Sp3-hybridization in superatomic clusters. Analogues to simple molecules involving the Au6 core

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The electronic and structural properties of [Au6{Ni3(CO)6}4]2- pave the way to describe a superatom analogue of the most simple and archetypical hydrocarbon, CH4. In this sense, our interest relies on the plausibility of finding superatomic clusters as analogues for archetypical molecules in organic chemistry, preserving relevant concepts of chemical significance, such as the hybridization of atomic orbitals. In [Au6{Ni3(CO)6}4]2-, a central Au6 core exhibits the formation of superatomic SP3 hybridized orbitals in order to account for the molecular shape and bonding. Inspired by this finding, several clusters were proposed exploring the capabilities of the metallic core to exhibit SP2 and SP superatomic hybrid orbitals. In addition, we include the evaluation of superatomic bonding involving SP3SP3, SP2SP2 and SPSP hybridized cores, which denote single, double and triple superatomic bonds. Our results describe the extension of the localized Lewis structure model to the understanding of clusters according to the superatom model, contributing to the tremendous opportunities for the design of functional clusters and nanoparticles. This journal is