Structure and Properties of Substituted Gold Clusters

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Abstract: Structure and stability of some substituted gold nanoparticles were investigated by quantum chemical calculations. It was found that terminal SH and SiO_4H_3 groups can substitute gold atoms without changes of regular structure in positions, where the number of Au-Au bonds does not exceed three. It was also revealed that neutral and charged endohedral clusters $Au_{12}M$ (M = Hf, Ta, W, Re, Os) form stable symmetrical or quasi-symmetrical structures for different values of total cluster charge. The latter property makes possible attachment/ detachment of functional ligands, and could have a potential for drug delivery.

Keywords: Nanoparticles, cage structure, endohedral gold clusters, gold nanoparticles, 5d-elements.

INTRODUCTION

Gold nanoparticles (AuNPs) attract great attention due to their perfect symmetrical structure and wide range of functional properties [1]. Interaction of Au nanocrystals with organometallic thiols leads to the formation of hybrid metal-organic nanostructured systems [2,3], which are considered as perspective microelectronic materials. Generation of light in AuNPs laser (i.e. spaser [4]) is believed to be explained by the presence of surface plasmon excitations in AuNPs. The plasmon excitations in nanoclusters containing HOMO-LUMO gap can be described as transitions between molecular orbitals [5] and hence the investigation of electron structure of AuNPs and gold clusters is required for the proper descriptions of plasmons. Plasmonic effects determine many biological applications of AuNPs [6]. AuNPs were widely used as compounds of antimicrobial agents, as well as in medicine for diagnostics and target drugs delivering to specific organs under treatment. Employment of small AuNPs for drugs delivery could be very promising for a large number of biological applications due to their low toxicity [7]. It was found that AuNps increase the sensitivity of cancer cells to X-ray and proton radiation in a broad spectrum of relevant clinical energies, and potentially could be used to increase their therapeutic effects [8]. Functionalized AuNPs can play a relevant role as intercellular gene regulation agents and in study of mechanism of tumor progression [9].

The specificity of chemical bonding in AuNPs is determined by the relativistic effects, which induce splitting of Au5d shell followed by the shift of $Au5d_{5/2}$ subshell toward the higher energy level. This shift increases the electron density of 5d-orbitals at Fermi level, and provides the structural features of gold nanoclusters [10]. Structure of flat gold clusters exists due to $6s$-$5d_{zz}$ hybridization [11]. Electronic level structure predicted by theoretical calculations for noble metals is in a good agreement with the results obtained by photoelectron spectroscopy. According to the experiment [12], contribution of Au5d-orbitals at Fermi level of gold is significantly higher than that of silver. Theoretical calculations predict that small energetically stable Au_n clusters should have a planar shape [11,13]. Small deviation from this rule have been obtained theoretically for Au_6 [11, 13] and Au_8 [14]. Transformation of the planar structure into a hollow cage occurs at n=17 [15]. Density Functional Theory (DFT) calculations predicts that Au_n clusters (n=32, 33, 34 and 35) have a cage-like shape [16].

At n=13, which is called the magic number, some of metal clusters have a symmetrical icosahedral or cuboctahedral shape. According to the DFT calculations [17], there are a lot of low-energy isomers of M_{13} nanoclusters (M = Cu, Ag, Au) with similar values of binding energy. However, Au_{32}, Au_{42}, and Au_{72} clusters have icosahedral structure [18,19], whereas Au_{20} cluster has a tetrahedral shape [19,20] with bond length of 2.68, 2.83, 2.97, and 3.12 Å. These values are close to the bond length in a bulk gold (2.88 Å). Symmetric cell structures are usually associated with

