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Aiiso Yufeng Li Family Department of
Chemical and Nano Engineering

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DEPARTMENT SEMINAR

Wednesday, October 16th, 2024

11:00 AM - 12:00 PM

SME 248



Dr. Lai-Sheng Wang, PhD

“Nanoclusters of Boron and Metal Borides”

Chair, Department of Chemistry

Jesse H. and Louisa D. Sharpe Metcalf Professor of Chemistry

Brown University

Abstract: As neighbors in the periodic table, boron and carbon share some similarities. They both have multiple allotropes with high melting temperatures and can form strong covalent bonds through catenation. While the investigation of carbon clusters led to the discovery of a rich variety of nanostructures from the fullerenes to carbon nanotubes and graphenes, relatively little was known about boron nanoclusters. Using photoelectron spectroscopy of size-selected anions in combination with computational chemistry, my lab and our collaborators have systematically investigated small boron clusters and found that they all possess planar structures,¹ in contrast to that of bulk boron, which is dominated by three-dimensional polyhedral building blocks. The propensity for planarity was found to be a result of both σ and π electron delocalization over the molecular plane. We discovered that the B₃₆ cluster has a highly stable planar structure with a central hexagonal vacancy, providing the first experimental evidence for the viability of single-atom boron-sheets with hexagonal vacancies, and coined the name “borophene”.² Borophenes have since been synthesized and characterized on inert substrates, becoming a new class of synthetic 2D materials. We have found recently that the B₄₈ cluster possesses a bilayer structure, suggesting the feasibility of bilayer borophenes. I will discuss these advance on boron nanoclusters, as well recent work on metal boride clusters. We have found that transition metals can be doped into the plane of boron clusters, suggesting the possibility of metallo-borophenes.³ However, lanthanide doped boron clusters form half-sandwich or inverse-sandwich structures,⁴ as well as unprecedented lanthanide boron cage clusters.⁵

References:

1. L. S. Wang. Photoelectron Spectroscopy of Size-Selected Boron Clusters: From Planar Structures to Borophenes and Borospherenes. *Int. Rev. Phys. Chem.* 2016, 35, 69-142.
2. Z. A. Piazza, H. S. Hu, W. L. Li, Y. F. Zhao, J. Li, and L. S. Wang. Planar Hexagonal B₃₆ as a Potential Basis for Extended Single-Atom Layer Boron Sheets. *Nature Commun.* 2014, 5, 3113.
3. W. L. Li, X. Chen, T. Jian, T. T. Chen, J. Li, and L. S. Wang. From Planar Boron Clusters to Borophenes and Metalloborophenes. *Nature Rev. Chem.* 2017, 1, 0071.
4. W. L. Li, T. T. Chen, D. H. Xing, X. Chen, J. Li, and L. S. Wang. Observation of Highly Stable and Symmetric Lanthanide Octa-Boron Inverse Sandwich Clusters. *Proc. Natl. Acad. Sci. (USA)* 115, E6972-E6977 (2018).
5. T. T. Chen, W. L. Li, W. J. Chen, X. H. Yu, X. R. Dong, J. Li, and L. S. Wang. Spherical Trihedral Metallo-Borospherenes. *Nature Commun.* 2020, 11, 2766.

Bio: Lai-Sheng Wang is the Jesse H. and Louisa D. Sharpe Metcalf Professor of Chemistry at Brown University. He received his B.S. degree in chemistry from Wuhan University and his PhD from the University of California at Berkeley. His research group has developed photoelectron spectroscopy techniques to investigate the size-dependent electronic structure and chemical bonding of nanoclusters. More recent work in his lab has focused on the study of the structures and bonding of size-selected boron and boride clusters. His lab has also pioneered electrospray and cryogenic ion trap techniques for photoelectron spectroscopic studies of free multiply-charged anions and complex solution molecules in the gas phase. Recently, they have been focusing on the investigation of polycyclic aromatic hydrocarbon anions and nonvalence excited states in anions using cryogenic photodetachment spectroscopy and resonant photoelectron imaging.

Seminar Host: Wanlu Li