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Aluminum anions and water: nucleophilic reactivity and free-electron metal clusters PATRICK ROACH, The Pennsylvania State University, ARTHUR REBER, The Virginia Commonwealth University, W. HUNTER WOODWARD, The Pennslyvania State University, SHIV KHANNA, The Virginia Commonwealth University, A. WELFORD CASTLEMAN, JR., The Pennsylvania State University — When coupled with appropriate theoretical considerations, the presence or absence of a reaction under strictly controlled conditions can be used to gain insight into electronic structure, bond strength, overall stability, and the general nature of a cluster of atoms. It will be shown that aluminum cluster anions react selectively with water molecules based on cluster size. Additionally, it will be suggested using first principles density functional theory that for certain cluster sizes reactivity events can be attributed mainly to the geometric, rather than electronic structure of a cluster. These findings provide a representative example of a hitherto unsubstantiated variable capable of governing and tuning reactivity, namely the energetics of a dissociative transition state at the cluster surface .

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