Undergraduate Research Highlights

Janzen DE, Bruening MA, Mamiya AA, Driscoll LE, da Silva Filho DA. Hemilabile Bonding of 1-oxa-4,7-Dithiacyclononane in Cyclometallated Palladium(II) Complexes. *Dalton Transactions*. 2019; 48: 11520–11535, doi: 10.1039/c9dt02059d (St. Catherine University; Universidade de Brasilia)

This study examined weak metal-ligand interactions in a series of cyclometallated complexes of Pd(II) incorporating the mixed donor ligand 1-oxa-4,7-dithiacyclononane. Understanding and manipulation of these weak-interactions is important to catalyst design. Variable temperature solution NMR studies revealed dynamic endodentate and exodentate bonding modes of the oxathioether ligand while single-crystal X-ray structures revealed only exodentate bonding. Density functional theory calculations helped elucidate a transition state for this conversion and estimated an energy barrier consistent with the solution NMR data. Daron E. Janzen is a professor of chemistry and biochemistry at St. Catherine University. Arthur A. Mamiya recently completed his PhD at the Universidade de Brasilia. Demetrio A. da Silva Filho is a professor of physics at the Universidade de Brasilia. Meaghan A. Bruening was an undergraduate who collaborated on this study from 2014 through 2017 in the Summer Scholars Undergraduate Research Program and as independent study. She is now in her third year of the PhD chemistry program at Caltech and received a National Science Foundation Graduate Research Fellowship. Laura E. Driscoll was an undergraduate who collaborated on this study in 2016 as a course-based research project. She is now in her second year of the physician assistant program at Bethel University. This research was supported by grants from St. Catherine University (Summer Scholars Program and the Endowed Chair in the Sciences), the National Science Foundation (MRI-1125975, Janzen, principal investigator; CCLI-0836842, Janzen, principal investigator), CNPq (420836/2018-7, 304020/2016-8 and 407682/2013-9), FAP-DF (193.001.596/2017 and 193.001.284/2016), and CAPES.

Davis SN, Wagner SE. Research Motivations and Undergraduate Researchers' Disciplinary Identity. *SAGE Open*. doi: 10.1177/2158244019861501 (George Mason University)

Disciplinary identity, or connection to a particular academic discipline, is constructed through a developmental process across a scholar's academic life course. Using unique data from an online survey of students at four diverse colleges and universities, we investigate the extent to which disciplinary identity among undergraduate researchers reflects motivations for participating in research and differs by student discipline. We document key differences in disciplinary identity based upon two internal motivators, intellectual interest and grit, as well as demographic characteristics. We discuss implications for institutions and undergraduate programs desiring to encourage students to participate in undergraduate research. Shannon N. Davis is professor and director of PhD programs in sociology at George Mason University. During the time of the research, Sarah E. Wagner was a fourth-year sociology major at George Mason and is currently employed at Mathematica Policy Research. Wagner's research was supported by the American Sociological Association's Carla B. Howery Teaching Enhancement Fund.

McCollum B, Morsch L, Pinder C, Ripley I, Skagen D, Wentzel M. Multi-Dimensional Trust between Partners for International Online Collaborative Learning in the Third Space. *International Journal for Students as Partners*. 2019; 3: 1: 50–59. doi: 10.15173/ijsap.v3i1.3730 (University of Illinois at Springfield)

Learners partner with an international peer at another university to complete online collaborative assignments (OCAs). We present OCAs as an example of the Third Space, where control over interactions and learning is negotiated between unfamiliar remote students, empowering students as emerging experts. This digital Third Space results in the formation of trust (a) between student partners to prepare for—and contribute during—the OCAs and (b) between students and faculty as partners in teaching and learning. Brett McCollum is professor of chemistry and the Mount Royal University Board of Governors Teaching Chair in Educational Leadership. Layne Morsch is associate professor of organic chemistry at University of Illinois at Springfield, and Michael T. Wentzel is associate professor of chemistry at Augsburg University. Chantz Pinder worked on this project as a third- and fourth-year undergraduate at University of Illinois at Springfield as both a student in an undergraduate research course and as a research associate funded by the UIS Competitive Scholarly Research Grant program. He graduated in spring 2019. Isaiah Ripley is an undergraduate student in chemistry at Augsburg University, and Darlene Skagen is an undergraduate student at Mount Royal University.

