



PHYSICAL SEMINAR ~ 4:00 P.M.
MONDAY, NOVEMBER 2, 2015
HUTCHISON HALL 473
DEPARTMENT OF CHEMISTRY
UNIVERSITY OF ROCHESTER



Guest Speaker:
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Department of Chemistry

Photoelectron Spectroscopy of Size-Selected Boron Clusters: From Planar Structures to Borophenes and Borospherenes

Abstract: Photoelectron spectroscopy in combination with computational studies over the past decade has shown that boron clusters possess planar or quasi-planar structures, in contrast to that of bulk boron, which is dominated by three-dimensional cage-like building blocks. All planar or quasi-planar boron clusters are observed to consist of a monocyclic circumference with one or more interior atoms. The propensity for planarity has been found to be a result of both σ and π electron delocalization over the molecular plane. An interesting question is if infinitely large planar boron clusters are possible, giving rise to atom-thin boron nanostructures analogous to graphene. Because of its electron deficiency, boron cannot form graphene-like structures with a honeycomb hexagonal framework. Computational studies suggested that extended boron sheets with partially filled hexagonal holes are stable. We have found that B36 is a highly stable quasi-planar boron cluster with a central hexagonal hole, providing the first indirect experimental evidence that single-atom layer boron-sheets with hexagonal vacancies are potentially viable. B36 can be viewed as a potential basis for extended two-dimensional boron sheets, dubbed "borophene". Our most recent studies revealed that the B40 cluster has an unprecedented cage structure (Fig. 1), which is the first all-boron fullerene to be characterized and is named "borospherene". Further studies show that the B39 – cluster consists of two nearly degenerate cage global minima, which are both chiral. Thus, there may exist a family of borospherenes.

Host: Professor James Farrar, email: farrar@chem.rochester.edu