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**Sequential Oxidation of Gallium Oxide Clusters - A First-Principles Study** S. GOWTHAM, Michigan Technological University, AURORA COSTALES, Universidad de Oviedo, Spain, RAVINDRA PANDEY, Michigan Technological University, USA — The structural and electronic properties of gallium oxide lusters ( $\text{Ga}_3\text{O}_n$ ;  $n = 4-8$ ) are studied under the framework of density functional theory, with respect to sequential oxidation. The focus is on changes induced by the addition or removal of an electron from the neutral species as well as similarities/differences between aluminum oxide clusters of the same size. Lowest energy isomers in case of neutral clusters were found in doublet electronic state, and except for  $\text{Ga}_3\text{O}_4^-$ ,  $\text{Ga}_3\text{O}_4^+$ , and  $\text{Ga}_3\text{O}_5^-$ , all ionized clusters were found in triplet electronic state. We observed that both addition and removal of an electron from the neutral cluster leads to significant changes in the structure of the lowest energy isomer, apart from altering the sequence of other low-lying geometries. Structural resemblance to corresponding alumina clusters is limited to a few cases while we predict new results for others. Binding energy remains almost constant throughout the oxidation process, with values for ionized systems bracketing the neutral ones. All clusters considered in this study are found to be stable against fragmentation via O and  $\text{O}_2$  channels. Analysis of vibrational frequencies confirms the tendency of  $\text{Ga}_3\text{O}_6^+$ ,  $\text{Ga}_3\text{O}_7$  and  $\text{Ga}_3\text{O}_8$  to form O-O bonds. HOMO-LUMO gap values show an oscillatory trend while calculated values of electron affinity and ionization potential are in good agreement with the corresponding values for alumina clusters.

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