Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2017

Supporting Information for:

σ-Holes and σ-Lumps Directs the Lewis Basic and Acidic Interactions of Noble Metal Nanoparticles: Introducing Regium Bonds

Joakim Halldin Stenlid[a], Adam Johannes Johansson[b] and Tore Brinck[a*]

[a] *Applied Physical Chemistry, School of Chemical Science and Engineering, KTH Royal Institute of Technology, Stockholm, Sweden,* [b] *Swedish Nuclear Fuel and Waste Management Company (SKB), Stockholm, Sweden*

**Address correspondence to Tore Brinck. Address: Teknikringen 30, SE-100 44, Stockholm, Sweden; Email: tore@kth.se*

Contents

S1. The N_2, Cl_2 and Ag_2 dimers

Included below are complementary figures illustrating for the N_2, Cl_2 and Ag_2 dimers: the sigma*-orbitals of N_2 and Cl_2 are shown in Figure S1 to illustrate the formation of sigma-lump ($V_{S,min}$) and a sigma-hole ($V_{S,max}$) at the end of the N_2 and Cl_2 dimers respectively. Figure S2 demonstrates the favored interaction behavior of Ag_2: the Ag-dimer interacts head-on with the Lewis basic O-atom of formaldehyde (CH_2O) and edge-on with the Lewis acidic B-atom of the BF_3 molecule.

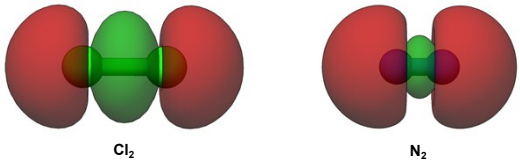

Figure S1. Displays the highest sigma*-orbitals of the Cl_2 and N_2 dimers.

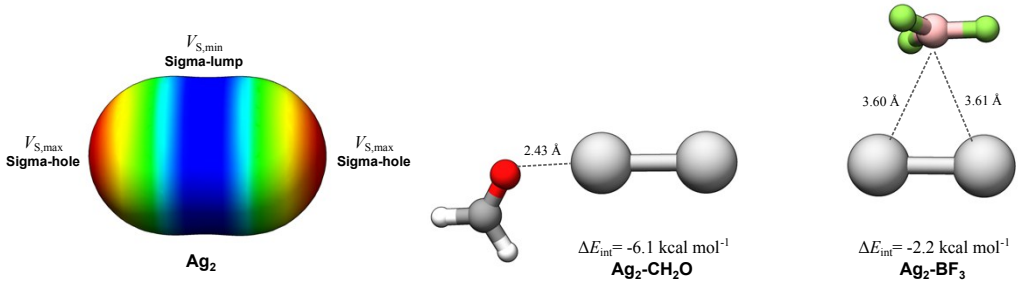

Figure S2. Electrostatic surface potential, $V_S(\mathbf{r})$, of Ag_2 on the 0.001 a.u. isodensity contour (left). Sigma holes and lumps are marked at the end and bridge sites respectively. The favored adsorption modes with the CH_2O (middle) electron donor and BF_3 (right) electron acceptor molecules are also included. All structures and energies are determined at the PBE0-D3(BJ)/def2-TVZPP level of theory[1–4] using effective core potentials (ECP)[4] for the Ag atoms.

S2. Nanoparticle orbitals

The virtual orbitals used in the evaluation of $E(\mathbf{r})$ are visualized in Figure S1 whereas Figure S2 contains all frontier molecular orbitals (FMO) of the studied metal nanoparticles.

