Coinage Metal Superatomic Cores: Insights into Their Intrinsic Stability and Optical Properties from Relativistic DFT Calculations

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Coinage-metal atomically precise nanoclusters are made of a well-defined metallic core embedded in a ligand-protecting outer shell. Whereas gold derivatives are particularly well documented, examples of silver nanoclusters are somewhat limited and copper species remain particularly scare. Our DFT relativistic calculations on superatomic metallic cores indicate that copper species are almost as stable as gold clusters and more stable than their silver counterparts. Thus, for silver superatomic cores, the role of the stabilizing ligands is more crucial in the stabilization of the overall structure, in comparison to copper and gold. Hence, the chemistry of the earlier counterparts of gold, especially copper, should grow quickly with at least characterizations of species related to that found in the heavier elements in the triad, which requires tackling synthetic challenges. Time-dependent (TD)-DFT calculations show that with an increase of the cluster core nuclearity, the absorption bands are redshifted, allowing us to differentiate between the clusters types. Moreover, the optical properties of the silver cores are fairly different from that of their Cu and Au relatives.

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