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Professional Appointments

2017 – present	Chair of Chemistry	University of Louisville
2011 – present	Professor of Chemistry	University of Louisville
2015 – 2017	Vice Chair of Chemistry	University of Louisville
2013 – present	Visiting Scientist-Regenerative Medicine Research Center	West China Hospital, Sichuan University
2009 – 2012	Vice Chair of Chemistry	University of Louisville
2005 – 2011	Associate Professor of Chemistry	University of Louisville
2005 – 2010	Chemistry Director of Graduate Studies	University of Louisville
2000 – present	Member of Graduate Faculty	University of Louisville
2000 – 2005	Assistant Professor of Chemistry	University of Louisville

Education

1998 – 2000	Alexander von Humboldt Postdoctoral Fellow Max Planck Institut for Bioinorganic Chemistry (née Strahlenchemie) Mülheim, Germany Advisor: Prof. Karl Wieghardt
1994 – 1998	Ph.D. in inorganic chemistry Texas A&M University College Station, TX Advisor: Prof. Marcetta Y. Darensbourg
1990 – 1994	B.S. in Chemistry, <i>Summa Cum Laude</i> , minor in Economics Southern Illinois University at Edwardsville Edwardsville, IL Advisor: Prof. Thomas Getman

Honors and Awards

2019-2020	ACC-Academic Leadership Network Participant
2017	Distinguished Faculty Award for Outstanding Scholarship, Research & Creative Activity in Applied Sciences – College of Arts and Sciences
2017	Research Exemplar Award
2011	Provost Award for Exemplary Advising
2001	Ralph E. Powe Junior Faculty Enhancement Award
1998 – 2000	Alexander von Humboldt Postdoctoral Fellowship
1997 – 1998	Dow Teacher/Scholar Fellowship, Texas A&M
1996 – 1997	NIH Chemistry/Biology Interface Training Program Fellowship, Texas A&M
1994 – 1996	Industry-University Cooperative Chemistry Program Fellowship, Texas A&M
1994	Medallion of Lincoln, Academy of Lincoln
1993	Council on Undergraduate Research Fellowship, SIUE

Professional Societies and Activities

2015	Pacificchem 2015 – Symposium Co-Organizer
2007	Local Organizing Committee – Kentucky Academy of Science Annual Meeting
2005	Invited Participant – Tenth Annual Congressional Visits Day
2001 – 2004	Founder and Chair: Kentuckiana Undergraduate Research Symposium
2001 –	Member of Society of Bioinorganic Chemistry
2000 – 2005	Member of Council on Undergraduate Research
1996 –	Member of the American Chemical Society

Publications (h-index: 21) (citations: total > 1700)

1. Grapperhaus, C. A.; Darensbourg, M. Y.; Sumner, L. W.; Russell, D. H. "Template effect for O₂ addition across cis-sulfur sites in nickel dithiolates" *J. Am. Chem. Soc.* **1996**, *118*, 1791-1792
2. Grapperhaus, C. A.; Maguire, M. J.; Tuntulani, T.; Darensbourg, M. Y. "Singlet oxygen and the production of sulfur oxygenates of nickel(II) and palladium(II) thiolates" *Inorg. Chem.* **1997**, *36*, 1860-1866
3. Mills, D. K.; Font, I.; Farmer, P. J.; Hsiao, Y. M.; Tuntulani, T.; Buonomo, R. M.; Goodman, D. C.; Musie, G.; Grapperhaus, C. A.; Maguire, M. J.; Lai, C. H.; Hatley, M. L.; Smees, J. J.; Bellefeuille, J. A.; Darensbourg, M. Y. "1,5-Diazacyclooctane, Pendant Arm Thiolato Derivatives and [(N,N'-bis(2-mercaptoethyl)-1,5-diazacyclooctanato)Nickel(II)]" *Inorg. Synth.* **1998**, *37*, 4052-4058
4. Grapperhaus, C. A.; Tuntulani, T.; Reibenspies, J. H.; Darensbourg, M. Y. "Methylation of tethered thiolates in (bme-daco)Zn₂ and (bme-daco)Cd₂ as a model of zinc sulfur-methylation proteins" *Inorg. Chem.* **1998**, *37*, 4052-4058
5. Bellefeuille, J. A.; Grapperhaus, C. A.; Buonomo, R. M.; Reibenspies, J. H.; Darensbourg, M. Y. "Alkylation-induced O-atom rearrangement in nickel S-oxygenates" *Organometallics* **1998**, *17*, 4813-4821
6. Grapperhaus, C. A.; Darensbourg, M. Y. "Oxygen Capture By Sulfur In Nickel Thiolates" *Acc. Chem. Res.* **1998**, *31*, 451-459
7. Grapperhaus, C. A.; Bill, E.; Wieghardt, K. "Ozone oxidation of iron(III) in a monofunctionalized cyclam: Spectroscopic characterization of high valent iron species" *J. Inorg. Biochem.* **1999**, *74*, 146-146
8. Grapperhaus, C. A.; Bellefeuille, J. A.; Reibenspies, J. H.; Darensbourg, M. Y. "Synthesis and dimer cleavage reactions of the N₂S thiolate bridged dimer [(mmp-dach)₂Ni]₂Cl₂" *Inorg. Chem.* **1999**, *38*, 3698-3703
9. Bellefeuille, J. A.; Grapperhaus, C. A.; Derecskei-Kovacs, A.; Reibenspies, J. H.; Darensbourg, M. Y. "Correlation of electrochemistry, nucleophilicity and density functional calculations of the cis-dithiolate (bme*-daco)Ni" *Inorg. Chim. Acta* **2000**, *300*, 73-81
10. Grapperhaus, C. A.; Mienert, B.; Bill, E.; Weyhermuller, T.; Wieghardt, K. "Mononuclear (nitrido)iron(V) and (oxo)iron(IV) complexes via photolysis of [(cyclam-acetato)Fe^{III}N₃]⁺ and ozonolysis of [(cyclam-acetato)Fe^{III}O₃SCF₃]⁺ in water/acetone mixtures" *Inorg. Chem.* **2000**, *39*, 5306-5317
11. Smees, J. J.; Miller, M. L.; Grapperhaus, C. A.; Reibenspies, J. H.; Darensbourg, M. Y. "Subtle bite-angle influences on N₂S₂Ni complexes" *Inorg. Chem.* **2001**, *40*, 3601-3605 (DOI 10.1021/ic0008619).
12. Grapperhaus, C. A.; Bill, E.; Weyhermuller, T.; Neese, F.; Wieghardt, K. "Molecular and electronic structure of [Mn^VN(cyclam-acetato)PF₆]. A combined experimental and DFT study" *Inorg. Chem.* **2001**, *40*, 4191-4198 (10.1021/ic001370r).