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the spherical aromaticity criterion for number of electrons *n* in the cluster: $n=2(N+1)^2$, where $N \geq 2$ is an integer number [19]. Embedding of W atom into the center of Au_{12} icosahedron cage provides 18-electrons closed-shell configuration. Icosahedral structure of 18-electrons clusters have been predicted theoretically [21] and observed experimentally for the cases of $Au_{12}W$ and $Au_{12}Mo$ [22]. Anionic clusters $Au_{12}V^-$, $Au_{12}Nb^-$, $Au_{12}Ta^-$ are also predicted to have an icosahedral structure [23], thus confirming the 18-electrons rule, which corresponds to the closed-shell configuration $s^2p^6d^{10}$ in spherical case or $a_g^2t_{1u}^6h_g^{10}$ in I_h case. On the other hand, for endohedral *p*-electron atoms the 20-electrons rule was theoretically confirmed for icosahedral $Au_{12}Sn^{4-}$ structure [24]. Small gold clusters attract great interest since in larger nanoparticles functional ligands are bonded to icosahedral or cuboctahedral cluster core [25-27]. In particular, surrounded by ligands Au_{102} nanoparticle was found to consist of 20 atom caps at poles and 13 atom equatorial level [28]. Thus the investigation of chemical properties of gold clusters can shed a light on the nature of functionalization of AuNPs.

MATERIALS AND METHODS

DFT calculations of structure and electronic properties of gold clusters have been performed using GAUSSIAN quantum chemical package by B3LYP method with Lanl2dz basis set for all atoms except of Si and S, for which 6-21G(d) basis set was used. In this paper we investigate two types of modified AuNPs. The first one contains the terminal SH and SiO_4H_3 groups, modeling attachment of functional ligands. The second one includes endohedral Au_{12} hollow clusters, which contain atom of elements surrounding Au in a periodic table enclosed into their inner cavity.

RESULTS AND DISCUSSION

Figure **1** shows theoretically predicted stable planar and quasi-planar $Au_6(D_{3h})$, Au_6 (C_{5v}) Au_{10}, Au_{12}, and Au_{13}^- clusters. Au_6 (C_{5v}) structure has pentagonal pyramidal shape.

Two cage-like Au_{20} and Au_{32} clusters are shown in Figure **2**. As can be seen from the Figures **1** and **2**, Au_{10}, Au_{12}, Au_{13}^-, Au_{20}, and Au_{32} consist of combinations of smaller elements $Au_6(D_{3h})$ and $Au_6(C_{5v})$. These

