

Department of Chemistry and Molecular Biology Seminar  
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3:45 pm in Dunbar 152

## Germanium and Arsenic Zintl Anions: Functionalization and Application in Multidimensional Cluster Based Materials

*Dr. Angel Ugrinov*

*The Pennsylvania State University, University Park, PA*

The deltahedral Zintl ions (for example Germanium Zintl anions) are five- and nine-atom cage-like clusters with triangular faces and delocalized bonding as in the deltahedral boranes. The reactivity of such species is expected to be different from Zintl ions with normal 2-center-2-electron bonds (Arsenic Zintl anions) and so far have not been sufficiently studied. Until 1999, the clusters were assumed to be highly reduced so that any attempt for oxidation was expected to destroy them. It has been shown, for the first time in Dr. Sevov's group that "normal" 2-center-2-electron bonds can be formed by such clusters with delocalized bonding.

My studies as a PhD student of  $\text{Ge}_9^{n-}$  ( $n = 2, 3, 4$ ) clusters revealed that they can bond to each other and to other groups in different modes and form oligomers such as trimer  $[\text{Ge}_9=\text{Ge}_9=\text{Ge}_9]^{6-}$  and tetramer  $[\text{Ge}_9=\text{Ge}_9=\text{Ge}_9=\text{Ge}_9]^{8-}$ . They can be functionalized as well and make Zintl ions as  $[\text{Ph}_2\text{Sb}-\text{Ge}_9-\text{SbPh}_2]^{2-}$ ,  $[\text{Ph}_2\text{Bi}-\text{Ge}_9-\text{BiPh}_2]^{2-}$ ,  $[\text{Ph}-\text{Ge}_9-\text{SbPh}_2]^{2-}$  and  $[\text{Ph}_2\text{Sb}-\text{Ge}_9-\text{Ge}_9-\text{SbPh}_2]^{4-}$ .

The possibility to involve Zintl anions in addition reactions opened amazing opportunity to use them as building blocks for the synthesis of materials with new properties. As the physical, chemical, electronic, optical, and magnetic properties of the clusters are controllable by size and composition, this approach may provide an unprecedented ability to synthesize customized materials.

The primary aim is to form clusters with different number of arsenic atoms and with different geometries that are held together by alkali metal cations. The expectation (borne out by theoretical calculations and preliminary band-gap measurements) is to build up a library of similar materials with tunable band gaps. So far we have made one, two, and three dimensional cluster assemblies based on  $\text{As}_7^{3-}$  and  $\text{As}_{11}^{3-}$  ions and their X-ray crystal structures will be presented.