Abstract Submitted
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Effect of ligand on the geometric and electronic structure of Au_{13} cluster[1] GHAZAL SHAFAI, SAMPYO HONG, TALAT RAHMAN, University of Central Florida, MASSIMO BERTINO, Virginia Commonwealth University — 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 ligand on the geometric and electronic structure of Au_{13} cluster. We find *bare* Au_{13} to form a flat flake, in agreement with previous theoretical calculations. This structure is lower in energy by 2.60 eV in comparison with the well ordered icosahedron geometry. Our results show, however, that the *Au_{13} cluster covered with ligands of phosphine (PH_3) forms a stable spherical structure (icosahedron)* in agreement with the experiment [1] which is by 0.08 eV lower in energy when compared to the flat-flake complex. If the phosphine is replaced by H, the spherical structure is no longer stable, but it still maintains a 3 dimensional form, signifying the effect of the ligand in stabilization of the structure. We observe a narrow d-band for flat-flake gold atoms in the complex, while in the icosahedron structure the d-band is wider. We also find a stronger overlap between the p orbitals of the P atom with d orbitals of gold atoms in the icosahedron complex. [1] M. F. Bertino et. al. Phys. Chem. B Lett. 110, 21416 (2006)

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