

**Title:** Group 12 Metal Halide Clusters: A Search for the Cause and Location of a Novel Transition in the Mode of Bonding in Mercury(II)Fluoride

Ziad Shafi and Kelling J. Donald

Department of Chemistry, Gottwald Center for the Sciences, University of Richmond,  
Richmond, Virginia 23173, United States

**Abstract:** Structure prediction remains a challenge for modern computational chemistry. The extraction of data from computationally-accessible, small, gas-phase clusters is one means of obtaining information to make predictions for structural preferences in extended solids. Generally, **the mode of bonding is conserved** as we climb the oligomerization ladder from gas-phase clusters to extended solids. For example: CO<sub>2</sub>, H<sub>2</sub>O, and MgF<sub>2</sub>, have gas-phase clusters which are held together by van der Waals, hydrogen bonding, and polar-covalent bonds respectively, and this mode of bonding is preserved when we look at dry ice, ice, and MgF<sub>2</sub> crystals. HgF<sub>2</sub> is the **only known exception** to this preservation of bonding. The work of Donald, Kretz, and Omorodion (2015) showed that HgF<sub>2</sub> clusters switch from weakly interacting to polar-covalently interacting somewhere between n=5 and n=11. Using Gaussian 09 along with a genetic algorithm method (CLUSTER), we have structural and energetic evidence to suggest that this novel *ionic switch* occurs at the **hexamer**.

