Supporting Information: Amino Acids Conjugated Gold Clusters: Interaction of Alanine and Tryptophan with Au_8 and Au_{20}

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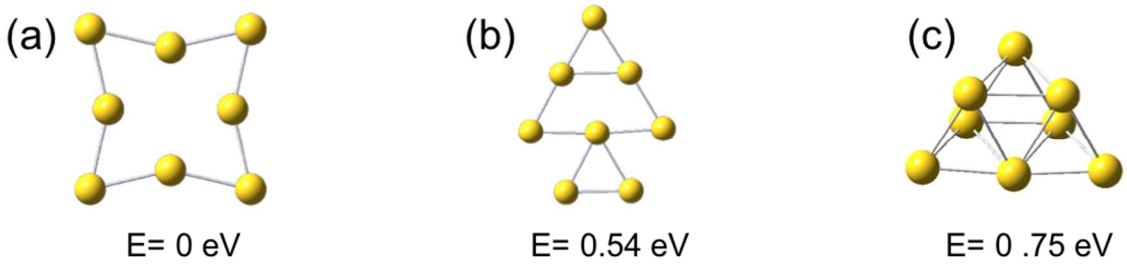


Figure S1. (a-c) Geometrical structures of Au_8 cluster. E is the energy difference between the given structure and the minimum energy geometry.

Table S1. Calculated structural parameters of Au_8 (D_{4h}) and Au_{20} (T_d) clusters in the gas and solvent phases.

Parameters	Au_8 (gas)	Au_8 (solvent)	Au_{20} (gas)	Au_{20} (solvent)
R (Au-Au)	2.7, 2.9	2.7, 2.9	2.8, 2.9, 3.1	2.8, 2.9, 3.1
ΔE_{BE}/dimer (eV)	-1.27	-1.12	-1.71	-1.51
Dipole moment, Debye	0.02	0.00	0.00	0.05
HOMO-LUMO gap (eV)	2.75	2.95	2.93	3.04

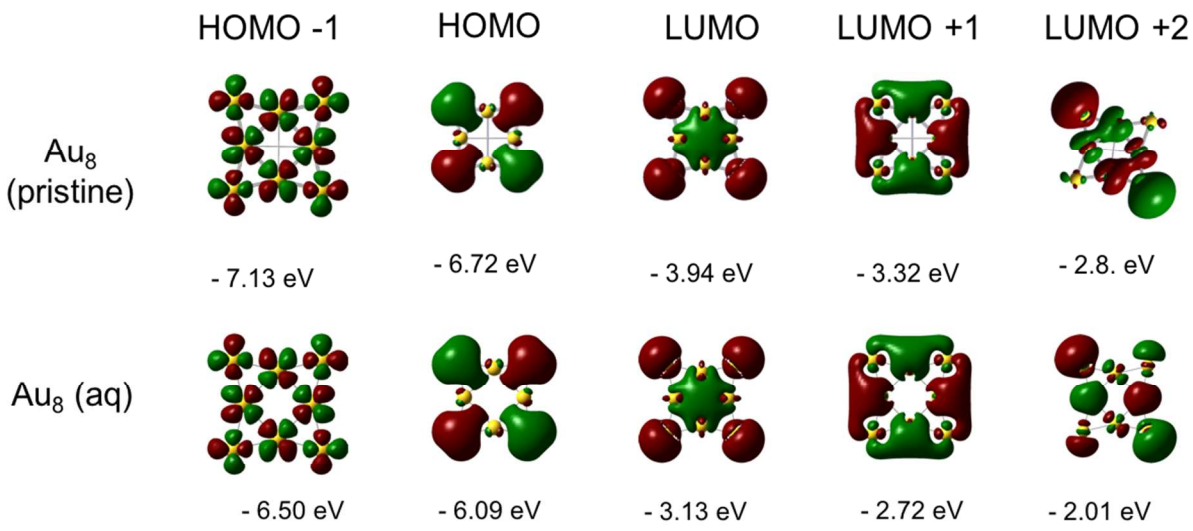


Figure S2. Frontier orbitals (HOMO-1 to LUMO+2) of Au_8 cluster in the gas and solvent (aq) phases.

