A Computational Investigation on the Atomic Behavior of Superatoms

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Because of their exceptional stability and similarities in the ordering and character of their molecular orbitals to those of actual elements, a number of mixed metal clusters have been labeled as 'Superatoms'. Khanna et al., have already identified several systems as superatoms. Those systems are usually metal clusters with a central transition metal surrounded by a polyhedra of group 1 metals or other various transition metals, in particular Na and Al. Apart from the novelty of having stable cages that imitate the electronic structure of atomic species, these 'superatom' show promises as quantum dots, component fragments in electronic devices, and can exceptional magnetic properties. In fact, a few of the computationally predicted super atoms have been identified experimentally including Na_7V^-, and Na_8V. Questions involving the actual atomic character of these clusters remain to be answered. In what ways are superatoms atomic? In what ways are they not? There are the obvious differences of size on constitution. It is difficult too, for instance, to assign a single value to the bond length of a superatom to an adjacent single atom. Nonetheless, we have initiated our study of the atomic properties of superatoms by studying the bonding and stability of systems in which the superatom is substituted for the actual atom. Computational methods, such as the ADF program, have been key tools in truly understanding the structural composition and overall potential of these superatoms as favorable substitutes to the current single atom structures. As studies continue, the possibility of a more favorable alternative is becoming more of a reality. Further investigation hopes to reveal the true potential of these superatoms.