Webb EW, Moerdyk JP, Sluiter KB, Pollock BJ, Speelman AL, Lynch EJ, Polik WF, Gillmore JG. Experimental and Computational Electrochemistry of Quinazolinespirohexadienone Molecular Switches —Differential Electrochromic vs Photochromic Behavior. *Beilstein Journal of Organic Chemistry*. 2019; 15: 2473–2485. doi: 10.3762/bjoc.15.240 (Hope College)

Our undergraduate research group has long focused on the preparation and investigation of electron-deficient analogs of the perimidinespirohexadienone (PSHD) family of photochromic molecular switches for potential application as “photochromic photooxidants” for gating sensitivity to photoinduced charge transfer. We previously reported the photochemistry of two closely related and more reducible quinazolinespirohexadienones (QSHDs), wherein the naphthalene of the PSHD is replaced with a quinoline. In the present work, we report our investigation of the electrochemistry of these asymmetric QSHDs. In addition to the short wavelength and photochromic long-wavelength isomers, we have found that a second, distinct long-wavelength isomer is produced electrochemically. This different, long-wavelength isomer arises from a difference in the regiochemistry of spirocyclic ring-opening. The structures of both long-wavelength isomers were ascertained by cyclic voltammetry and 1H NMR analyses, in concert with computational modeling. These results are compared to those for the symmetric parent PSHD, which due to symmetry possesses only a single possible regioisomer upon either electrochemical or photochemical ring-opening. Density functional theory calculations of bond lengths, bond orders, and molecular orbitals allow the rationalization of this differential photochromic vs. electrochromic behavior of the QSHDs. William F. Polik is the Edward & Elizabeth Hofman Professor of Chemistry and Schaap Research Fellow at Hope College. Jason G. Gillmore is professor of chemistry and Schaap Research Fellow at Hope College. Eric Webb (’15) worked on this project during his third and fourth years, as well as two summers. He is currently an organic chemistry PhD candidate at Princeton University. Jon Moerdyk (’09) worked on this project from his first through fourth years (including 3.5 summers). After completing his PhD in organic chemistry at UT Austin in 2014, he is an associate professor of chemistry at Seton Hill University. Kyndra Sluiter (’11) worked on this project during her third and fourth years (as well as one summer). She is currently employed as a chemist IV at Perrigo, a generic pharmaceutical manufacturer. Ben Pollock (’13) contributed computational work to this project during his fourth year. After earning his MS in organic chemistry from UW Madison, Pollock is currently in sales with Epic, a medical software and devices company in Madison. Amy Speelman (’10) worked on computational electrochemistry for this project during her second and third years. After earning her PhD in inorganic chemistry from University of Michigan in 2016, she is currently a postdoctoral scholar at Yale University. Eugene Lynch worked on computational electrochemistry for this project as an NSF REU student at Hope College in summer 2011 during his associate’s degree program at College of the Canyons. After completing his bachelor’s degree in chemistry at University of California, Berkeley in 2014, he is an engineer with Alice Financial and the cofounder and software engineer for Good Call NYC. This work was funded by a Camille & Henry Dreyfus Foundation Start-up Award (SU-04-040), a Cottrell College Science Award from Research Corporation (CC6653), and a Faculty Early Career Development Grant (CHE-0952768) from the US National Science Foundation (NSF). This work was also funded in part by a grant to Hope College from the Howard Hughes Medical Institute through the Undergraduate Science Education Program, which provided support for Hope College's Curie cluster and to ALS (Computational Science & Modeling Scholars Program) and JPM (HHMI Research Scholars Program). Additional computations were conducted on the MU3C cluster, supported by Major Research Instrumentation grants (CHE-0520704 and CHE-1039925) from the NSF. ALS acknowledges additional support from a Jean Dreyfus Boissevain Scholarship awarded to the Hope College Chemistry Department by the Camille & Henry Dreyfus Foundation. EJL (home institution College of the Canyons, Santa Clarita, CA) acknowledges support by a Research Experiences for Undergraduates Site award (CHE-0851194) to the Hope College Chemistry Department from NSF.