13. Grapperhaus, C. A.; Patra, A. K.; Poturovic, S. "Synthetic Models of Nitrile Hydratase" *J. Inorg. Biochem.* **2001**, *86*, 240-240
14. Grapperhaus, C. A.; Patra, A. K.; Mashuta, M. S. "First {Fe-NO}⁶ complex with an N₂S₃Fe-NO core as a model of NO-inactivated iron-containing nitrile hydratase. Are thiolates and thioethers equivalent donors in low-spin iron complexes?" *Inorg. Chem.* **2002**, *41*, 1039-1041
15. Kaasjager, V. E.; Bouwman, E.; Gorter, S.; Reedijk, J.; Grapperhaus, C. A.; Reibenspies, J. H.; Smee, J. J.; Darensbourg, M. Y.; Derecskei-Kovacs, A.; Thomson, L. M. "Unique reactivity of a tetradentate N₂S₂ complex of nickel: Intermediates in the production of sulfur oxygenates" *Inorg. Chem.* **2002**, *41*, 1837-1844 (10.1021/ic010784x).
16. Mashuta, M. S.; Pimenov, K. V.; Grapperhaus, C. A. "cis-Dioxocyclam" *Acta Crystallographica Section C-Crystal Structure Communications* **2002**, *58*, O226-O227 (Doi 10.1107/S0108270102003165).
17. Grapperhaus, C. A.; Li, M.; Mashuta, M. S. "1,5-Bis(benzothiazolyl)-3-thiapentane and its asymmetric dinuclear Ag(I) complex with three distinct intermolecular-stacking interactions" *Chem. Commun.* **2002**, 1792-1793
18. Grapperhaus, C. A.; Poturovic, S.; Mashuta, M. S. "Dichloromethane alkylates a trithiolato-ruthenium complex to yield a methylene-bridged thioether core. Synthesis and structural comparison to the thiolato-ruthenium precursor" *Inorg. Chem.* **2002**, *41*, 4309-4311
19. Grapperhaus, C. A.; Li, M.; Patra, A. K.; Poturovic, S.; Kozlowski, P. M.; Zgierski, M. Z.; Mashuta, M. S. "Synthesis and characterization of N₂S₃X-Fe models of iron-containing nitrile hydratase" *Inorg. Chem.* **2003**, *42*, 4382-4388
20. Grapperhaus, C. A.; Li, M.; Gibson, E. R.; Mashuta, M. S. "Hydrogen-bond networks in the mono- and diprotonated cyclic diamine 9aneN₂S" *J. Chem. Crystallogr.* **2004**, *34*, 5-11
21. Grapperhaus, C. A.; Mullins, C. S.; Kozlowski, P. M.; Mashuta, M. S. "Synthesis and oxygenation of a nickel(II) and zinc(II) dithiolate: An experimental and theoretical comparison" *Inorg. Chem.* **2004**, *43*, 2859-2866
22. Grapperhaus, C. A.; Poturovic, S. "Electrochemical investigations of the tris(2-(diphenylphosphino)thiaphenolato)ruthenate(II) monoanion reveal metal- and ligand-centered events: radical, reactivity, and rate" *Inorg. Chem.* **2004**, *43*, 3292-3298
23. 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+/+0}" *J. Am. Chem. Soc.* **2004**, *126*, 5138-5153 (10.1021/ja030645+).
24. Grapperhaus, C. A.; Kreso, M.; Burkhardt, G. A.; Roddy, J. V. F.; Mashuta, M. S. "Template synthesis of N₂S and N₃S chelates via alkylation of bis(2-aminoethanethiolato)Ni: sulfur and nitrogen-centered alkylations" *Inorg. Chim. Acta* **2005**, *358*, 123-130
25. Grapperhaus, C. A.; Mullins, C. S.; Mashuta, M. S. "Structural comparison of alkylated derivatives of (bmmp-dmed)Ni and (bmmp-dmed)Zn" *Inorg. Chim. Acta* **2005**, *358*, 623-632
26. Poturovic, S.; Mashuta, M. S.; Grapperhaus, C. A. "Carbon-sulfur bond formation between a ruthenium-coordinated thiyl radical and methyl ketones" *Angewandte Chemie-International Edition* **2005**, *44*, 1883-1887 (10.1002/anie.200462713).
27. Grapperhaus, C. A.; Poturovic, S.; Mashuta, M. S. "Oxygenation of a ruthenium(II) thiolate to a ruthenium(II) sulfinate proceeds via ruthenium(III)" *Inorg. Chem.* **2005**, *44*, 8185-8187 (10.1021/ic051211d).
28. Mullins, C. S.; Grapperhaus, C. A.; Kozlowski, P. M. "Density functional theory investigations of NiN₂S₂ reactivity as a function of nitrogen donor type and N-H...S hydrogen bonding inspired by nickel-containing superoxide dismutase" *J. Biol. Inorg. Chem.* **2006**, *11*, 617-625 (10.1007/s00775-006-0109-6).