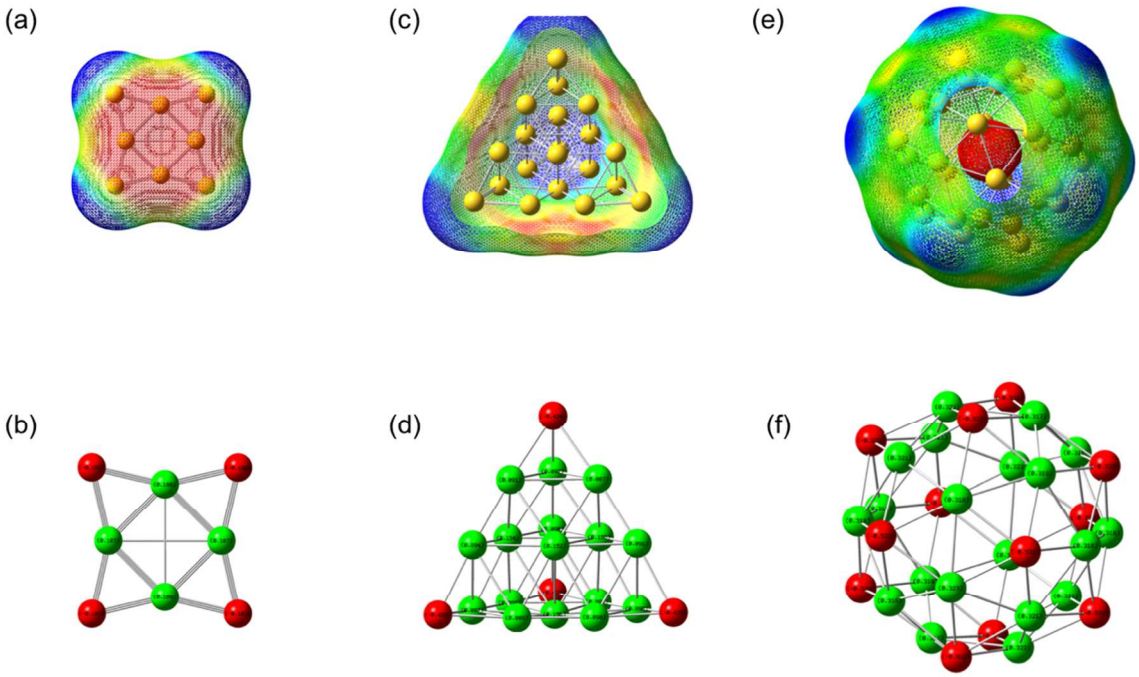
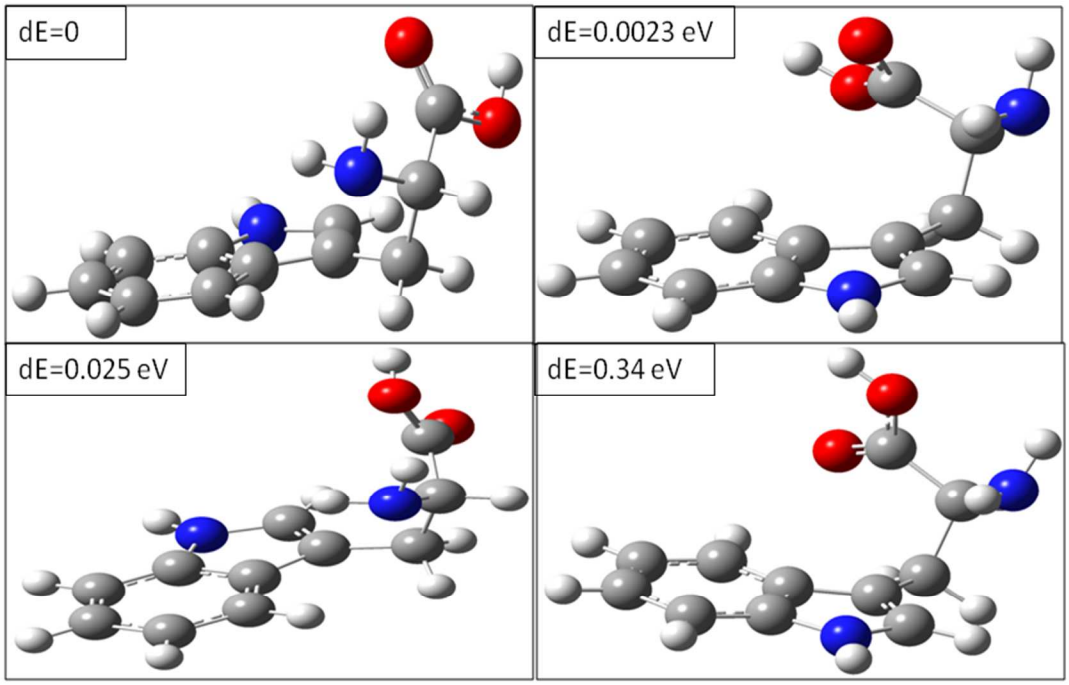


