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Electronic Structure of $Bi_3Ga_y^-$ Semiconductor Clusters and the Special Stability of $Bi_3Ga_2^-$ - A Gas Phase Zintl Analogue JOSE ULISES REVELES, Department of Physics, Virginia Commonwealth University, Richmond VA, 23284., UJJWAL GUPTA, JOSHUA J. MELKO, Departments of Chemistry and Physics, The Pennsylvania State University, University Park, PA 16802, SHIV N. KHANNA, Department of Physics, Virginia Commonwealth University, Richmond VA, 23284., A. W. CASTLEMAN, JR., Departments of Chemistry and Physics, The Pennsylvania State University, University Park, PA 16802, SHIV KHANNA RESEARCH GROUP COLLABORATION, THE CASTLEMAN GROUP COLLABORATION — Here we present evidence that the gap between the highest occupied and lowest unoccupied molecular orbitals (HOMO-LUMO gap) can be tuned (1.12eV-1.89eV) by changing the Ga composition of Bi_3Ga_y neutral and anionic clusters, some of which display special stability. Collaboratively, mass spectrometry, photoelectron spectroscopy and computational results show that $Bi_3Ga_2^-$ is a very stable cluster with a large calculated HOMO-LUMO gap of 1.89 eV, and can be viewed as a gas phase Zintl analogue of Sn_5^{2-}, already synthesized in the solution phase. The stability of $Bi_3Ga_2^-$ is further attributed to the fact that it has 12 valence electrons and possesses a closo structure in agreement with Wade's rules.

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