29. Frye, B. C.; Mashuta, M. S.; Mullins, C. S.; Grapperhaus, C. A.; Buchanan, R. M. "Ethyl 1-methylimidazole-2-carboxylate" *Acta Crystallographica Section E-Structure Reports Online* **2006**, 62, O1548-O1549 (10.1107/s1600536806010038).
30. Grapperhaus, C. A.; O'Toole, M. G.; Mashuta, M. S. "Synthesis and structure of the tetradeca-iron(III) oxide-alkoxide cluster $[\text{Bu}_4\text{N}]_2[\text{Fe}_{14}\text{O}_8(\text{OCH}_2\text{CH}_3)_{20}\text{Cl}_8]$ " *Inorg. Chem. Commun.* **2006**, 9, 1204-1206
31. Grapperhaus, C. A.; Kozlowski, P. M.; Kumar, D.; Frye, H. N.; Venna, K. B.; Poturovic, S. "Singlet diradical character of an oxidized ruthenium trithiolate: electronic structure and reactivity" *Angew. Chem., Int. Ed. Engl.* **2007**, 46, 4085-4088 (10.1002/anie.200700297).
32. Green, K. N.; Brothers, S. M.; Jenkins, R. M.; Carson, C. E.; Grapperhaus, C. A.; Darensbourg, M. Y. "An experimental and computational study of sulfur-modified nucleophilicity in a dianionic NiN_2S_2 complex" *Inorg. Chem.* **2007**, 46, 7536-7544 (10.1021/ic700878y).
33. Grapperhaus, C. A.; O'Toole, M. G.; Mashuta, M. S. "{3,3'-Ethane-1,2-diylbis(methylimino)-bis(propane-1-thiolato)}nickel(II)" *Acta Crystallogr., Sect. E: Struct. Rep. Online* **2007**, 63, M2281-U2317 (10.1107/s1600536807037725).
34. Grapperhaus, C. A.; Venna, K. B.; Mashuta, M. S. "Carbon-sulfur bond formation via alkene addition to an oxidized ruthenium thiolate" *Inorg. Chem.* **2007**, 46, 8044-8050 (10.1021/ic701078e).
35. Grant, G. J.; Botros, M. E.; Hassler, J. S.; Janzen, D. E.; Grapperhaus, C. A.; O'Toole, M. G.; VanDerveer, D. G. "Hg(II) and Cd(II) complexes with mixed donor macrocyclic thioethers: The oxophobicity of mercury(II)" *Polyhedron* **2008**, 27, 3097-3104 (10.1016/j.poly.2008.07.005).
36. O'Toole, M. G.; Kreso, M.; Kozlowski, P. M.; Mashuta, M. S.; Grapperhaus, C. A. "Spin-State-Dependent Oxygen Sensitivity of Iron Dithiolates: Sulfur Oxygenation or Disulfide Formation" *J. Biol. Inorg. Chem.* **2008**, 13, 1219-1230 (10.1007/s00775-008-0405-4).
37. O'Toole, M. G.; Bennett, B.; Mashuta, M. S.; Grapperhaus, C. A. "Substrate Binding Preferences and pK_a Determinations of a Nitrile Hydratase Model Complex: Variable Solvent Coordination to (bmmp-TASN)FeOTf" *Inorg. Chem.* **2009**, 48, 2300-2308 (10.1021/ic802180d).
38. Grapperhaus, C. A.; Ouch, K.; Mashuta, M. S. "Redox-regulated ethylene binding to a rhenium-thiolate complex" *J. Am. Chem. Soc.* **2009**, 131, 64-65 (10.1021/ja8086483).
39. $\text{N}_2\text{S}_3\text{X-Fe}$ Models of Nitrile Hydratase; O'Toole, M., G.; Grapperhaus, C., A. In *Bioinorganic Chemistry*; American Chemical Society: Washington, DC, 2009, p 99-113.
40. Mullins, C. S.; Grapperhaus, C. A.; Frye, B. C.; Wood, L. H.; Hay, A. J.; Buchanan, R. M.; Mashuta, M. S. "Synthesis and Sulfur Oxygenation of a $(\text{N}_3\text{S})\text{Ni}$ Complex Related to Nickel-Containing Superoxide Dismutase" *Inorg. Chem.* **2009**, 48, 9974-9976 (10.1021/ic901246w).
41. Grapperhaus, C. A.; Cui, J. L.; Buchanan, R. M.; Mashuta, M. S. "Supramolecular assembly of a dinuclear Ag(I) complex with discrete Ag_2S_2 centers" *Inorg. Chem. Comm.* **2009**, 12, 1091-1093 (10.1016/j.inoche.2009.08.027).
42. Masitas, C. A.; Mashuta, M. S.; Grapperhaus, C. A. "Asymmetric Oxygenation of a Ruthenium Dithiolate Mimics the Mixed Sulfenato/Sulfinato Donor Sets of Nitrile Hydratase and Thiocyanate Hydrolase" *Inorg. Chem.* **2010**, 49, 5344-5346 (10.1021/ic100414c).
43. Masitas, C. A.; Kumar, M.; Mashuta, M. S.; Kozlowski, P. M.; Grapperhaus, C. A. "Controlled Sulfur Oxygenation of the Ruthenium Dithiolate (4,7-Bis-(2'-methyl-2'-mercaptopropyl)-1-thia-4,7-diazacyclononane)RuPPh₃ under Limiting O₂ Conditions Yields Thiolato/Sulfinato, Sulfenato/Sulfinato, and Bis-Sulfinato Derivatives" *Inorg. Chem.* **2010**, 49, 10875-10881 (10.1021/ic101221z).
44. Cui, J.; Mashuta, M. S.; Buchanan, R. M.; Grapperhaus, C. A. "Synthesis, Structure, and Solution Properties of [(mim-TASN)FeCl₂]⁺ and Its μ -Oxo Derivative" *Inorg. Chem.* **2010**, 49, 10427-10435 (10.1021/ic1012999).