Figure S3. The ESP and Mulliken charge distribution of; (a)-(b) Au_8, (c)-(d) Au_{20}, and (e)-(f) Au_{32} clusters. ESP range: -0.1 (red) to +0.1 (blue). Mulliken charge: red corresponds to negative, and green corresponds to positive charge values.

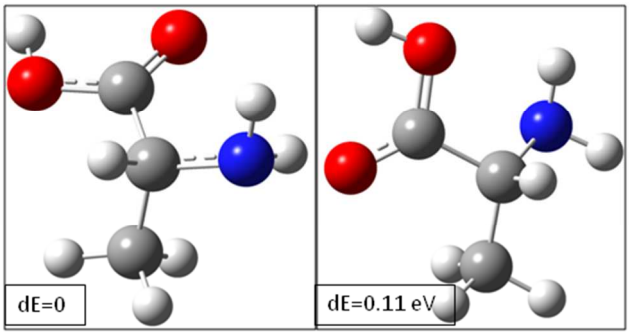
Table S2. Calculated structural parameters, dipole moments and energy gap of Trp and Ala in the gas and solvent phases. R is bond length in Å, A is the plane angle in degree, and D is the dihedral angles in degree.

Parameters	Trp (gas)	Trp (solvent)	$Trp_{(zw)}$ (solvent)	Ala (gas)	Ala (solvent)	$Ala_{(zw)}$ (solvent)
R(1-3) (Å)	1.21	1.21	1.27	1.21	1.22	1.27
R(2-3) (Å)	1.36	1.35	1.24	1.36	1.35	1.24
R(3-4) (Å)	1.53	1.53	1.57	1.53	1.53	1.57
R(4-5) (Å)	1.45	1.46	1.51	1.46	1.46	1.51
A(3, 4, 5) °	113.0	113.1	104.2	113.0	113.1	104.0
A(4, 3, 1) °	125.3	125.2	113.7	125.2	125.0	113.6
A (4, 3, 2) °	112.5	112.1	117.0	112.2	112.1	117.1
A(6, 4, 5) °	111.5	110.4	113.8	-	-	-
D(5, 4, 3, 1) °	3.2	-5.1	10.5	13.1	13.6	-2.8
D(5, 4, 3, 2) °	-178.8	174.5	-170.5	-167.5	-167.1	177.5
D (7, 6, 4, 5) °	65.4	66.5	53.4	-	-	-
D(7, 6, 4, 3) °	-61.7	-60.0	-65.2	-	-	-
Dipole moment, Debye	2.0	1.7	14.1	1.3	1.7	11.4
Energy gap, eV	5.2	5.2	5.3	6.6	7.6	7.6

(a) Isomers of Trp and their energies relative to the ground state



(b) Isomers of Ala and their energy relative to the ground state



Scheme S1. The isomers of canonical Trp (a) and Ala (b) in the gas phase.