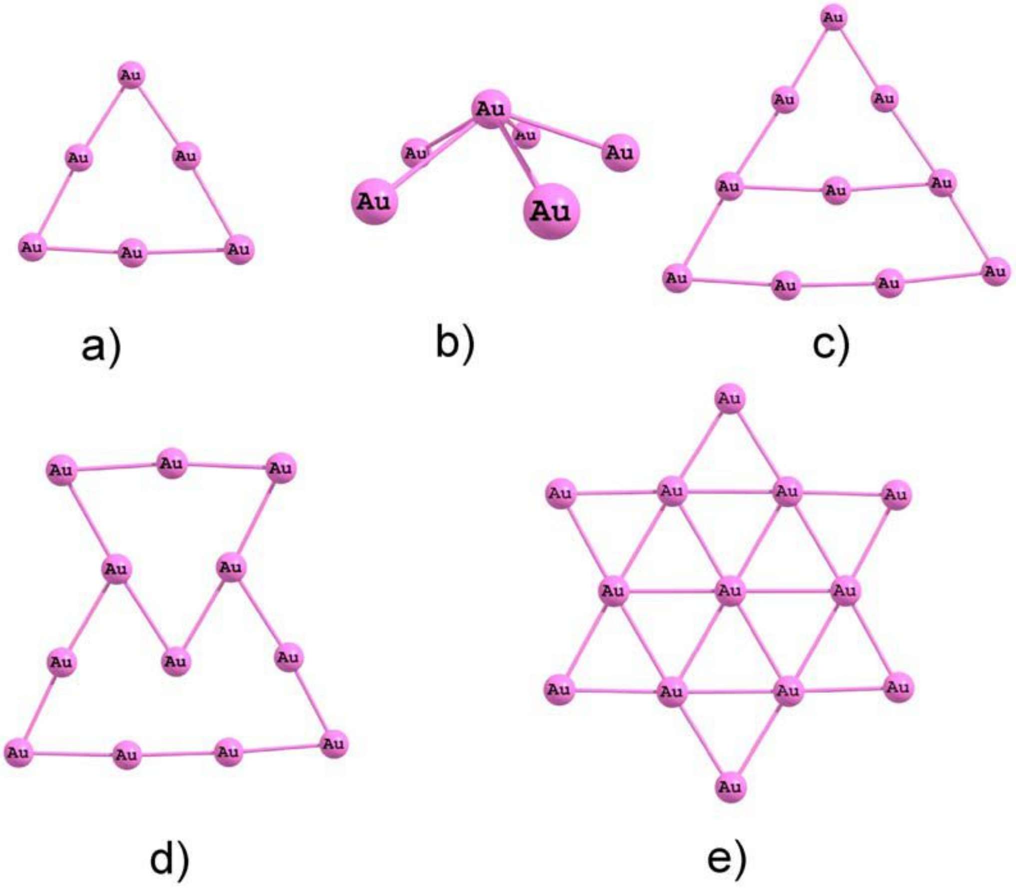


Figure 1: Small planar and quasi-planar gold clustered: **a**) $Au_6(D_{3h})$, **b**) $Au_6(C_{5v})$, **c**) Au_{10}, **d**) Au_{12} and **e**) Au_{13}^-.

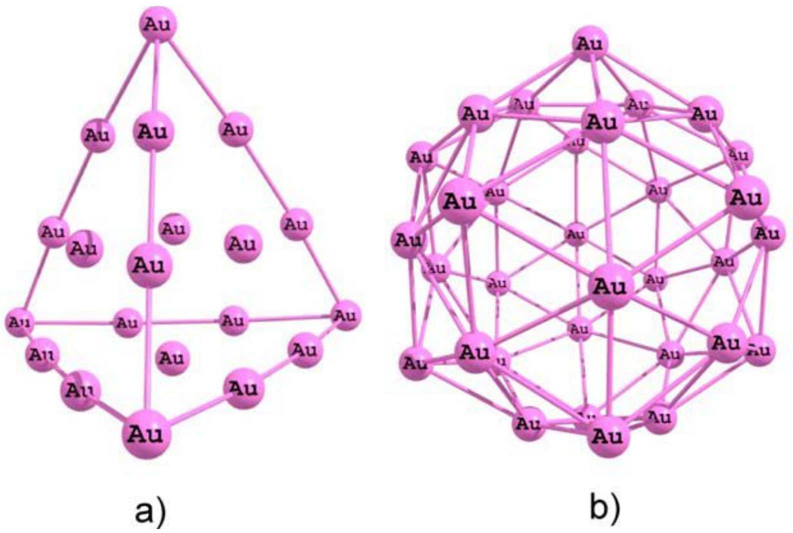


Figure 2: Two cage structures **a**) Au_{20} and **b**) Au_{32}.

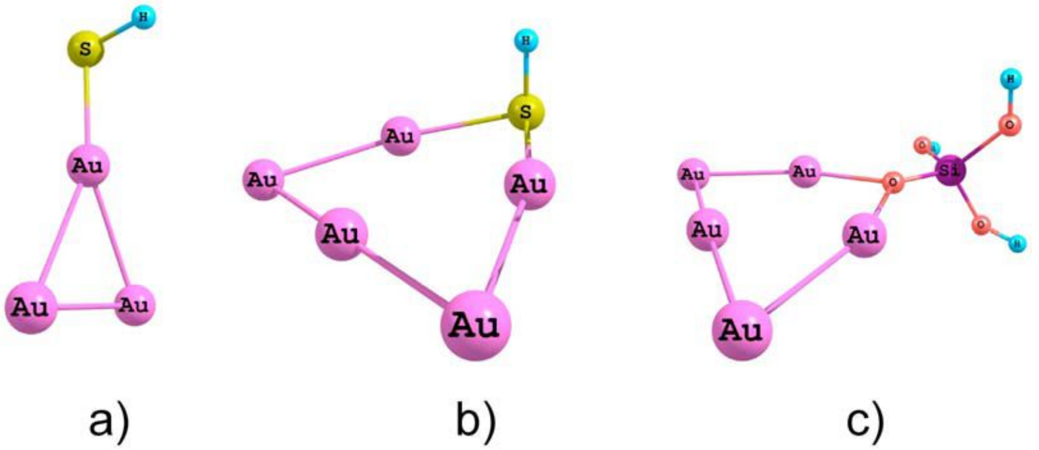


Figure 3: Modified gold clusters: **a**) Au_3SH with single Au-S bond, **b**) Au_5SH obtained by replacement of Au in Au_6 by SH and **c**) $Au_5SiO_4H_3$ obtained by replacement of Au in Au_6 by SiO_4H_3.

structures were found recently in [11,18,19] and described as fractals. In the present work we investigate modifications some of the above considered gold clusters.

