

Dimitrios Maganas – List of publications

Researcher ID: [E-9031-2013](#) ORCID: [0000-0002-1550-5162](#)

Publications 2019

38. Dittmer, A.; Izsák, R. b.; Neese, F.; Maganas, D., Accurate Band Gap Predictions of Semiconductors in the Framework of the Similarity Transformed Equation of Motion Coupled Cluster Theory. *Inorganic chemistry* **2019**.
37. 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 $[\text{Fe}^{(\text{II/III})}\text{Cl}_4]^{2-/1-}$ Molecules. *The Journal of chemical physics* **2019**, 150, 104106.
36. Neese, F.; Atanasov, M.; Bistoni, G.; Maganas, D.; Ye, S., Chemistry and Quantum Mechanics in 2019: Give Us Insight and Numbers. *Journal of the American Chemical Society* **2019**, 141, 2814-2824.

Publications 2018

35. 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. *Journal of chemical theory and computation* **2018**, 14, 3686-3702.
34. 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. *The Journal of Physical Chemistry A* **2018**, 122, 1215-1227.
33. 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. *Journal of chemical theory and computation* **2018**, 14, 4320-4334.
32. 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. *Inorganic Chemistry* **2018**, 57, 6421-6438

Publications 2006-2017

31. Suturina, E. A.; Nehr Korn, J.; Zadrozny, J. M.; Liu, J.; Atanasov, M.; Weyhermüller, T.; Maganas, D.; Hill, S.; Schnegg, A.; Bill, E., Magneto-Structural Correlations in Pseudotetrahedral Forms of the $[\text{Co}(\text{SPh})_4]_2$ Complex Probed by Magnetometry, Mcd Spectroscopy, Advanced Epr Techniques, and Ab Initio Electronic Structure Calculations. *Inorganic chemistry* **2017**, 56, 3102-3118.

30. 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. *Inorganic chemistry* **2017**, *56*, 11819-11836.
29. Kubas, A.; Noak, J.; Trunschke, A.; Schlögl, 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 MoVO_x. *Chemical science* **2017**, *8*, 6338-6353.
28. Van Kuiken, B. E.; Hahn, A. W.; Maganas, D.; DeBeer, S., Measuring Spin-Allowed and Spin-Forbidden d–d Excitations in Vanadium Complexes with 2p3d Resonant Inelastic X-Ray Scattering. *Inorganic chemistry* **2016**, *55*, 11497-11501.
27. Rees, J. A.; Wandzilak, A.; Maganas, D.; Wurster, N. I. C.; Hugenbruch, S.; Kowalska, J. K.; Pollock, C. J.; Lima, F. A.; Finkelstein, K. D.; DeBeer, S., Experimental and Theoretical Correlations between Vanadium K-Edge X-Ray Absorption and K α Emission Spectra. *JBIC Journal of Biological Inorganic Chemistry* **2016**, *21*, 793-805.
26. Maganas, D.; Trunschke, A.; Schlögl, R.; Neese, F., A Unified View on Heterogeneous and Homogeneous Catalysts through a Combination of Spectroscopy and Quantum Chemistry. *Faraday discussions* **2016**, *188*, 181-197.
25. 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). *The journal of physical chemistry letters* **2016**, *7*, 4207-4212.
24. Campbell, C.; van Santen, R.; Stamatakis, M.; Collis, N.; Freund, H.-J.; Plaisance, C.; Sauer, J.; Garrett, B.; Gross, E.; Kotarba, A., Catalyst Design from Theory to Practice: General Discussion. *Faraday discussions* **2016**, *188*, 279-307.
23. 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. *Inorganic chemistry* **2015**, *54*, 9948-9961.
22. Jiang, S.-D.; Maganas, D.; Levesanos, N.; Ferentinos, E.; Haas, S.; Thirunavukkuarasu, K.; Krzystek, J.; Dressel, M.; Bogani, L.; Neese, F., Direct Observation of Very Large Zero-Field Splitting in a Tetrahedral Ni^{II}Se₄ Coordination Complex. *Journal of the American Chemical Society* **2015**, *137*, 12923-12928.
21. 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.
20. Martin-Diaconescu, V.; Gennari, M.; Gerey, B.; Tsui, E.; Kanady, J.; Tran, R.; Pécaut, J.; Maganas, D.; Krewald, V.; Gouré, E., Ca K-Edge Xas as a Probe of Calcium Centers in Complex Systems. *Inorganic chemistry* **2014**, *54*, 1283-1292.