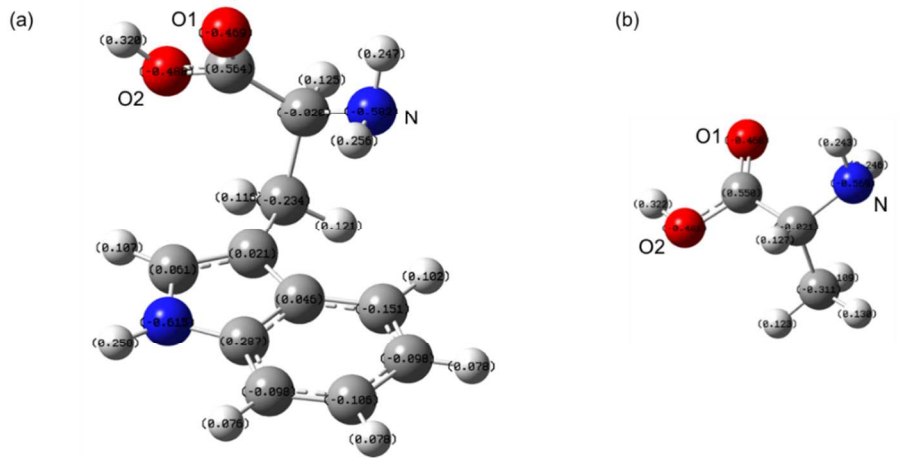


Figure S4. Trp and Ala in the canonical configurations in the gas phase: Mulliken charges (a) Trp; N. -0.58 e, NH_2. -0.08, O1. -0.47, O2. -0.49, and COOH. -0.07 e. (b) Ala; N. -0.57 e, NH_2. -0.08, O1. -0.47, O2. -0.48, and COOH. -0.08 e.

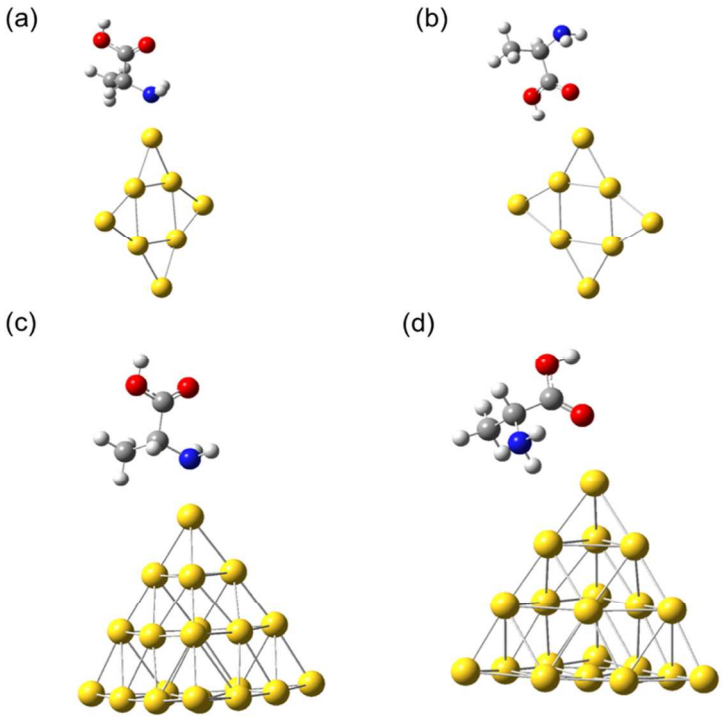


Figure S5. Au_n-Ala clusters in the solvent phase; (a) Au_8-Ala, with Au-N single site interaction via amine site. (b) Au_8-Ala, with Au-O single site interaction via carboxylic site. (c) Au_{20}-Ala, with Au-N single site interaction via amine site. (d) Au_{20}-Ala, with Au-O single site interaction via carboxylic site.