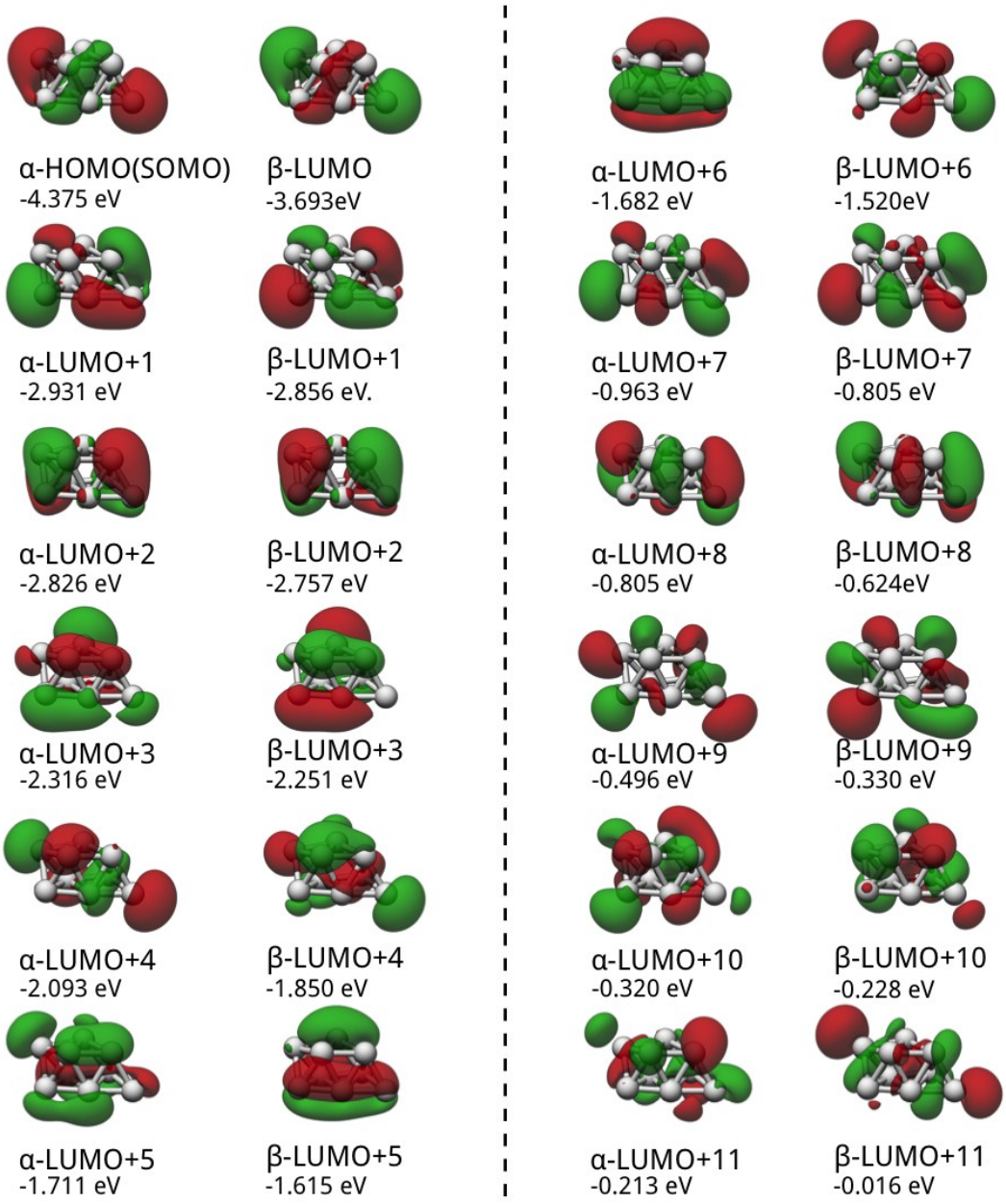

Figure S3. Displays all the virtual orbitals of Ag_9 with eigenvalues below zero, i.e. the orbitals used in the determination of the $E(\mathbf{r})$ descriptor values.