Smolyaninova VN, Korzi W, Zimmerman W, Searfoss S, Jensen C, Yong G, Schaefer D, Prestigiacomo JC, Osofsky MS, Heungsoo K, Zhen X, Qazilbash MM, Smolyaninov II. Superconducting Properties of Tin-Based ENZ and Hyperbolic Metamaterials. *Physica C: Superconductivity and Its Applications*. 2019; 565: 1353511. doi: 10.1016/j.physc.2019.1353511 (Towson University)

Recent experiments have demonstrated that the superconducting critical temperature may be improved in various metamaterial superconductor geometries. Here, we present the results of a study of tin-based metamaterial superconductors in the epsilon-near-zero (ENZ) and hyperbolic metamaterial configurations. It was observed that critical temperature enhancement is significantly reduced when the metamaterial structural dimensions exceed 240 nm, the superconducting coherence length in pure tin. Vera Smolyaninova is a professor of physics at the Department of Physics, Astronomy, and Geosciences at Towson University. Christopher Jensen is a graduate student at Towson. Grace Yong is a lecturer in the Department of Physics at Loyola University Maryland. David Schaefer is professor and chair of the Department of Physics, Astronomy, and Geosciences at Towson. Joseph C. Prestigiacomo and Michael S. Osofsky are research physicists at the US Naval Research Laboratory. Heungsoon Kim is a materials engineer at the US Naval Research Laboratory. At the time of the research, Zhen Xing was a PhD candidate at the College of William & Mary. Mumtaz Qazilbash is associate professor of physics at William & Mary. Igor I. Smolyaninov works at Saltenna LLC in McLean, VA. William Zimmerman was an undergraduate student at Towson at the time of the research. William Korzi is a fourth-year physics major at Towson who worked on this project from 2018 through 2019. Sabrina Searfoss is an undergraduate dual-degree student who worked on this project from 2017 through 2018. She is now studying engineering at the University of Maryland–College Park. The research was supported by grants from DARPA (Award No: W911NF-17-1-0348), Office of Naval Research (Award N00014-18-1-2681; V. Smolyaninova, principal investigator), and FCSM Undergraduate Research Grants and the Sweeting Summer Research Fellowship at Towson University.

McNally JR, Mehlenbacher MR, Luscieti S, Smith GL, Reutovich AA, Poli M, Arosio P, Bou-Abdallah F. Mutant L-Chain Ferritins that Cause Neuroferritinopathy Alter Ferritin Functionality and Iron Permeability. *Metallomics*. 2019; 11: 1635–647, doi: 10.1039/c9mt00154a (State University of New York at Potsdam)

In mammals, the iron storage and detoxification protein ferritin is composed of two functionally and genetically distinct subunit types, H (heavy) and L (light). The two subunits co-assemble in various ratios, with a tissue specific distribution, to form shell-like protein structures of 24 subunits within which a mineralized iron core is stored. The H-subunits possess ferroxidase centers that catalyze the rapid oxidation of ferrous ions, whereas the L-subunit does not have such centers and is believed to play an important role in electron transfer reactions that occur during the uptake and release of iron. Pathogenic mutations on the L-chain lead to neuroferritinopathy, a neurodegenerative disease characterized by abnormal accumulation of ferritin inclusion bodies and iron in the central nervous system. Here, we have characterized the thermal stability, iron loading capacity, iron uptake, and iron release properties of ferritin heteropolymers carrying the three pathogenic L-ferritin mutants (L154fs, L167fs, and L148fs, which for simplicity we named Ln1, Ln2 and Ln3, respectively), and a nonpathogenic variant (L135P) bearing a single substitution on the 3-fold axes of L-subunits. Our data support the hypothesis that hereditary neuroferritinopathies are due to alterations of ferritin functionality and lower physical stability which correlate with the frameshifts introduced at the C-terminal sequence and explain the dominant transmission of the disorder. SUNY Potsdam alumnus Justin McNally is a scientist in preclinical research and development at Millendo Therapeutics Inc. in Ann Arbor, MI. SUNY Potsdam alumnus Matthew Mehlenbacher is pursuing a PhD in chemistry at Dartmouth College. Paolo Arosio is professor of molecular biology, Maura Poli is research professor, and Sara Luscietiis is a research associate at the University of Brescia in Brescia, Italy. Fadi Bou-Abdallah is professor of chemistry at SUNY Potsdam. Gideon Smith and Aliaksandra Reutovich are second-year majors in biochemistry at SUNY Potsdam. This work was supported by the National Institute of Health, Award Number R15GM104879 (F. B. A.) and the Henry Dreyfus Teacher-Scholar Award (F. B. A., award TH-16-007) of the Camille & Henry Dreyfus Foundation. It also was partially supported by Grant PRIN10-11 of MIUR, from the Italian Ministry of Research (P. A.). McNally and Mehlenbacher were partly supported by Kilmer Undergraduate Research Apprenticeships (SUNY Potsdam).