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Theoretical Study of Gallium Oxide Clusters GOWTHAM S, Michigan Technological Univ., AURORA COSTALES, Universidad de Oviedo, Spain, MRINALINI DESHPANDE, RAVINDRA PANDEY, Michigan Technological Univ.
— Gallium oxide is an important semiconducting oxide with applications in the areas of optics and micro-electronics. It is, therefore, not surprising that considerable efforts have been made in the past to understand the structural, optical and electronic properties of gallium oxide. On the other hand, interest in studying the properties of nanostructures and nanoclusters of gallium oxide is relatively recent. Small clusters of gallium oxide can be taken as a prototype to understand the Physics and Chemistry of surfaces and nanostructures. In this talk, we report the equilibrium structure, bonding and electronic properties of small clusters of gallium oxide which are studied under the framework of Density Functional Theory. All the clusters studied so far have shown a preference for planar arrangement of constituent atoms. The ionization induced structural distortions in the neutral clusters are relatively small, except those for Ga_3O_2. In anionic (cationic) clusters, the added (removed) electron is shared by gallium atoms, except in case of GaO_3. All the isomers are dominated by ionic Ga-O bond. The HOMO-LUMO gap in oxygen deficient Ga_mO_n clusters depends upon the gallium content, i.e., the gap will change with particle size even if n/m is fixed. Ionization potential and electron affinity of these clusters have been calculated, for the first time, in this study, and both values increase with the increase in oxygen to metal ratio.

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