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Interpretation of Cp(*) - protected Aluminum Clusters as Superatom Complexes[1] P. ANDRE CLAYBORNE, OLGA LOPEZ-ACEVEDO, Department of Chemistry, NSC, University of Jyväskylä, ROBERT WHETTEN, University of Jyväskylä and Georgia Insitute of Technology, HENRIK GRÖNBECK, Competence Centre for Catalysis and Department of Applied Physics, Chalmers University of Technology, HANNU HÄKKINEN, Department of Chemistry and Department of Physics, NSC, University of Jyväskylä — Metal clusters stabilized by a surface ligand shell represent an interesting intermediate state of matter between molecular metal-ligand complexes and bulk metal. Such "metalloid" particles are characterized by the balance between metal-metal bonds in the core and metal-ligand bonds at the exterior of the cluster. In previous studies, the electronic stability observed for selected ligand-protected aluminum clusters is not fully understood. By density functional theory calculations, we illustrate here that the electronic stability of various experimentally isolated Cp(*) – protected aluminum clusters can be explained using the electron shell model for the aluminum core, coupled with an ionic Al-Cp(*) interaction at the surface. Thus, one may classify ligand-protected aluminum clusters as "superatom complexes" similar to the ligand-protected gold clusters.

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