45. Cheruzel, L. E.; Cui, J. L.; Mashuta, M. S.; Grapperhaus, C. A.; Buchanan, R. M. "N-(2-formyl-1-methylimidazol-4-yl)-2,2-dimethylpropanamide: A versatile reagent for preparing imidazole-amine ligands with variable second-coordination spheres" *Tetrahedron Lett.* **2011**, 52, 4771-4774
46. Ouch, K.; Mashuta, M. S.; Grapperhaus, C. A. "Metal-Stabilized Thiyl Radicals as Scaffolds for Reversible Alkene Addition via C–S Bond Formation/Cleavage" *Inorg. Chem.* **2011**, 50, 9904-9914 (10.1021/ic200416y).
47. Ouch, K.; Mashuta, M. S.; Grapperhaus, C. A. "Alkyne Addition to a Metal-Stabilized Thiyl Radical: Carbon–Sulfur Bond Formation between 1-Octyne and [Ru(SP)₃]⁺" *Eur. J. Inor. Chem.* **2012**, 2012, 475-478 (10.1002/ejic.201101016).
48. Herdt, D. R.; Grapperhaus, C. A. "Kinetic study of nickel-thiolate oxygenation by hydrogen peroxide. Implications for nickel-containing superoxide dismutase" *Dalton Trans.* **2012**, 41, 364-366 (10.1039/C1DT11300C).
49. Shearer, J.; Callan, P. E.; Masitas, C. A.; Grapperhaus, C. A. "Influence of Sequential Thiolate Oxidation on a Nitrile Hydratase Mimic Probed by Multiedge X-ray Absorption Spectroscopy" *Inorg. Chem.* **2012**, 51, 6032-6045 (10.1021/ic202453c).
50. Chauhan, R.; Mashuta, M. S.; Grapperhaus, C. A. "Selective and Reversible Base-Induced Elimination of a Ruthenium Dithioether Yields a Vinyl Metallosulfonium Complex" *Inorg. Chem.* **2012**, 51, 7913-7920 (10.1021/ic300983x).
51. Kumar, D.; Masitas, C. A.; Nguyen, T. N.; Grapperhaus, C. A. "Bioinspired catalytic nitrile hydration by dithiolato, sulfinato/thiolato, and sulfenato/sulfinato ruthenium complexes" *Chem. Commun.* **2013**, 49, 294-296 (10.1039/C2CC35256G).
52. Sampson, K. O.; Kumar, D.; Mashuta, M. S.; Grapperhaus, C. A. "Addition of polysubstituted alkenes, aromatic alkynes, and dienes to a metal-stabilized thiyl radical via carbon–sulfur bond formation: Electrochemical, chemical, and computational investigations" *Inorg. Chim. Acta* **2013**, 408, 1-8 (10.1016/j.ica.2013.08.003).
53. Sulfur-Oxygenation Enhances Ligand Exchange in Nitrile Hydratase Inspired Ruthenium(II) Complexes; Masitas, C. A.; Mashuta, M. S.; Grapperhaus, C. A.; In *Biochalcogen Chemistry: The Biological Chemistry of Sulfur, Selenium, and Tellurium* Bayse, C. A., Brumaghim, J. L., Eds.; ACS Books, accepted for publication 2013.
54. Lu, M.; Campbell, J. L.; Chauhan, R.; Grapperhaus, C. A.; Chen, H. "Probing the Reactivity and Radical Nature of Oxidized Transition Metal-Thiolate Complexes by Mass Spectrometry" *J. Am. Soc. Mass. Spectrom.* **2013**, 24, 502-512 (10.1007/s13361-012-0537-1).
55. Chauhan, R.; Mashuta, M. S.; Grapperhaus, C. A. "Reinvestigation of the first structurally characterized metal-coordinated sulfenic acid complex" *Inorg. Chem. Commun.* **2013**, 37, 186-188 (DOI 10.1016/j.inoche.2013.09.045).
56. Kumar, D.; Nguyen, T. N.; Grapperhaus, C. A. "Kinetic Effects of Sulfur Oxidation on Catalytic Nitrile Hydration: Nitrile Hydratase Insights from Bioinspired Ruthenium(II) Complexes" *Inorg. Chem.* **2014**, 53, 12372-12377 (Doi 10.1021/IC501695N).
57. Chauhan, R.; Moreno, M.; Banda, D. M.; Zamborini, F. P.; Grapperhaus, C. A. "Chemiresistive metal-stabilized thiyl radical films as highly selective ethylene sensors" *Rsc Adv* **2014**, 4, 46787-46790 (Doi 10.1039/C4ra07560a).
58. Kumar, D.; Mashuta, M. S.; Grapperhaus, C. A. "Metal-centered oxidation decreases nitrile hydration activity of bioinspired (N2S3)Ru-PPh₃ precatalysts" *Inorg. Chem. Commun.* **2015**, 61, 197-199 (10.1016/j.inoche.2015.10.001).
59. Haddad, A. Z.; Kumar, D.; Sampson, K. O.; Matzner, A. M.; Mashuta, M. S.; Grapperhaus, C. A. "Proposed Ligand-Centered Electrocatalytic Hydrogen Evolution and Hydrogen Oxidation at a Noninnocent Mononuclear Metal-Thiolate" *J. Am. Chem. Soc.* **2015**, 137, 9238-9241 (10.1021/jacs.5b05561).

