5), 1368-1381.

15. **Neese, F.**; Solomon, E. I., MCD C-term signs, saturation behavior, and determination of band polarizations in randomly oriented systems with spin S >= 1/2. Applications to S = 1/2 and S = 5/2. *Inorg. Chem.* **1999,** *38* (8), 1847-1865.

14. **Neese, F.**; Hedman, B.; Hodgson, K. O.; Solomon, E. I., Relationship between the dipole strength of ligand pre-edge transitions and metal-ligand covalency. *Inorg. Chem.* **1999,** *38* (21), 4854-4860.

13. **Neese, F.**; Solomon, E. I., Detailed Spectroscopic and Theoretical Studies on $[Fe(EDTA)(O_2)]^{3-}$: Electronic Structure of the Side-on Ferric−Peroxide Bond and Its Relevance to Reactivity. *J. Am. Chem. Soc.* **1998,** *120* (49), 12829-12848.

12. **Neese, F.**; Solomon, E. I., Calculation of zero-field splittings, g-values, and the relativistic nephelauxetic effect in transition metal complexes. Application to high-spin ferric complexes. *Inorg. Chem.* **1998,** *37* (26), 6568-6582.

11. **Neese, F.**; Kappl, R.; Huttermann, J.; Zumft, W. G.; Kroneck, P. M. H., Probing the ground state of the purple mixed valence Cu(A) center in nitrous oxide reductase: a CW ENDOR (X-band) study of the ^{65}Cu, ^{15}N-histidine labeled enzyme and interpretation of hyperfine couplings by molecular orbital calculations. *J. Biol. Inorg. Chem.* **1998,** *3* (1), 53-67.

10. Solomon, E. I.; Zhou, J.; **Neese, F.**; Pavel, E. G., New insights from spectroscopy into the structure/function relationships of lipoxygenases. *Chemistry & Biology* **1997,** *4* (11), 795-808.

9. Schumacher, W.; **Neese, F.**; Hole, U.; Kroneck, P. M. H., Cytochrome c Nitrite Reductase and Nitrous Oxide Reductase: two Metalloenzymes of the Nitrogen Cycle with Novel Metal Sites. In *Transition Metals in Microbial Metabolism*, Winkelmann, G.; Carrano, C. J., Eds. Harwood Academic Publisher: **1997**; pp 329-356.

8. Kroneck, P. M. H.; Kastrau, D. H. W.; Schumacher, W.; Hole, U.; **Neese, F.**; Zumft, W. G.,

Novel Binuclear Metal Centers in Cytochrome c Nitrite Reductase and Nitrous Oxide Reductase: A Spectroscopic and Molecular Orbital Study. In *Bioinorganic Chemistry - Transition Metals in Biology and their Coordination Chemistry* Trautwein, A. X., Ed. Wiley-VCH: Weinheim, **1997**; pp 710-724.

7. Farrar, J. A.; Grinter, R.; **Neese, F.**; Nelson, J.; Thomson, A. J., The electronic structure of the mixed-valence copper dimer $[Cu_2\{N(CH_2CH_2N{=}CHCH{=}NCH_2CH_2)_3N\}]^{3+}$. *J. Chem. Soc., Dalton Trans.* **1997**, 4083-4087.

6. **Neese, F.**; Zumft, W. G.; Antholine, W. E.; Kroneck, P. M. H., The Purple Mixed-Valence CuA Center in Nitrous-oxide Reductase: EPR of the Copper-63-, Copper-65-, and Both Copper-65- and [15N]Histidine-Enriched Enzyme and a Molecular Orbital Interpretation. *J. Am. Chem. Soc.* **1996,** *118* (36), 8692-8699.

5. Farrar, J. A.; **Neese, F.**; Lappalainen, P.; Kroneck, P. M. H.; Saraste, M.; Zumft, W. G.; Thomson, A. J., The electronic structure of Cu_A: A novel mixed-valence dinuclear copper electron-transfer center. *J. Am. Chem. Soc.* **1996,** *118* (46), 11501-11514.

4. Singh, R. J.; Hogg, N.; **Neese, F.**; Joseph, J.; Kalyanaraman, B., Trapping of nitric oxide formed during photolysis of sodium-nitroprusside in aqueous and lipid phases: an electron spin resonance study. *Photochemistry and Photobiology* **1995,** *61* (4), 325-330.

3. **Neese, F.**, The Program EPR. *Quantum Chemistry Program Exchange Bulletin* **1995,** *15* (1), 5.

2. Hogg, N.; Singh, R. J.; Joseph, J.; **Neese, F.**; Kalyanaraman, B., Reactions of Nitric Oxide with Nitronyl Nitroxides and Oxygen: Prediction of Nitrite and Nitrate Formation by Kinetic Simulation. *Free Rad. Res.* **1995,** *22* (1), 47-56.

1. Kroneck, P. M. H.; Antholine, W. E.; Koteich, H.; Kastrau, D. H. W.; **Neese, F.**; Zumft, W. G., The EPR detectable Copper of Nitrous Oxide Reductase as a Model for CuA in Cytochrome c Oxidase: A Multifrequency Electron Paramagnetic Resonance Investigation. In *Bioinorganic Chemistry of Copper*, Karlin, K. D.; Tyeklar, Z., Eds. Chapman and Hall Inc.: New York, **1993**; pp 419-426.