Figure **3a** shows the theoretically predicted stable Au_3SH cluster with single Au-S bond. Figures **3b** and **3c** present structures obtained by replacement of one Au atom in Au_6 particle by SH and SiO_4H_3 functional groups.

Theoretically calculated Au-S bond lengths are given in Table **1**. Both $Au_6(D_{3h})$ and $Au_6(C_{5v})$ structures after replacement of one Au atom by SH group give the same structure shown in Figure **3b**. Replacement of one atom in Au_{10} by the same functional groups also keeps the shape almost unchanged (see Figure **4**).

In a large cage-like tetrahedral Au_{20} cluster we investigated replacement of Au by functional groups at different positions and attachment of SH group to the cage. The results are shown in Figure **5a-d**.

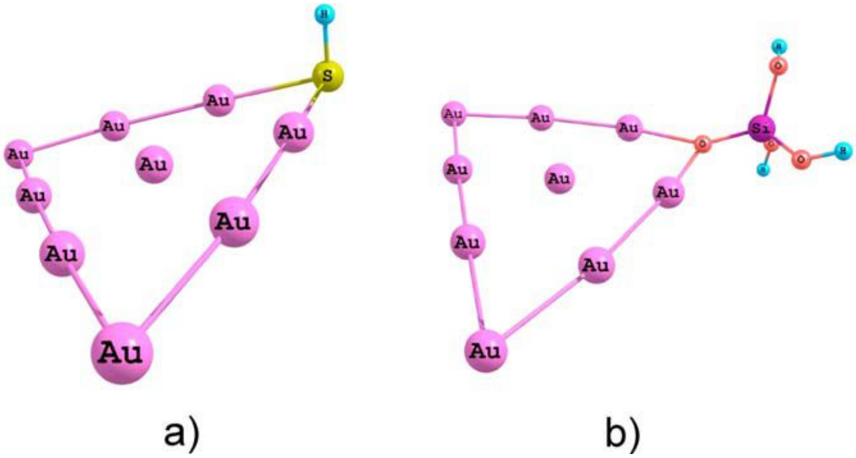
Table 1: Calculated Au-S Bond Lengths and Au-S-Au Bond Angles

	Bond order	Bond lengths (in Å)[1]	Bond angles[2]
Au_3SH	1	2.323	
Au_5SH	2	2.454, 2.454	79°
Au_9SH	2	2.527, 2.527	70°
$Au_{19}SH$ (a)	3	2.646, 2.646, 2.646	87°
$Au_{19}SH$ (b)	2	2.472, 2.472	103°
$Au_{20}SH$ (c)	2	2.468, 2.581	78°

