

# *The Department of Chemistry and Biochemistry*

## **Seminar Series**

*Presents a Seminar Titled:*

*“Sigma Holes Along a Continuum from Electrostatic Interactions to Dative Bonding”*

*Presented By*



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The sensitivity of the size and strength of sigma holes on terminal halides (X) bonded and on group 14 central atoms has been investigated at the MP2(full) level of theory for small Lewis Acids, including the  $MH_{4-n}X_n$  systems (M = C, Si, Ge, Sn, and Pb). The charge redistribution in these molecules and the (in)stability of the sigma hole at X as a function of M and n will be discussed. A substituent-induced reversal in the relative strengths of halogen bond energies is identified and explained. We explore as well a complicated dependence of the relative halogen bond strengths on M and m for the mixed halide  $MH_{3-m}F_mI$  compounds. We analyze halogen bonds formed by  $MF_3I$  acids to a wide class of Lewis bases and consider the viability of competing interactions (e.g. hydrogen bonding) for the haloethanes. A few (experimental) observations by other groups of halogen bonding by larger organic systems will be mentioned during the talk. These sub-covalent interactions are not unique to terminal atoms. We examine in some detail the so-called sigma-hole interactions induced on the central M centers when X = F. These interactions - supported by an increasing covalent contribution as M gets larger - help to stabilize species that span the spectrum from weak non-covalent to dative bonding in  $MFR_3 \bullet R'$  adducts.

**Friday, March 28, 2014 at 3:00 p.m. in OCNPS 100**