Abstract Submitted
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Signature of the Superatom to Superhalogen Behavior of $Au_n(BO_2)_m$ clusters[1] ANIL KANDALAM, McNeese State University, MATTHIAS GOTZ, University of Konstanz, MARY WILLIS, Virginia Commonwealth University, GERD GANTEFOR, University of Konstanz, PURU JENA, Virginia Commonwealth University — We report the discovery of a new class of clusters consisting of $Au_n(BO_2)_m$ which formed during the oxygenation of gold clusters when boron nitride was used as insulation in the pulsed arc cluster ion source (PACIS). Using DFT based calculations, we trace the origin of these species to be due to the unusual stability of the BO_2 moiety as well as shed light on their formation process. PES measurements and the corresponding DFT calculations further reveal some rather remarkable properties of $Au_n(BO_2)_m$ clusters such as large HOMO-LUMO gaps in the range of 3.00 eV – 3.95 eV and electron affinities substantially larger than that of F, the most electronegative element in the periodic table. In addition, some of the most predominant features of the electronic structure of the bare Au clusters, namely odd-even alternation in the electron affinity, are preserved in the $Au_n(BO_2)$ species. The synergy between theory and experiment illustrates that $Au_n(BO_2)_m$ clusters, behave as superatoms and superhalogens, opening the door for the synthesis of a new class of cluster-assembled materials.

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