"Mechanistic and Electronic Structural Insights into the Metallobiochemistry of Nitrification "



INORGANIC SEMINAR MONDAY, OCTOBER 3RD, 2016 4:00 P.M. HUTCHISON HALL 473 DEPARTMENT OF CHEMISTRY UNIVERSITY OF ROCHESTER

GUEST SPEAKER: PROFESSOR KYLE M. LANCASTER CORNELL UNIVERSITY DEPARTMENT OF CHEMISTRY AND CHEMICAL BIOLOGY

Abstract:

Nitrification, the oxidation of ammonia to nitrite and nitrate, is a key entry point for fixed nitrogen to return to the atmosphere as dinitrogen. Nitrification is the root of tremendous economic loss in agriculture as well as a major ecological hazard via nitrogenous eutrophication. Molecular details concerning the elementary, multi-electron chemical steps whereby ammonia is oxidized to hydroxylamine and ultimately to nitrite remain elusive. This may be attributable in part to the difficulty associated with accessing sufficient quantities of relevant enzymes for biophysical characterization. Nevertheless, such insights are attractive because they hold the promise of inspiring novel, green chemical methods for difficult bond activations and multi-electron transformations. This talk will describe our investigation of the crucial molecular steps of nitrification revealed through the application of rapid kinetics, spectroscopy, and electronic structure calculations. Key insights include the establishment of a direct link between nitrification and nitrous oxide pollution, the identification of important intermediates in hydroxylamine oxidation by both Fe and Cu, a revision of the enzymatic steps involved in hydroxylamine oxidation, and a tentative identification of the elusive archaeal hydroxylamine oxidoreductase. The seminar will conclude with reinterpretation of the electronic structure of high-valent copper-oxygen species toward rationalizing competence of these species for challenging E-H bond activations.

Host: Professor Michael Neidig, email: neidig@chem.rochester.edu