## Abstract Submitted for the MAR08 Meeting of The American Physical Society

Ligand-spacer controlled size selectivity of gold clusters¹ 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<sub>3</sub>, L<sub>5</sub>, and L<sub>6</sub>) leads to the formation of Au clusters of characteristic size [1]. In particular, in the presence of L<sub>3</sub>,  $Au_{13}^{+1}$  clusters are formed, while the presence of L<sub>5</sub> 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  $Au_{8}(X)_{4}^{+2} + Au_{3}X^{+1}$  (X= L<sub>3</sub> and L<sub>5</sub> ligands) and find that  $Au_{11}^{+3}$  is indeed preferred by L<sub>3</sub> rather than L<sub>5</sub>, 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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