60. Haddad, A. Z.; Garabato, B. D.; Kozlowski, P. M.; Buchanan, R. M.; Grapperhaus, C. A. "Beyond Metal-Hydrides: Non-Transition-Metal and Metal-Free Ligand-Centered Electrocatalytic Hydrogen Evolution and Hydrogen Oxidation" *J. Am. Chem. Soc.* **2016**, *138*, 7844-7847 (10.1021/jacs.6b04441).
61. Zhang, W.; Saraei, N.; Hanlin, N.; Vaugh, J. R.; Jones, A. S.; Mashuta, M. S.; Buchanan, R. M.; Grapperhaus Craig, A. "Reversible Methanol Addition to Copper Schiff Base Complexes: A Kinetic, Structural, and Spectroscopic Study of Reactions at Azomethine C=N Bonds" *Dalton Trans.* **2016**, Advance Article (10.1039/C6DT01955B) (featured on front cover).
63. Zhang, W.; Haddad, A. Z.; Garabato, B. D.; Kozlowski, P. M.; Buchanan, R. M.; Grapperhaus Craig, A. "Translation of Ligand-Centered HER Activity and Mechanism of a Rhenium-Thiolate from Solution to Modified Electrodes: A Combined Experimental and DFT Study" *Inorg. Chem.* **2017**, *56*, 2177 -2178 (10.1021/ic6b02829)
64. Vishnosky, N. S.; Mashuta, M. S.; Buchanan, R. M.; Grapperhaus C. A. "Syntheses, Structures, and Electrochemical Studies of N,N'-bis(alkylthiocarbamate)butane-2,3-diimine Cu(II) Complexes as Pendant Alkoxy Derivatives of Cu(ATSM)" *Inorg. Chim. Acta* **2017**, *416*, 45 -51 (10.1016/j.ica.2017.01.020)
65. Jain, R.; Mashuta, M. S.; Buchanan, R. M.; Grapperhaus C. A. "Electrocatalytic Hydrogen Evolution and Hydrogen Oxidation with a Ni(PS)₂Complex" *Eur. J. Inorg.* **2017**, *2017*, 3714 -3719 (10.1002/ejic.201700590)
66. Haddad, A. Z.; Cronin, S. P.; Mashuta, M. S.; Buchanan, R. M.; Grapperhaus, C. A. *Inorg. Chem.* **2017**, *56*, 11254–11265 (10.1021/acs.inorgchem.7b01608).
67. "Ligand-Assisted Metal-Centered Electrocatalytic Hydrogen Evolution upon Reduction of a Bis (thiosemicarbazonato) Ni (II) Complex" Jain, R.; al Mamun, A.; Buchanan, R. M.; Kozlowski, P. M.; Grapperhaus C. A. *Inorg. Chem.*, **2018**, *57*, 13486-13493 (10.1021/acs.inorgchem.8b02110)
68. "Streams, cascades, and pools: various water cluster motifs in structurally similar Ni(II) complexes" Sarei, N.; Hietsoi, O.; Mullins, C. S.; Gupta, A. J.; Frye, B. C.; Mashuta, M. S.; Buchanan, R. M.; Grapperhaus C. A. *CrystEngComm* **2018**, *20*, 7071-7081 (10.1039/C8CE01153B) –featured on journal cover
69. "Active uptake of hydrophilic copper complex Cu(II)-TETA in primary cultures of neonatal rat cardiomyocytes" Fu, C.; Ding, X.; Lihao, J.; Luo, Z.; Grapperhaus C. A. Kang, Y. J. *Metallomics* **2019**, *11*, 565-575 (10.1039/C8MT00277K)
70. "Water wire clusters in isostructural Cu(II) and Ni(II) complexes: Synthesis, characterization, and thermal analysis" Saraei, N.; Hietsoi, O.; Frye, B. C.; Gupta, A. J.; Mashuta, M. S.; Gupta, G.; Buchanan, R. M.; Grapperhaus, C. A. *Inorg. Chim. Acta* **2019**, *492*, 268-274 (10.1016/j.ica.2019.04.012)
71. "Photocatalytic hydrogen evolution on Si photocathodes modified with bis(thiosemicarbazonato) nickel(II)/Nafion" Gulati, S.; Hietsoi, O.; Calvary, C. A.; Strain, J. M.; Pishgar, S.; Brun, H. C.; Grapperhaus, C. A.; Buchanan, R. M.; Spurgeon, J. M. *Chem. Commun.* **2019**, *55*, 9440-9443 (10.1039/c9cc04117f)
72. "Synthesis, Characterization, and HER Activity of Pendant Diamine Derivatives of NiATSM" Calvary, C. A.; Hietsoi, O.; Strain, J. M.; Mashuta, M. S.; Spurgeon, J. M.; Buchanan, R. M.; Grapperhaus, C. A. *Eur. J. Inorg. Chem.* accepted (10.1002/ejic.201900721).
73. "Effect of Stacking Interactions on the Translation of Structurally Related Bis(thiosemicarbazonato) nickel(II) HER Catalysts to Modified Electrode Surfaces" Gupta, A. J.; Vishnosky, N. S.; Hietsoi, O.; Losovyj, Y.; Strain, J.; Spurgeon, J.; Mashuta, M. S.; Jain, R.; Buchanan, R. M.; Gupta, G.; Grapperhaus, C. A. *Inorg. Chem.* accepted (10.1021/acs.inorgchem.9b01209)
74. "Utilizing Charge Effects and Minimizing Intramolecular Proton Rearrangement to Improve Overpotential of a Thiosemicarbazonato Zinc HER Catalyst" Cronin, S. P.; Mamun, A. A.; Toda, M.

