Reviving the Cluster-Surface Analogy

Heterogeneous materials underpin most industrial-scale catalytic applications, but the extreme reaction conditions and ill-defined surface structures create difficulties in studying and controlling reaction outcomes. Since the 1970’s, molecular cluster chemistry (~2-4 metal atoms) has been pursued in the hopes of modeling the chemistry occurring on the surfaces of heterogeneous catalysts. This “cluster-surface analogy” is rooted in an early desire to merge the control and selectivity of homogeneous catalysts with the rates, robustness, and scope of catalytically active metallic surfaces. Still, work in this area is limited by i) a lack of control over the coordination sphere of the cluster, and ii) a limited conceptual link between the electronic structures of metal surfaces and those of molecular clusters.

The research described in this talk is aimed at a new approach to the cluster-surface analogy, in which ligands are specifically designed to mimic the properties of metallic surfaces. These macrocyclic, redox-active ligands offer electronic and geometric flexibility for the cluster core, offering a way of modelling both the “sea-of-electrons” available at a metallic surface and the local geometric changes that occur during surface restructuring events. In particular, the chemistry of Fe$_2$ and Co$_2$ bridging nitrides will be described, including their connection to the chemistry that underpins the Haber-Bosch synthesis of ammonia.

BIO
Neil C. Tomson received a Ph.D. in 2009 from the University of California, Berkeley, after performing research involving organometallic chemistry of the Group 5 elements. He then worked as a post-doctoral research associate at the Max Planck Institute for Bioinorganic Chemistry, where he used a range of physical inorganic techniques and computational methods to describe the electronic structures of metal nitrosyl (M–NO) and metal nitrosoalkane (M–N(R)O) complexes. From 2011-2012, Prof. Tomson was an Adjunct Assistant Professor at the College of St. Benedict | St. John’s University, before moving to Los Alamos National Laboratory, where he held Glenn T. Seaborg Institute and Director’s Post-doctoral Research Fellowships in support of his work on uranium imido chemistry. Prof. Tomson joined the faculty at the University of Pennsylvania in 2015 and is currently pursuing molecular inorganic chemistry aimed at developing unique approaches to energy storage and catalysis.