

Potential of N-heterocyclic carbene derivatives from Au₁₃(dppe)₅Cl₂ gold superatoms. Evaluation of electronic, optical and chiroptical properties from relativistic DFT

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Atomically precise gold superatoms offer useful templates to evaluate tunable properties via ligand engineering. Herein, the role of different linked N-heterocyclic carbene (NHC) protecting ligands ranging from strong to weak σ -donors was evaluated according to the Tolman electronic parameter (TEP), in species related to the classical [Au₁₃Cl₂(dppe)₅]³⁺ nanocluster (1). Our results show a strong dependency on the nature of NHC, providing a useful design principle for the efficient tuning of the structural, optical, chiroptical and emission properties of the Au₁₃Cl₂ core. A sizable decrease is observed in the HOMO-LUMO gap for weaker σ -donor ligand cases, with a change in the LUMO nature from core-based orbitals in 1, to a π -ligand nature. Furthermore, a shorter bridge results in interesting structural changes between the eclipsed σ staggered Au₁₃Cl₂ core unraveling the potential to convert light energy into mechanical work. Thus, the noticeable modulation of [Au₁₃Cl₂(NHC)₅]³⁺ properties by different ligands underlies design rules for tunable clusters towards nanostructured materials, by taking advantage of the recent introduction of NHC-protected gold clusters. © 2019 the Partner Organisations.