J.; Mashuta, M. S.; Losovyj, Y.; Kozlowski, P. M.; Buchanan, R. M.; Grapperhaus, C. A. *Inorg. Chem.* accepted

Patents

1. Provisional Patent Application: Compounds, their preparation, related compositions, catalysts, electrochemical cells, fuel cells, and uses thereof. Grapperhaus, C. A.; Buchanan, R. M.; Haddad, A. Z. December 2016 US 62/436,490
2. Provisional Patent Application: Therapeutic applications of various metal N_2S_2 compounds. Grapperhaus, C. A.; Buchanan, R. M.; Vishnosky N. S., Young, J. O. E., Bates, P. J., Andres, S. A. June 2017 US 62/501,553

Presentations

A. Scholarly Meetings

1. Grapperhaus, C. A.; Maguire, M. J.; Tuntulani, T.; Darensbourg, M. Y. "Reactions of sulfur in nickel- and palladium-bound thiolates with $^1\Delta O_2$: Production of metallosulfoxides and metallosulfones" 211th American Chemical Society National Meeting, New Orleans, LA (1996) poster presentation
2. Grapperhaus, C. A.; Bellefeuille, J. A.; Darensbourg, N. Y. "Alkylation induced oxygen transfer in nickel sulfoxides" 215th American Chemical Society National Meeting, Dallas, TX (1998) oral presentation
3. Grapperhaus, C. A.; Darensbourg, M. Y.; Bellefeuille, J. A. "Sulfur Site Reactivity of Nickel Thiolates and Implications for Degradation of Metalloenzymes by Oxygenation" Graduate Research Seminar: Bioinorganic Chemistry (Gordon), Ventura, CA (1998) oral presentation
4. Grapperhaus, C. A.; Bill, E.; Weighardt, K. "Ozone Oxidation of Iron(III) in a Monofunctionalized Cyclam: Spectroscopic Characterization of High Valent Iron Species" 9th International Conference on Biological Inorganic Chemistry, Minneapolis, MN (1999) poster presentation
5. Grapperhaus, C. A.; Bill, E.; Weyhermüller, T.; Weighardt, K. "Ozonolysis and Photolysis of Fe(III) Precursors in a Monofunctionalized Cyclam: Spectroscopic Characterization of Fe(IV)=O and Fe(V)=N Species" TMR (Training and Mobility of Researchers) – NOHEMIP Research Network Mid-Term Review and Second Annual Meeting, Toulouse, France (2000) oral presentation
6. Grapperhaus, C. A.; Patra, A. K.; Poturovic, S. "Synthetic Models of Nitrile Hydratase" 1st Annual Kentuckiana Undergraduate Research Symposium, Louisville, KY (2001) oral presentation
7. Grapperhaus, C. A.; Patra, A. K.; Poturovic, S. "Synthetic Models of Nitrile Hydratase" 10th International Conference on Bioinorganic Chemistry, Florence, Italy (2001) poster presentation
8. Grapperhaus, C. A.; Patra, A. K.; Poturovic, S.; Kozlowski, P. M.; Mashuta, M. S. "A Structural and Electronic Model of NO-Inactivated Iron-Containing Nitrile Hydratase. A Comparison of Thiolate and Thioether Donor Atoms in Low-Spin Iron Complexes" Metals in Biology Gordon Conference Ventura, CA (2002) poster presentation
9. Grapperhaus, C. A.; Patra, A. K.; Li, M.; Poturovic, S.; Mashuta, M. S. "Modeling oxygenated cysteine thiolates with a thiolate/thioether donor set. A structural and spectroscopic model of no-inactivated iron-containing nitrile hydratase" 224th American Chemical Society National Meeting, Boston, MA (2002) oral presentation
10. Grapperhaus, C. A.; Poturovic, S.; Mashuta, M. S. "Ligand versus metal oxygen sensitivity of ruthenium(II) thiolates" 225th American Chemical Society National Meeting, New Orleans, LA (2003) oral presentation
11. Grapperhaus, C. A.; Poturovic, S.; Mashuta, M. S. "Understanding ruthenium thiolate reactivity: radicals, oxygen, and alkylation" Inorganic Chemistry Gordon Research Conference, Newport, RI (2003) poster presentation