[1] Experimental [28] Au-S bond lengths are 2.2-2.6 Å

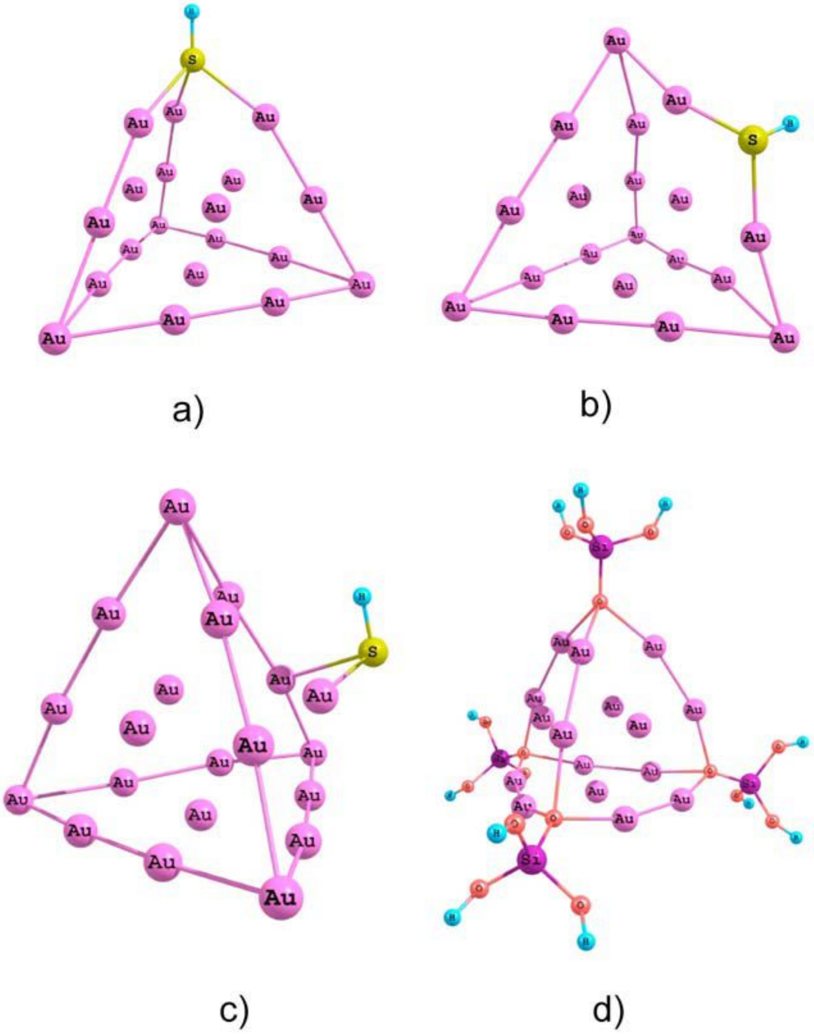
[2] Experimental [28] Au-S-Au bond angles are 80°-115°

Replacement of the vertex Au atoms by SH-group a) and by SiO_4H_3 group d) does not lead to significant changes in the shape. But replacement of one Au atom



a) b)

Figure 4: Modified structures of Au_{10}: **a**) Au_9SH and **b**) $Au_9SiO_4H_3$.



a) b)

c) d)

Figure 5: Modified structures of Au_{20}: **a**) Au atom in a vertex position is replaced by SH group, **b**) Au atom of a side face is replaced by SH group, **c**) SH group is attached to the side face of Au_{20}, **d**) four vertex Au atoms are replaced by SiO_4H_3 groups.

in the side face of the tetrahedron leads to pushing of the functional group out from the plane (Figure **5b**) and forming of only two bonds between sulfur and gold atoms. If SH group is attached to a face side of Au_{20} cluster, S atom also forms two bonds with Au atoms (Figure **5c**). Thus, sulfur atom may form single, double and triple bonds with gold clusters. Theoretically calculated bond lengths and angles (see Table **1**) are in agreement with experimental data [28].

Adding of one 5d-element to Au_{12} formula results in all cased stable endohedral structure instead of plane