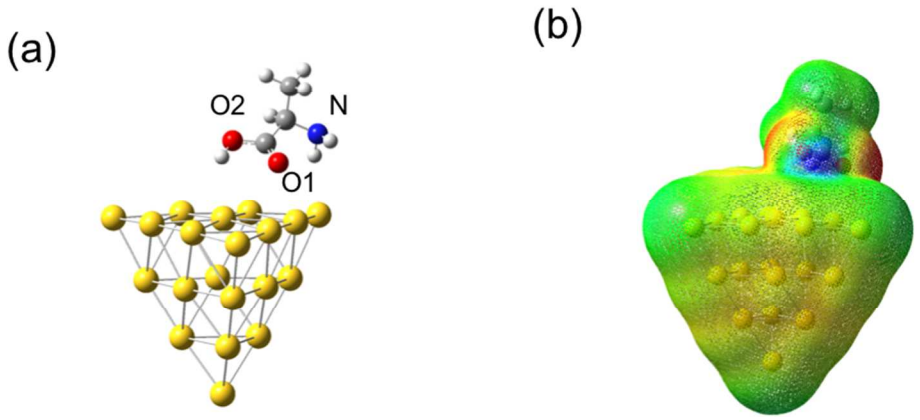


Figure S6. (a) The gas phase equilibrium configuration of Au_{20}-Ala representing single site interaction through the face atoms, (b) ESP of Au_{20}-Ala. ESP range: -0.025 (red) to 0.045 (blue).

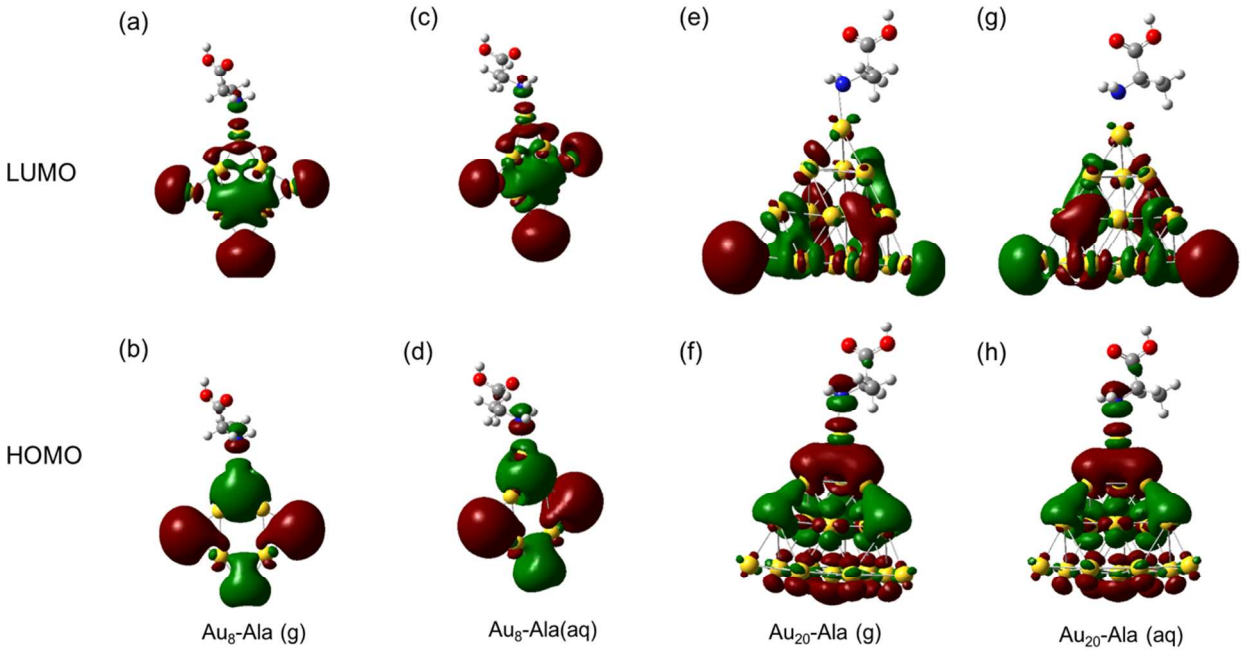


Figure S7. The frontier orbitals corresponding to the HOMO and the LUMO of; (a)-(b) Au_8-Ala (g), (c)-(d) Au_8-Ala (aq), (e)-(f) Au_{20}-Ala (g) and (g)-(h) Au_{20}-Ala (aq) complexes interacting through the amine site with the isovalue of 0.02 (e/Å^3).

