Electronic structure of ligated transition-metal superatoms and assemblies of superatoms

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Superatoms are compact clusters of spherical shape, the electronic structure of which can be related to that of polyelectronic atoms [1]. As for simple atoms or atomic ions, chemical stability is most often reached for superatoms when they satisfy the closed-shell requirement. In a similar way, as unstable open-shell atoms can bind together to form stable molecules, open-shell superatoms can also assemble to form "supermolecules" [2]. As for molecules, closed-shell stability (octet rule, for example) is also most often required for such assemblies of superatoms. In this presentation we analyse the electronic structure of stable ligated Cu- [3-5], Ag- [6], and Pd-rich superatoms, as well as on "supermolecules", made of several icosahedral superatoms, which we predict to be stable systems isolobal to I_3^- [7], I_4^{2-}, SF_2 or CO_2.

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