12. Grapperhaus, C. A. "Modeling Oxygenated Cysteine Thiolates at the Active Site of Iron-Containing Nitrile Hydratase with a Thiolate/Thioether Donor Set" Third German-American Symposium on Frontiers of Chemistry (*invited*), Kloster Seeon, Germany (2004) poster presentation (*withdrawn due to illness*)
13. Grapperhaus, C. A.; Patra, A. K.; Li, M.; Poturovic, S.; Mashuta, M. S. "Modeling Oxygenated Cysteine Thiolates at the Active Site of Iron-Containing Nitrile Hydratase with a Thiolate/Thioether Donor Set" CERC3 Young Chemists' Workshop: Biocatalysis, Erlangen, Germany (2004) oral presentation
14. Grapperhaus, C. A. "Understanding Ruthenium Thiolate Reactivity: Radicals, Oxygen, and Alkylation" Inorganic Chemistry Gordon Conference, Newport, RI (2004) poster presentation (*withdrawn due to illness*)
15. Grapperhaus, C. A.; Poturovic, S.; Mashuta, M. S. "Reactivity Studies of a Metal-Coordinated Thiyl Radical: C-S Bond Formation" Inorganic Reaction Mechanisms Gordon Conference, Ventura, CA (2005) poster presentation
16. Grapperhaus, C. A.; Poturovic, S.; Mashuta, M. S. "Reactivity Studies of a Proposed Metal-Coordinated Thiyl Radical: C-S Bond Formation" 12th International Conference on Biological Inorganic Chemistry, Ann Arbor, MI (2005) poster presentation
17. Grapperhaus, C. A.; Mullins, C. S.; Buchanan, R. M.; Frye, B. C.; Mashuta, M. S.; Kozlowski, P. M. "Probing thiolate reactivity of Ni-SOD model complexes" 232nd American Chemical Society National Meeting, Atlanta, GA (2006) oral presentation (delivered by Martin G. O'Toole due to illness)
18. Grapperhaus, C. A.; Poturovic, S.; Frye, H. N.; Mashuta, M. S.; Kozlowski, P. M. "Reactivity studies of a proposed metal-coordinated thiyl radical" 231st American Chemical Society National Meeting, Atlanta, GA (2006) poster presentation (delivered by Martin G. O'Toole due to illness)
19. Grapperhaus, C. A. "Substrate Binding & Oxygenation Studies of Iron-Dithiolates as Models of Nitrile Hydratase" Metals in Biology Gordon Conference, Ventura, CA (2007) poster presentation
20. Grapperhaus, C. A.; O'Toole, M. G.; Mashuta, M. S. "N₂S₃FeX model complexes of nitrile hydratase: Substrate binding and spin state dependent oxygen reactivity" 233rd American Chemical Society National Meeting, Chicago, IL (2007) oral presentation
21. Grapperhaus, C. A. "Reactivity of Nitrile Hydratase Model Complexes" CERMACS2007 – Central Regional Meeting of the American Chemical Society, Cincinnati, OH (2007) oral presentation (*invited*)
22. Grapperhaus, C. A. "[9]aneN₂S Based Models of the Sulfur-Oxygenated Active Site of Nitrile Hydratase" SERMACS2007 - Southeastern Regional Meeting of the American Chemical Society, Greenville, SC (2007) oral presentation (*invited*)
23. Grapperhaus, C. A.; Ouch, K.; Venna, K. B.; Mashuta, M. S. "One way or reversible: Alkene addition to metal-coordinated thiyl radicals" 236th American Chemical Society National Meeting, Philadelphia, PA (2008) oral presentation
24. Grapperhaus, C. A.; Cui, J. L.; Buchanan, R. M.; Mashuta, M. S. "Supramolecular assembly of a dinuclear Ag(I) complex with discreet Ag₂S₂ centers" *Inorg. Chem. Comm.* **2009**, *12*, 1091-1093 (10.1016/j.inoche.2009.08.027).
25. Grapperhaus, C. A.; Ouch, K.; Mashuta, M. S. "Redox Regulated Binding of Alkenes to a Rhenium Thiolate" 39th IRMG: Inorganic/Bioinorganic Reaction Mechanisms Group Meeting, Kloster Banz, Germany (2010) poster presentation
26. Grapperhaus, C. A. "A Tame Metal-Coordinated Thiyl Radical: Redox Regulation of Alkene Binding to Metal Thiolates" International Symposium on Molecular Coordination Chemistry (In honor of Prof. K. Wieghardt's retirement), Mülheim, Germany (2010) oral presentation (*invited*)