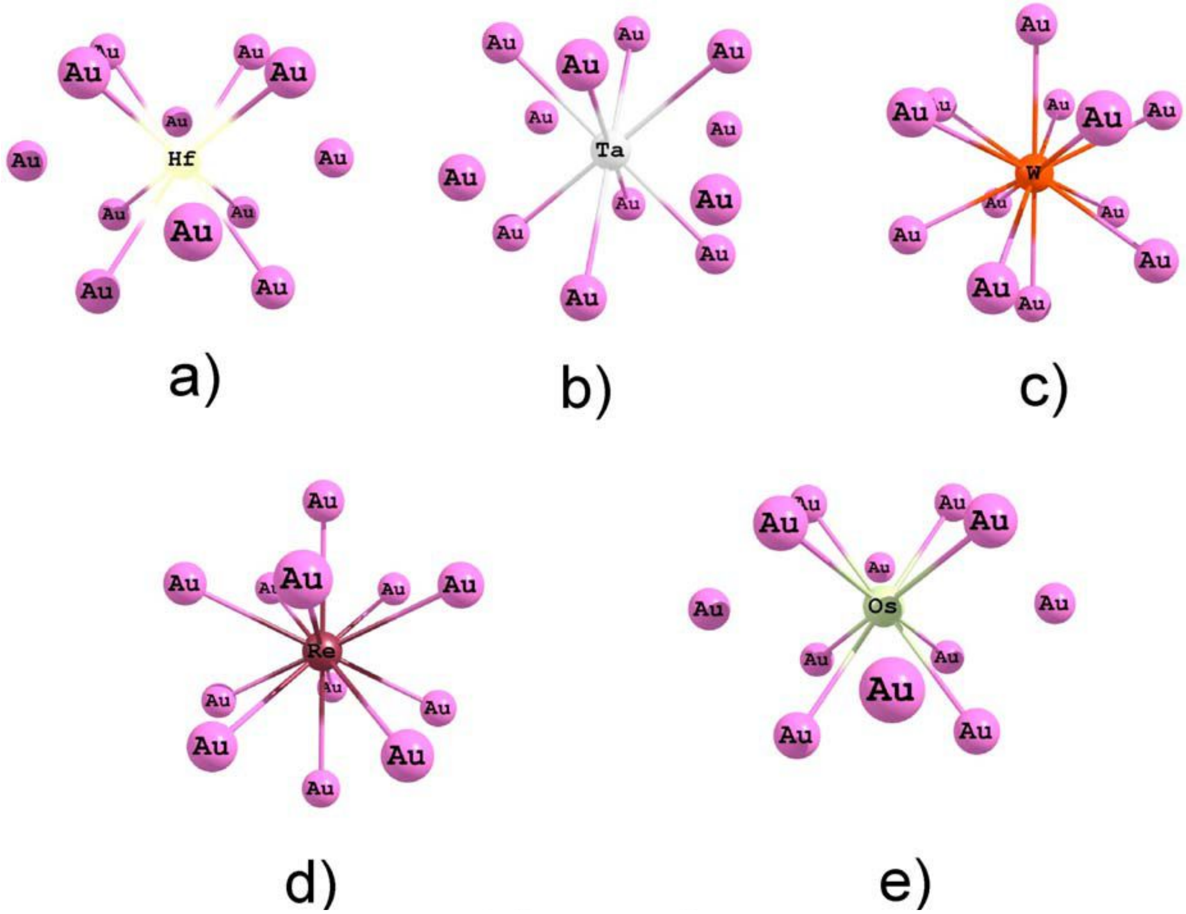


Figure 6: $Au_{12}M$ clusters: **a**) $Au_{12}Hf$ (distorted cuboctahedron), **b**) $Au_{12}Ta$ (distorted cuboctahedron), **c**) $Au_{12}W$ (icosahedron), **d**) $Au_{12}Re$ (distorted cuboctahedron), and **e**) $Au_{12}Os$ (distorted cuboctahedron).

Au_{13}^{-} structure shown in Figure **1e**). Theoretically predicted endohedral $Au_{12}M$ (M=Hf, Ta, W, Re and Os) clusters are shown in Figure **6**. All these structures are stable, and central atom forms 12 bonds with Au atoms. Symmetry of $Au_{12}Hf$ cluster is D_{4h}, and corresponds approximately to the distorted cuboctahedron. Eight short bonds 2.87 Å are directed toward the top and bottom faces of distorted cube, whereas four long bonds 2.97 Å (not shown in the Figure **6**), are directed toward the atoms in the equatorial plane. Similar structure was obtained for $Au_{12}Ta$, with length of short and long bonds of 2.85 Å and 2.92 Å, respectively. $Au_{12}W$ cluster has a perfect icosahedral shape with the value of W-Au bond length of 2.81 Å. Similar perfect octahedral $Au_{12}W$ structure with Au-W bond length of 2.68 Å was obtained earlier in [21]. Symmetry of $Au_{12}Re$ is also D_{4h}, with eight short bonds (2.78 Å), and four long bonds (3.06 Å). $Au_{12}Os$ cluster also has a distorted cuboctahedral shape with eight short bonds (2.74 Å) and four long bonds (3.21 Å).

Our DFT calculations of 18-electron clusters $Au_{12}Hf^{2-}$, $Au_{12}Ta^{-}$, $A_{12}Re^{+}$, $Au_{12}Os^{2+}$ revealed that they have almost perfect icosahedral shape with Au-M bond lengths of 2.85 Å, 2.82 Å, 2.82 Å, and 2.82 Å that confirms the 18-electrons rule. Calculations of negatively charged 20-electron $Au_{12}W^{2-}$ cluster predict slightly distorted icosahedral shape, with bond lengths of 2.81-2.82 Å. Thus, we found two stable forms of 13-atomic clusters $Au_{12}Hf$, $Au_{12}Ta$, $Au_{12}Re$, and $Au_{12}Os$: perfect icosahedron and distorted cuboctahedron. The perfect icosahedral shape corresponds to the 18-electron ionic clusters, whereas the distorted cuboctahedral shape corresponds to the neutral clusters. It should be noted that calculations of clusters $Au_{12}M$ (M element from Hf to Hg) in X_{α} ZORA approximation resulted in that in all case except W, the O_h clusters are more stable than I_h isomers [29].