19. 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. *Physical Chemistry Chemical Physics* **2014**, *16*, 264-276.
18. Maganas, D.; Kristiansen, P.; Duda, L. C.; Knop-Gericke, A.; DeBeer, S.; Schlögl, 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*, 20163-20175.
17. Maganas, D.; DeBeer, S.; Neese, F., Restricted Open-Shell Configuration Interaction Cluster Calculations of the L-Edge X-Ray Absorption Study of TiO₂ and CaF₂ Solids. *Inorganic chemistry* **2014**, *53*, 6374-6385.
16. Tzima, T. D.; Ferentinos, E.; Maganas, D.; Melissas, V. S.; Sanakis, Y.; Kyritsis, P., Electronic and Magnetic Properties of the Binuclear [Mn₂{(OPPh₂)₂}]₄ Complex, as Revealed by Magnetometry, Epr and Density Functional Broken-Symmetry Studies. *Polyhedron* **2013**, *52*, 706-712.
15. 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. *The Journal of chemical physics* **2013**, *138*, 204101.
14. 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 V₂O₅ Using Local Pair Natural Orbital Coupled Cluster Theory and Spin-Orbit Coupled Configuration Interaction Approaches. *Physical Chemistry Chemical Physics* **2013**, *15*, 7260-7276.
13. Grigoropoulos, A.; Maganas, D.; Symeonidis, D.; Giastas, P.; Cowley, A. R.; Kyritsis, P.; Pneumatikakis, G., Synthesis of Chalcogenidoimidodiphosphinato-Rh^I Complexes and DFT Investigation of Their Catalytic Activation in Olefin Hydroformylation. *European Journal of Inorganic Chemistry* **2013**, *2013*, 1170-1183.
12. Mathies, G.; Chatziefthimiou, S. D.; Maganas, D.; Sanakis, Y.; Sottini, S.; Kyritsis, P.; Groenen, E. J. J., High-Frequency EPR Study of the High-Spin Fe^{II} Complex Fe[(SPPH₂)₂]₂. *Journal of Magnetic Resonance* **2012**, *224*, 94-100.
11. 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}{(OPPh₂)(EPPH₂)N}₂(Sol)₂] Complexes (E= S, Se; Sol= DMF, THF) by Magnetometry, HFEPR, and Ab Initio Quantum Chemistry. *Inorganic chemistry* **2012**, *51*, 7218-7231.
10. Maganas, D.; Sottini, S.; Kyritsis, P.; Groenen, E. J. J.; Neese, F., Theoretical Analysis of the Spin Hamiltonian Parameters in Co (II) S₄ Complexes, Using Density Functional Theory and Correlated Ab Initio Methods. *Inorganic chemistry* **2011**, *50*, 8741-8754.

9. Ferentinos, E.; Maganas, D.; Raptopoulou, C. P.; Terzis, A.; Psycharis, V.; Robertson, N.; Kyritsis, P., Conversion of Tetrahedral to Octahedral Structures Upon Solvent Coordination: Studies on the $M[(OPPh_2)(SePPh_2)N]_2$ ($M = Co, Ni$) and $[Ni\{(OPPh_2)(EPPh_2)N\}_2(DMF)_2](E = S, Se)$ Complexes. *Dalton Transactions* **2011**, 40, 169-180.
8. Maganas, D.; Grigoropoulos, A.; Staniland, S. S.; Chatziefthimiou, S. D.; Harrison, A.; Robertson, N.; Kyritsis, P.; Neese, F., Tetrahedral and Square Planar $Ni[(SPR_2)_2]_2$ Complexes, $R = Ph$ & iPr Revisited: Experimental and Theoretical Analysis of Interconversion Pathways, Structural Preferences, and Spin Delocalization. *Inorganic chemistry* **2010**, 49, 5079-5093.
7. Sottini, S.; Mathies, G.; Gast, P.; Maganas, D.; Kyritsis, P.; Groenen, E. J. J., A W-Band Pulsed EPR/Endor Study of $Co^{II}S_4$ Coordination in the $Co[(SPPh_2)(SP^iPr_2)N]_2$ Complex. *Physical Chemistry Chemical Physics* **2009**, 11, 6727-6732.
6. Maganas, D.; Milikisyants, S.; Rijnbeek, J. M. A.; Sottini, S.; Levesanos, N.; Kyritsis, P.; Groenen, E. J. J., A Multifrequency High-Field Electron Paramagnetic Resonance Study of $Co^{II}S_4$ Coordination. *Inorganic chemistry* **2009**, 49, 595-605.
5. Maganas, D.; Kyritsis, P.; Aullón, G.; Alvarez, S., Ligands That Enforce Unnatural Stereospinomers. *Dalton Transactions* **2008**, 2235-2237.
4. Levesanos, N.; Robertson, S. D.; Maganas, D.; Raptopoulou, C. P.; Terzis, A.; Kyritsis, P.; Chivers, T., $Ni[(EP^iPr_2)_2]_2$ Complexes: Stereoisomers ($E = Se$) and Square-Planar Coordination ($E = Te$). *Inorganic chemistry* **2008**, 47, 2949-2951.
3. Maganas, D., Covalency of M-S in Transition Metal Complexes with Ms_4 Coordination, Phd Thesis. **2007**.
2. Maganas, D., *DFT Studies on the Electronic Properties of Multinuclear Complexes Involving Cu (I) Ions and Chelate Ligands Containing Either S, Se or Te in the Coordination Sphere*; ISBD 978-88-86037-21-1, 2007; Vol. HPC-Europa, Science and supercomputing in Europe.
1. Maganas, D.; Staniland, S. S.; Grigoropoulos, A.; White, F.; Parsons, S.; Robertson, N.; Kyritsis, P.; Pneumatikakis, G., Structural, Spectroscopic and Magnetic Properties of $M[R_2P(E)NP(E)R_2]_2$ Complexes, $M = Co, Mn$, $E = S, Se$ and $R = Ph$ or iPr . Covalency of Ms Bonds from Experimental Data and Theoretical Calculations. *Dalton Transactions* **2006**, 2301-2315.