Abstract Submitted
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Ligand-spacer controlled size selectivity of gold clusters[1] GHAZAL SHAFAI, SAMPYO HONG, TALAT RAHMAN, University of Central Florida, MASSIMO BERTINO, Virginia Commonwealth University — It has been observed in the experiment that the presence of diphosphine ligands with varying spacers (L_3, L_5, and L_6) leads to the formation of Au clusters of characteristic size [1]. In particular, in the presence of L_3, Au_{11}^{+3} clusters are formed, while the presence of L_5 leads to the formation of Au_8^{+2}, Au_9^{+2} and Au_{10}^{+2} clusters. We have carried out calculations based on the density functional theory in the projector augmented wave scheme (PAW) and the pseudopotential approach, to examine the effect of the diphosphine ligand spacer size on the stability of Au clusters containing 2 to 11 atoms through evaluations of the cluster total energy and proper corrections of spurious interactions between charged supercells. For example, to investigate the stability of Au_{11}^{+3}, we compare the total energy of $Au_{11}(X)_5^{+3}$ and $Au_8(X)_4^{+2}$ + Au_3X^{+1} (X= L_3 and L_5 ligands) and find that Au_{11}^{+3} is indeed preferred by L_3 rather than L_5, in agreement with the experiment. The electronic structural changes brought about by the various local environments of these clusters are presented with full details. [1] Bertino et al. Phys. Chem. B Lett. 110, 21416 (2006)

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