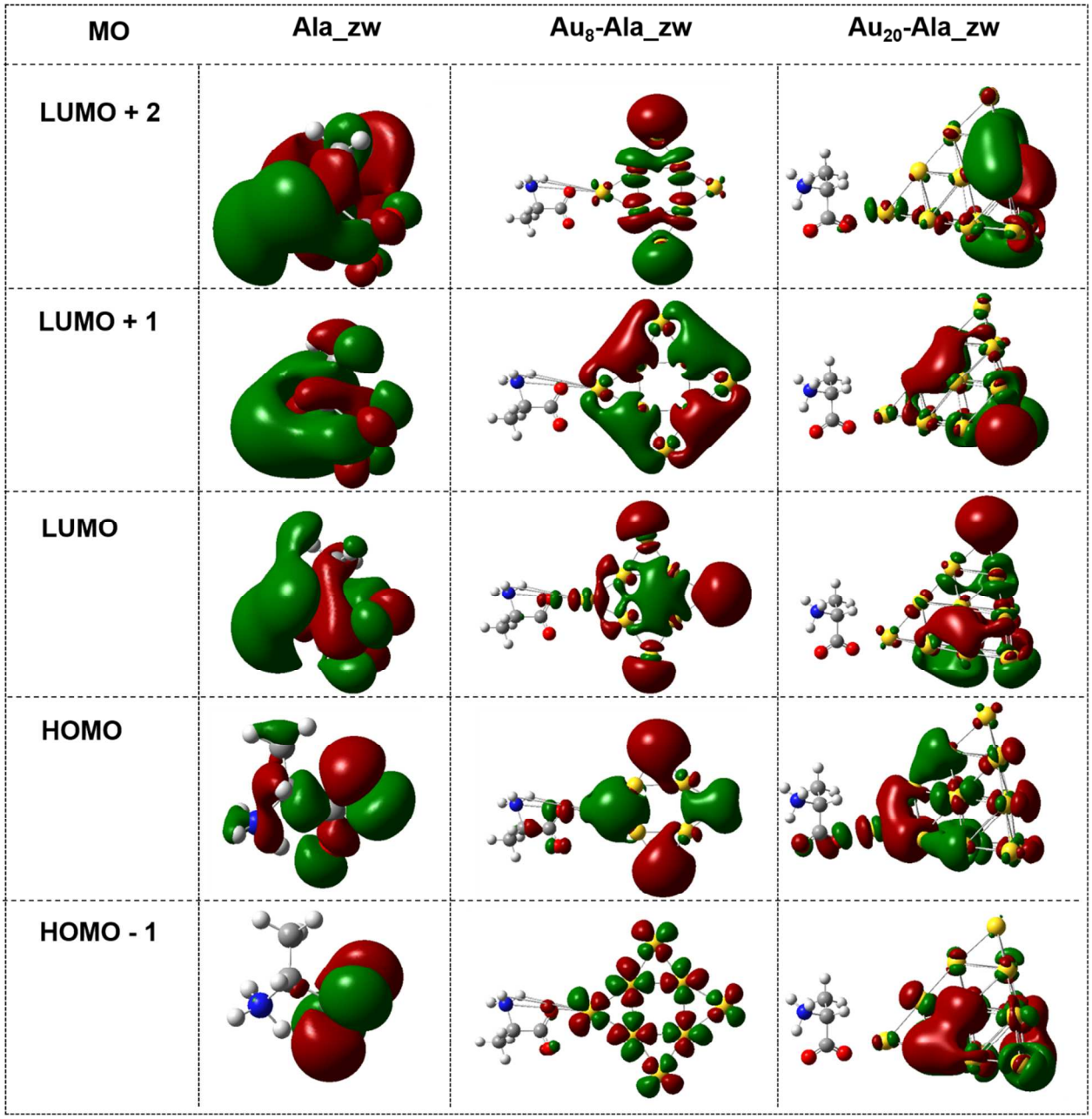


Figure S8. Frontier orbitals corresponding to HOMO-1 to LUMO+2 for $Ala_{(zw)}$, Au_8-$Ala_{(zw)}$, and Au_{20}-$Ala_{(zw)}$ complexes in solvent phase.