27. Chauhan, R.; Mashuta, M. S.; Grapperhaus, C. A. "Alkene addition to a Ru-coordinated thiyl radical: Synthesis by chemical oxidants and reactivity studies" Pacifichem 2010, Honolulu, HI (2010) poster presentation
28. Grapperhaus, C. A.; Ouch, K.; Chauhan, R.; Mashuta, M. S. "Alkene addition and reactivity with oxidized metal thiolates" Pacifichem 2010, Honolulu, HI (2010) oral presentation (*invited*)
29. Grapperhaus, C. A.; Ouch, K.; Mashuta, M. S. "Redox regulated binding of alkenes to rhenium thiolates" Pacifichem 2010, Honolulu, HI (2010) poster presentation
30. Grapperhaus, C. A.; Masitas, C. A.; Mashuta, M. S. "Sulfur Oxygenation of Nitrile Hydratase Mimic Enhances Ligand Lability and Hydrolysis Activity" Inorganic Reaction Mechanisms Gordon Conference, Galveston, TX (2011) poster presentation
31. Grapperhaus, C. A. "Controlled sulfur oxygenation of a nitrile hydratase mimic: Enhanced ligand lability and hydrolysis activity" 244th American Chemical Society National Meeting, Philadelphia, PA (2012) oral presentation (*invited*)
32. Kumar, D.; Grapperhaus, C. A. "Sulfur-Oxidation Effects on the Hydration Activity of Bioinspired Ru Catalysts" Metals in Biology Gordon Conference, Ventura, CA (2013) poster presentation
33. Grapperhaus Craig, A.; Chauhan, R.; Moreno, M.; Haddad, A.; Mashuta, M. S.; Zamborini, F. P. "Metal-stabilized thiyl radicals as scaffolds for ethylene sensing, alkene activation, and proton reduction" Inorganic Reaction Mechanisms Gordon Conference, Galveston, TX (2013) poster presentation
34. Grapperhaus Craig, A.; Zamborini, F. P.; Chauhan, R.; Moreno, M. "Chemiresistive metal-stabilized thiyl radical films as highly selective ethylene sensors" 248th American Chemical Society National Meeting, San Francisco (2014) oral presentation
35. Grapperhaus Craig, A.; Jain, R.; Zhang, W.; Gibson, T.; Nie, H. L.; Mashuta, M. S.; Buchanan, R. M. "Reversible binding of aliphatic alcohols and benzyl alcohol oxidation using N4 – Schiff base and reduced Schiff base Copper (II) complexes." Inorganic Reaction Mechanisms Gordon Conference, Galveston, TX (2015) poster
36. Grapperhaus Craig, A. "Redox-Active Metal-Thiolates: Ligand-Centered Alkene Binding and Proton Reduction" International Conference on Inorganic Chemistry (CIC 2015), Suzhou, China (2015) oral (and session chair)
37. Grapperhaus Craig, A.; Haddad, A. Z.; Jain, R.; Kumar, D.; Sampson, K. O.; Mashuta, M. S. "Redox-Active Metal-Thiolates: Ligand-Centered Electrocatalytic Proton Reduction & Hydrogen Oxidation" Pacifichem 2015, Honolulu, HI (2015) oral (symposium co-organizer)
38. Grapperhaus Craig, A.; Haddad, A. Z.; Garabato, B.; Buchanan, R. M.; Kozlowski, P. M. "Hydrogen evolution without metal-hydrides: Ligand-centered HER catalysts with transition metals and non-transition metals" 253rd American Chemical Society National Meeting, San Francisco (2017) oral presentation
39. Grapperhaus, Craig A. "Ligand-Centered HER Catalysis using Bis(thiosemicarbazones)" Inorganic Reaction Mechanisms Gordon Conference, Galveston, TX (2017) poster
40. Grapperhaus Craig, A.; Zhang, W.; Buchanan, R. M. "Modification of glassy carbon electrodes with Cu- and Zn-bis(thiosemicarbazones) as heterogeneous HER catalysts" 254th American Chemical Society National Meeting, Washington D.C. (2017) oral presentation
41. Grapperhaus Craig, A. "Bisthiosemicarbazone Electrocatalysts for the Hydrogen Evolution Reaction: Influence of Metal Ion on Activity and Mechanism" Chem-Connect Colloquium in Southeast Texas, Lamar University, Beaumont, TX (2018) invited keynote speaker
42. Grapperhaus Craig, A. "Bisthiosemicarbazone Electrocatalysts for the Hydrogen Evolution Reaction: Influence of Metal Ion on Activity and Mechanism" 2019 ACS Great Lakes Regional Meeting: Gibbs Symposium. Lisle, IL (2019) oral presentation, session organizer.

Invited Oral Presentations at Academic Institutions

Western Kentucky University (2000)	Ohio University (2008)
Southern Illinois University at Edwardsville (2001)	Wayne State University (2008)
Kentucky State University (2002)	Berea College (2009)
Indiana State University (2003)	Western Kentucky University (2009)
University of Nevada – Reno (2004)	University of Missouri, St. Louis (2009)
University of Cincinnati (2004)	University of Louisville, Department of Chemical Engineering (2010)
University of Würzburg (2004)	Technische Universität Kaiserslautern (2010)
University of Delaware (2004)	University of Nevada, Reno (2011)
Indiana University (2004)	Marquette University (2011)
Texas A&M University (2004)	Duquesne University (2012)
Rice University (2004)	University of Memphis (2012)
University of Miami (Ohio) (2004)	Sichuan University (2013)
University of Kentucky (2004)	National Taiwan Normal University (2013)
College of Mount St. Joseph (2005)	National Tsing Hua University (2013)
Purdue University (2005)	University of Toronto (2013)
University of North Carolina – Charlotte (2005)	Auburn University (2015)
Marshall University (2007)	Tulane University (2016)
Virginia Commonwealth University (2008)	Indiana University (2017)
Old Dominion University (2008)	University of Science and Technology of China (2018)
Bellarmino University (2008)	Dalian University of Technology (2018)

Persons Mentored

Post-Doctoral Researchers

Oleksandr Heitsoi (2017 – 2019)
Jinlan Cui (2008 – 2012)
Ming Li (2001 – 2002)
Apurba Patra (2000 – 2001)

Ph.D. Students

current

Caleb Calvary	Nina Sarei	Steven Cronin
Emtias Chowdhury	Kritika Bajaj	Peter Armstrong
Sashil Chapagain		

2019 Nicholas Vishnosky	2017 Wuyu Zhang	
2017 Rahul Jain	2017 Andrew Haddad	2015 Davinder Kumar
2014 Rajat Chauhan	2012 Kagna Ouch	2012 Cesar Masitas
2008 Martin O'Toole	2006 Christopher S. Mullins	2005 Selma Poturovic

M.S. Thesis Students

2008 Kagna Ouch	2007 Kiran Venna
2006 Majda Kreso	

>40 Undergraduate Research Students mentored