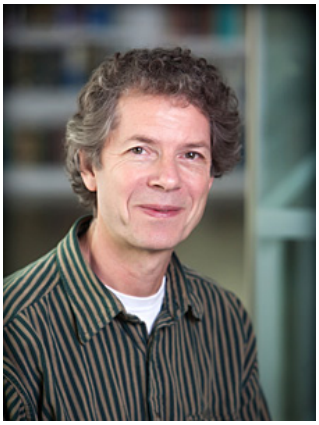
Physical Chemistry Seminar

Tuesday, February 2, 2016 | **11:00 am** | **Room 1315 Chemistry Building**

The unique bonding characteristics of beryllium and the Group IIA metals



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Host: Ned Sibert

Having closed valence sub-shells, the alkaline earth atoms participate in covalent bonding via orbital hybridization and exchange interactions, with additional contributions from dispersion interactions. Starting from a closed ns^2 configuration imparts different characteristics to the chemistry of this group, as compared to metals that have open-shell atomic ground states. Theoretical studies of the bonding of the Group IIA metals have been pursued for many years, and they are known to be challenging for ab initio electronic structure methods. The bonding motifs have been examined, and the differences between beryllium and the remainder of the group explored. Experimental studies that probe the bonding, particularly for beryllium, have lagged behind the theoretical work. I will describe recent spectroscopic and theoretical investigations of simple beryllium compounds, and discuss these results in terms of their relationship to the properties of the heavier Group IIA elements. Diatomic molecular ions that contain alkaline earth atoms are of interest for experiments involving cold molecular ions. The advantage of using ions is that they can be readily trapped using external fields. The alkaline earth atomic cations are well suited for laser cooling as they have transitions that are analogous to those of the alkali metals. Hence, Coulomb crystals are readily formed in rf traps. Reactions of these atomic ions yield diatomic products that are sympathetically cooled to low translational temperatures by the surrounding atomic ions. In principle, spectroscopic measurements may be used to probe the internal energies of the molecular ions. However, there are no gas phase spectroscopic data for the ions of interest (e.g., BaO^+, $BaCl^+$, CaO^+). I will discuss our recent studies of these ions that rely on pulsed field ionization – zero kinetic energy (PFI-ZEKE) photoelectron techniques.

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315

Graduate Students can meet with the speaker in Room 8305F at 1:00 pm