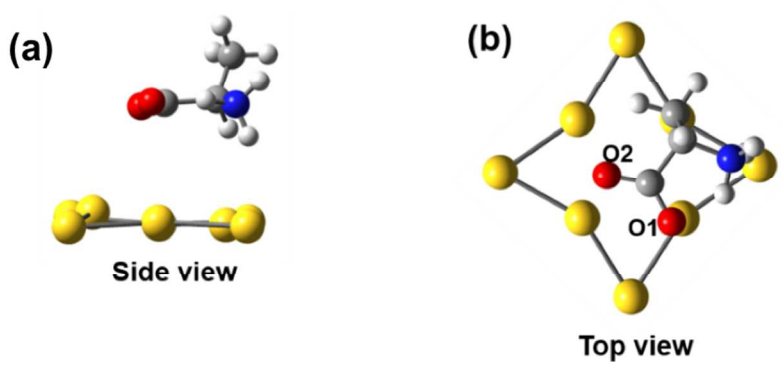


Figure S9. (a) Side view and (b) Top view of Au_8-$Ala_{(zw)}$ complex stabilized via multi-site interaction in solvent phase.

Table S3. Calculated electronic properties of Au_8-$Ala_{(zw)}$ complex stabilized via multi-site interaction in solvent phase.

Parameter	Au_8-$Ala_{(zw)}$
E_{Total} (eV)	-38306.6123
$\Delta E_{B.E}$ (eV)	-0.20
R (Au-N) Å	3.69
R(Au-O1) Å	3.47
R(Au-O2) Å	3.57
Q-Au (e)	-0.19
Dipole moment (Debye)	11.92

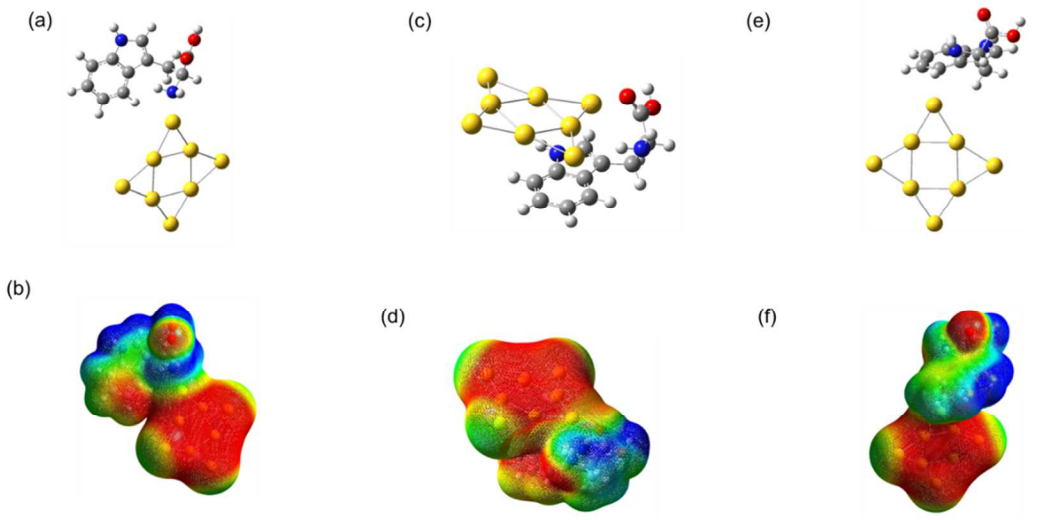


Figure S10. The equilibrium configuration and ESP of Au_8-Trp complexes in the solvent phase. (a)-(b) Amine site with Au-N single site interaction, (c)-(d) Carboxylic site with Au-O single site interaction, Au_8 ~ 4 Å above indole plane and parallel to it, and (e)-(f) Indole site with Au-C single site interaction. ESP range: -0.025(red) to 0.045 (blue).