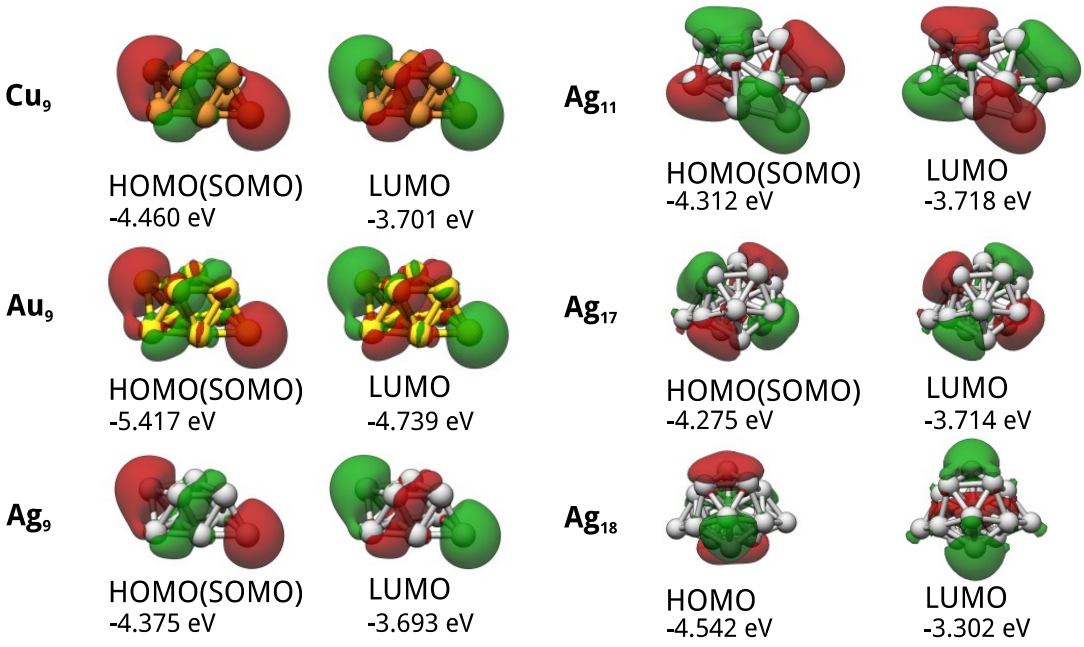

Figure S4. HOMO (SOMO) and LUMO orbitals of the studied nanoparticles.

S3. Descriptor values and geometric information

Tables S1, S3, S6-S10 contains the local descriptor values ($V_{S,max}$, $E_{S,min}$, $\bar{I}_{S,ave}$, and partial charges from NBO, Mulliken and Bader analysis) of the Ag, Cu and Au nanoparticles used in this study. Interaction energies and adsorption distances for the studied probe compound interactions are summarized in Tables S2, S4 and S5.

Table S1. Ag_9 Lewis acidity details at the atomic sites: $V_{S,max}$ [kcal mol^{-1}], $E_{S,min}$ [eV] and $\bar{I}_{S,ave}$ [eV] as determined at the PBE0*/LACV3P*//PBE0*/LANL2-DZ level of theory with PBE0* indicating 10% HF admixture and atomic partial charges (q_{NBO}, q_{Bader} and $q_{Mulliken}$) obtained at the PBE0-D3(BJ)/def2-TVZPP//PBE0-D3(BJ)/def2-TVZP level of theory. $V_{S,max}$ and $E_{S,min}$ are reported at both the 0.001 and 0.004 a.u. isodensity surface.

Site	$V_{S,max}^{0.001}$	$V_{S,max}^{0.004}$	$E_{S,min}^{0.001}$	$E_{S,min}^{0.004}$	$\bar{I}_{S,ave}$	q_{NBO}	q_{Bader}	$q_{Mullliken}$
1	7.47	24.63	-5.94	-3.01	6.28	-0.073	0.037	0.015
2	3.24	18.49	-3.99	-2.07	6.3	-0.432	0.069	0.005
3	10.78	28.64	-7.32	-3.82	6.24	0.141	0.114	-0.066
4	18.31	38.46	-9.73	-4.62	6.57	0.201	0.037	0.029
5=6	8.92	26.47	-6.47	-3.29	6.3	-0.070	0.062	0.029
7=8	14.93	34.48	-8.36	-4.05	6.57	0.042	0.059	-0.007
9	13.72	32.04	-8.49	-4.34	6.4	0.219	0.085	-0.026

Table S2. Interaction information for the adsorption of electron donating probe molecules on Ag_9: Interaction energy (ΔE_{int}) in kcal mol^{-1} and average interaction distances (d_{mean}) in Å from the central atom of electron-donator to the closest Ag atom. Structures and energies were obtained at the PBE0-D3(BJ)/def2-TVZPP//PBE0-D3(BJ)/def2-TVZP level of theory.

