

UNIVERSITY OF RHODE ISLAND
Department of Chemistry
SEMINAR

Room 215 Beupre Center
10:00 a.m., Tuesday November 26, 2019

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Catalysis with Boron, University of Würzburg, Am Hubland, D-97074
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***“Metallomimetic Chemistry of Boron:
Metal-Free Catalysis and Nitrogen
Fixation at a Main Group Element”***

HOST

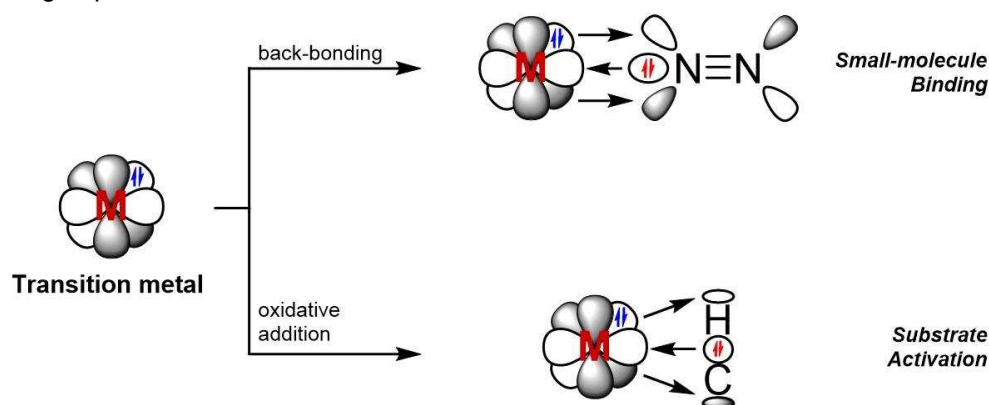
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Metallomimetic Chemistry of Boron: Metal-Free Catalysis and Nitrogen Fixation at a Main Group Element

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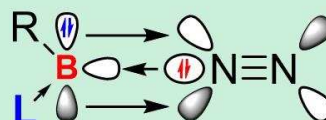
The importance of transition metals (TMs) in modern catalysis cannot be overstated. TM-based catalysts enable processes that are of tremendous human and economic importance; they have innumerable applications in many industrial sectors. However, the toxicity, price and natural scarcity of many elements that are used in TM catalysis fuel an interest for the development of metal-free catalysts based on the main-group elements.



Metal-free strategies (metallomimetics):



Frustrated Lewis Pairs
C-H Activation



Low-valent Boron
N₂ Activation

However, contrary to many catalytically-active TM complexes, classical main-group compounds do not possess the combination of empty and filled orbitals that is crucial for the complex electronic processes involved in the elemental steps of catalytic cycles. The development of catalysts based on the p-block elements thus requires the design and application of unique strategies. In this seminar, I will present an approach for the rational design of such strategies: combining predictive computational calculations with a bottom-up experimental investigation of metal-free reactions.

Results obtained through this method include the use of boron compounds for small-molecule activation, reduction processes, and organic functionalization reactions. I will discuss systems that involve the combination of single and multiple active sites in order to mimic the electronic environment of TM complexes. Similarities and differences in the reactivity of main-group compounds and TM complexes will also be highlighted.