Electron count and electronic structure of bare icosahedral Au_{32} and Au_{33} ionic nanoclusters and ligated derivatives. Stable models with intermediate superatomic shell fillings

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Abstract
DFT calculations were carried out on bare Au32 and Au33 nanoclusters with various charges, in order to analyze their stability with respect to different cluster electron numbers. Results indicate that in addition to the neutral Au32 hollow species, significant HOMO-LUMO gaps are computed for [Au32]8+ (hollow) and [Au32]4+ (two-shell structure). Species with smaller HOMO-LUMO gaps can reach stability upon "passivation" by a ligand shell, as experimentally exemplified. Icosahedral frameworks of Ih or lower symmetry are favored for the cationic nanoclusters whereas different structures are computed for the anionic ones.

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