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RESEARCH OVERVIEW

Take a deep breath! About 80% of the air we breathe is nitrogen gas. Nitrogen gas (N_2) is everywhere! N_2 is cheap and abundant…but it is also extremely inert and unreactive. What if we could use renewable sources of energy like the sun to transform N_2 into an energy-dense fuel such as ammonia (NH_3). The energy stored in the N-H bonds can be used when need, producing N_2 and/or H_2O as the only waste product. This is the concept of a nitrogen-based fuel cycle! We focus on designing molecular transition metal catalysts to convert N_2 to NH_3, and then oxidize NH_3 back to N_2. Efficient catalysts for NH_3 synthesis from N_2, protons, and electrons, could augment the energy intensive Haber-Bosch process that uses high-temperatures and fossil-derived H_2, to enable distributed on-demand NH_3 production. Catalysts for the reverse reaction, NH_3 oxidation, will be essential to utilize the energy stored in N-H bonds. These fundamental studies employ synthesis, spectroscopy, and theory to study monometallic transition metal compounds with chromium, iron, ruthenium, and nickel using bidentate or tetradentate phosphine and carbene ligands to enhance the reactivity of N_2 and NH_3. We seek to develop strategies for making and breaking N≡N and N-H bonds by the delivery and removal of H-atoms, while moving toward the development of electrocatalytic schemes. This work uses electrochemistry, chemical kinetics, and thermochemical studies to understand the reaction mechanism of these catalytic processes. We are also designing novel multi-metallic systems to control catalytic conversions of molecules with strong bonds by understanding metal cooperativity in molecular systems. In addition, transition metal

Inorganic Chemistry, Organometallic Chemistry, Molecular Catalysis

REPRESENTATIVE PUBLICATIONS

Bhattacharya, P., Heiden, Z. M., Chambers, G. M., Johnson, S. I., Bullock, R. M., **Mock, M.T.** (2019) Catalytic Ammonia Oxidation to Dinitrogen by Hydrogen Atom Abstraction. *Angewandte Chemie International Edition*: v. 58 p. 11618-11624.

Kendall, A. J., Johnson, S. I., Bullock, R. M., **Mock, M.T.** (2018) Catalytic Silylation of N_2 and Synthesis of NH_3 and N_2H_4 by Net Hydrogen Atom Transfer Reactions using a Chromium P_4 Macrocycle. *Journal of the American Chemical Society*: v. 140 p. 2528-2536.

Prokopchuk, D. E., Wiedner, E. S., Walter, E. D., Popescu, C. V., Piro, N. A., Kassel, W. S., Bullock, R. M., **Mock, M. T.** (2017) Catalytic N_2 Reduction to Silylamines and Thermodynamics of N_2 Binding at Square Planar Fe. *Journal of the American Chemical Society*: v. 139 p. 9291-9301.

Bhattacharya, P., Prokopchuk, D. E., **Mock, M.T.** (2016) Exploring the Role of Pendant Amines in Transition Metal Complexes for the Reduction of N_2 to Hydrazine and Ammonia. *Coordination Chemistry Reviews*: v. 334 p. 67-83.

compounds with sulfur-based ligands are being used to model the iron-molybdenum cofactor (FeMoco) of the nitrogenase enzyme, and to activate small molecules such as H_2, N_2, and CO_2.	

Announcement of a Summer Chemistry Research Opportunity at Montana State University

Prof. Michael Mock (Faculty member in the Department of Chemistry and Biochemistry) is seeking a junior or senior undergraduate chemistry major interested in performing synthetic inorganic chemistry at Montana State University from May 23 – July 31. This summer research opportunity is funded by the National Science Foundation and will run concurrently with a separate NSF sponsored REU program (Research Experience for Undergraduates) hosted by MSU. Research activities will entail the synthesis and characterization of transition metal complexes for energy related applications and small molecule activation. Research will be performed in Prof. Mock's research laboratory. Summer dorm housing and a 100-meal dining plan will be provided on the MSU campus. A $3,500 summer research stipend will be offered for the 10-week session. Interested candidates should contact Prof. Michael Mock by email: michael.mock@montana.edu