Table **2** shows the total energy differences between neutral and charged clusters. Energy differences between neutral and negatively charged $Au_{12}Ta$ clusters is about 3-4 eV, which is close to the vertical detachment energies of small gold clusters [30] and hollow golden cages [31]. This energy difference for $Au_{12}Hf^{2-}$, normalized by the number of electron, is 1.47 eV, i.e. twice less, than for pure gold clusters. Thus the chemical properties of combined endohedral clusters $Au_{12}M$ are similar to that of pure gold ones, but there are two differences. The structure of endohedral clusters is more compact then that of plane small gold clusters. Depending on the atomic number of 5d element, they can attach/detach one or two electrons with the changes of their endohedral structures. This attachment/detachment is accompanied by structure changes between icosahedron and distorted cuboctahedron.

Table 2: Total Energies of Ionic Clusters Relatively the Total Energies of Neutral Clusters (eV)

Positively charged ions	Negatively charged ions		
Au_6^+	+8.46	Au_6^-	-2.31
Au_{10}^+	+7.38	Au_{10}^-	-4.21
Au_{12}^+ Au_{12}^+	+7.23	Au_{12}^-	-4.66
Au_{20}^+	+7.41	Au_{20}^-	-2.57
$Au_{12}Re^+$	+5.89	$Au_{12}Hf^{2-}$	-2.94
$Au_{12}Os^{2+}$	+15.61	$Au_{12}Ta^-$	-3.40

Table 3: HOMO-LUMO Gaps in Neutral and Charged Clusters $Au_{12}M$ (in eV)

18-electron clusters	Clusters with the number of electrons differing from 18		
$Au_{12}Hf^{2-}$	2.40	$Au_{12}Hf$	1.52
$Au_{12}Ta^-$	2.39	$Au_{12}Ta$	0.81
$Au_{12}W$	2.90^1)		
$Au_{12}Re^+$	2.79	$Au_{12}Re$	1.54
$Au_{12}Os^{2+}$	2.85	$Au_{12}Os$	1.47

1) Gap value 3.0 eV was obtained in [21].

Filling of 18 electron closed shell is accompanied by increasing of HOMO-LOMO gap (see Table **3**), which indicates stabilization of a cluster. All HOMO-LUMO gaps are close to that of $Au_{12}W$ [21].

The electronic structure of gold clusters differs significantly from that of the bulk one due to the energy gap, which decreases almost monotonic from 1.91 eV for Au_{20} to 0.72 eV for Au_{72} [19]. The exclusion from monotonic rule is Au_{42}, for which gap equals to 0.42. Note that in our B3lyp approach the gap in Au_{20} equals to 2.49 eV [13], thus it is somewhat overestimated relative to more sophisticated mp2 approach [19]. This trends for band gap variation when going from clusters to nanoparticles and then to solids are quite general. For example the gap decreases from small Se chains to larger chains and further to semiconducting solid [32].

In a conclusion, it was found that attachment of functional group (SH and SiO_4H_3) to gold clusters, or replacement of an Au atom by the functional groups leads to formation of single, double or triple bonds depending of position of the group. This result is in good agreement with experimental data, which reveals broad range of S-Au distances [28]. I was also found that doubly charged 18-electrons clusters $Au_{12}Hf^{2-}$ and $Au_{12}Os^{2+}$ have the icosahedral structure, thus confirming the 18-electrons rule in two mores cases. Neutral $Au_{12}Hf$, $Au_{12}Ta$, $Au_{12}Re$, and $Au_{12}Os$ clusters are stable and have the distorted cuboctahedral shape. So, bimetallic clusters considered above have some new properties with respect to pure gold clusters. Their coboctahedral or icosahedral shape is more adapted for attachment and transport of functional ligands than the planar shape of small gold clusters.

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