Theoretical Investigation of Metal Doped Gold Nano-Clusters

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Abstract

A major interest of cluster science is to discover highly stable clusters which may be used as building blocks for novel materials. While colloidal gold nanoparticles were used in stained glass windows in the middle ages, gold nanoclusters have attracted considerable interest over the past two decades due to their catalytic properties,[1-3] applications as sensors[1],and use in molecular electronics. They have been employed as bioconjugate probes for amplification tags in gene analysis[2], antibody or antigen detection[3], DNA sequencing, and gene mapping[4, 5]. The existence of the endohedral gold clusters, $M@Au_{12}$ confirmed both theoretically and experimentally.[6,7] In addition, element-centered ligated gold cluster compounds, such as the octahedral $[\{C@Au_6\}(Ph_3P)_6X_2]$ or the icosahedral $[\{Pd@Au_{12}\}(Ph_3P)_8Cl_4]$[8] clusters, are known.

Despite the tremendous research progress on gold clusters, many open questions remain. For example, can a cage with a transition metal encapsulated within a cluster of less than 12 gold atoms exist? Also, what types of electronic or boding interactions between the transition metal and the gold atoms are involved? Although significant progress has been made on endohedral gold $M@Au_{12}$ clusters, studies of metal-encapsulated gold ($M@Au_n$) clusters containg less than 12 gold atoms are still in their preliminary stages. In this presentation, we will discuss the relative stabilities, highest occupied and lowest unoccupied molecular orbital (HOMO-LUMO) gaps, and vertical ionization potentials of metal doped gold clusters, $M@Au_9$ (M = Mo, W, Co, and Ir) and $M@Au_{10}$ (M = Mo, W, and Ru) investigated by using the different density functional theories (DFT).

References:

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