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On the Unusual Reactivity Patterns in Copper doped Aluminum Cluster Anions[1] ARTHUR REBER, Department of Physics, Virginia Commonwealth University, PATRICK ROACH, W. HUNTER WOODWARD, A. WELFORD CASTLEMAN JR., Departments of Chemistry and Physics, Pennsylvania State University, SHIV KHANNA, Department of Physics, Virginia Commonwealth University — We have measured the relative reactivity of Al_nCu^- clusters (n=11-34) with O_2. An odd-even alternation is observed that is in accordance with spin-dependant etching, and $CuAl_{22}^-$ is observed as a "magic peak." As $CuAl_{22}^-$ has 68 valence electrons, it has an open shell within a spherical jellium model and would be expected to be reactive. First principles electronic structure studies indicate that the results from an unusually large splitting of the $2D^{10}$ sub-shell in the jellium model leading to a HOMO-LIMO gap of 1.24 eV. We show that the splitting results from a geometric distortion of the cluster that may also be understood as a crystal field splitting of the superatomic orbitals.

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