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Reactivity of Aluminum and Doped Aluminum Clusters[1]
ARTHUR REBER, SHIV KHANNA, Virginia Commonwealth University, PATRICK ROACH, WILLIAM WOODWARD, A. WELFORD CASTLEMAN JR., Penn State University — We examine the reactivity of aluminum cluster anions with water, and other nucleophiles. The clusters reveal size dependent reactivity which primarily results in either the chemisorption of one or more water molecules, or no observable reactivity. The reactivity of the clusters is found to be dependent on surface sites which facilitate the splitting of the water on the surface of the cluster. Clusters with two sets of active sites are found to selectively release molecular Hydrogen. We also investigated the reactivity of aluminum clusters doped with another metal and their reactivity with molecular Oxygen. As the reactivity of aluminum clusters with oxygen depends on the electronic shell closing, this serves as a probe of the effects of doping on the electronic shell structure. The results reveal variable effects of doping on the electronic structure depending on the precise geometry and electron count.

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