Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

DFT investigation for low-energy structures of 22- atom and 23-atom Boron Clusters KEVIN FRANCIS, CHRISTOPHER VARNEY, HIKMAT BC, University of West Florida — Using density functional theory, we investigate low-energy structures of B22 and B23 clusters. Our study shows that a 22-atom boron cluster prefers a three-dimensional double ring structure for all of its charged states where as the 23-atom boron cluster prefers a planar structure. It is found that boron clusters with an odd number of atoms in this size regime tend to form planar structures, while clusters with an even number of atoms prefer three-dimensional ring structures. We have also studied several isomers of cationic and anionic B22 and B23 clusters.

Kevin Francis
University of West Florida

Date submitted: 14 Nov 2016 Electronic form version 1.4