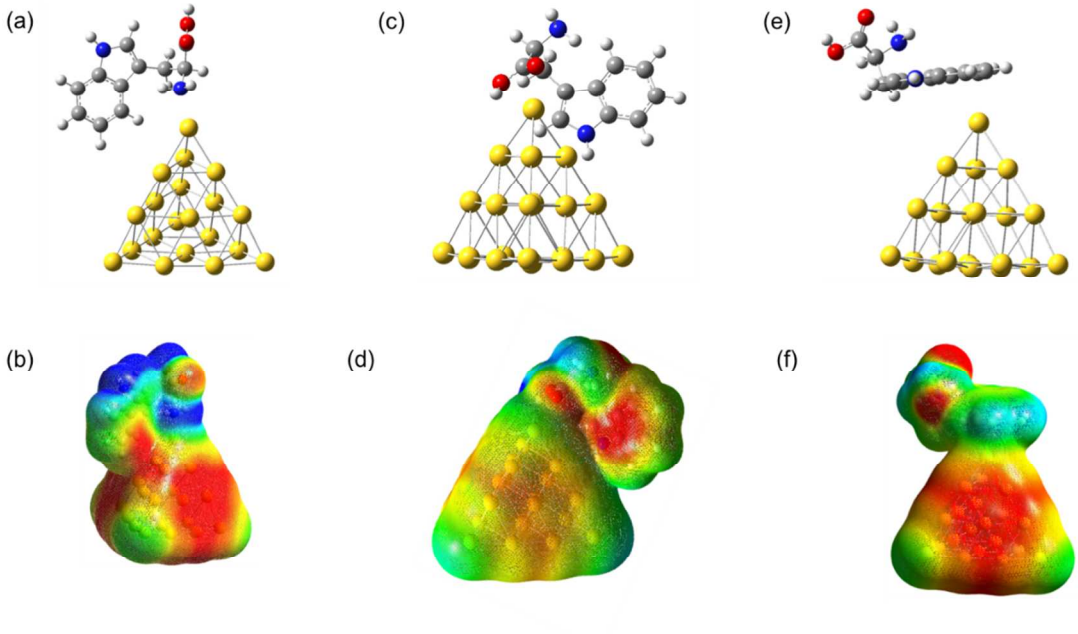


Figure S11. The equilibrium configuration and ESP of Au_{20}-Trp complexes in the solvent phase. (a)-(b) Amine site with Au-N single site interaction, (c)-(d) Carboxylic site with Au-O single site interaction, and (e)-(f) Indole site with Au-C single site interaction. ESP range: -0.025(red) to 0.045 (blue).

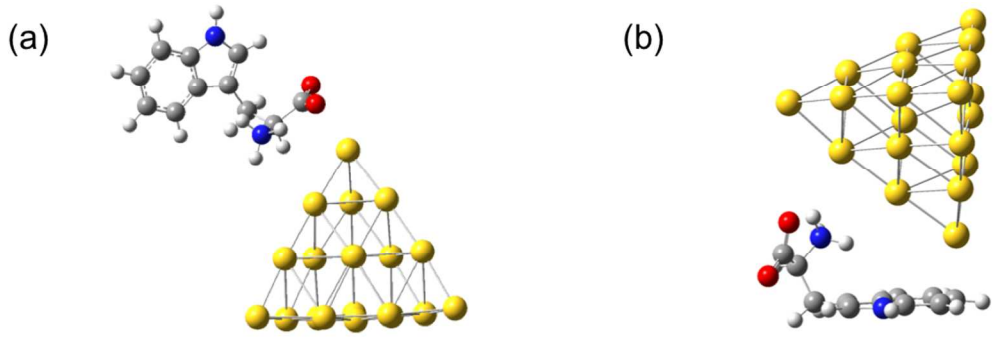


Figure S12. The equilibrium configuration of Au_{20}-$Trp_{(zw)}$ which are (a) 0.23 eV and (b) 0.28 eV above the minimum energy configuration.