Site	ΔE_{int} (H_2O)	d_{mean} (H_2O)	ΔE_{int} (H_2S)	d_{mean} (H_2S)	ΔE_{int} (NH_3)	d_{mean} (NH_3)	ΔE_{int}[a)] (CO)	d_{mean}[b)] (CO)
1	-4.8	2.55	-6.8	2.69	-9.0	2.38	-6.7	2.19
2	-3.7	2.63	-5.1	2.77	-7.2	2.41	-4.6	2.21
3	-5.7	2.49	-8.0	2.65	-10.9	2.34	-8.9	2.18
4	-6.8	2.46	-9.8	2.61	-12.8	2.33	-10.5	2.14
5=6	-5.1	2.53	-7.5	2.66	-9.8	2.36	-7.7	2.15
7=8	-6.4	2.46	-9.4	2.61	-12.0	2.33	-10.3	2.13
9	-6.4	2.47	-8.7	2.64	-12.1	2.34	-8.6	2.19

[a)] from ref 5. [b)] reoptimized at the PBE0-D3(BJ)/def2-TVZP level of theory.

Table S3. Ag_9 Lewis basicity details: $V_{S,min}$ and $\bar{I}_{S,min}$ at the 0.001 a.u. isosurface as determined at the PBE0*/LACV3P*//PBE0*/LANL2-DZ level of theory with PBE0* indicating 10% HF admixture.

Site	$V_{S,min}$ [kcal mol^{-1}]	$\bar{I}_{S,min}$ [eV]
h_{138}/h_{158}	-10.76	5.76
h_{245}/h_{258}	-10.26	5.95
h_{178}	-0.24	6.50
h_{345}	0.13	6.42
h_{789}	1.68	6.59

Table S4. Interaction information for the adsorption of electron-acceptors on Ag_9: Interaction energy (ΔE_{int}) in kcal mol^{-1} and average interaction distances (d_{mean}) in Å from central atom of electron-acceptor to the three closest Ag atoms. Structures and energies were obtained at the PBE0-D3(BJ)/def2-TVZPP//PBE0-D3(BJ)/def2-TVZP level of theory.

Site	ΔE_{int} (BH_3)	d_{mean} (BH_3)	ΔE_{int} (BF_3)	d_{mean} (BF_3)	ΔE_{int} (HCl)	d_{mean} (HCl)	ΔE_{int} (Na^+)	d_{mean} (Na^+)
h_{138}/h_{158}	-28.8	2.42	-4.6	3.68	-5.6	2.83	-37.1	3.11
h_{245}/h_{258}	-24.6	2.47	-4.7	3.75	-5.8	2.86	-38.2	3.08
h_{178}	-21.6	2.48	-3.9	3.66	-5.1	2.75	-30.7	3.16
h_{345}	-22.4	2.48	-3.5	3.72	-4.4	2.81	-30.7	3.15
h_{789}	-23.3	2.49	-3.3	3.72	-4.6	2.75	-27.2	3.18

Table S5. Interaction information for the adsorption of H_2O and H_2S on Cu_9 and Au_9: Interaction energy (ΔE_{int}) in kcal mol^{-1} and average interaction distances (d_{mean}) in Å from central atom of electron-donator to the closest metal atom. Structures and energies were obtained at the PBE0-D3(BJ)/def2-TVZPP//PBE0-D3(BJ)/def2-TVZP level of theory.

Site	ΔE_{int} (Cu_9-H_2O)	d_{mean} (Cu_9-H_2O)	ΔE_{int} (Cu_9-H_2S)	d_{mean} (Cu_9-H_2S)	ΔE_{int} (Au_9-H_2O)	d_{mean} (Au_9-H_2O)	ΔE_{int} (Au_9-H_2S)	d_{mean} (Au_9-H_2S)
1	-5.9	2.19	-8.6	2.36	-5.4	2.51	-14.0	2.49
2	-3.5	2.28	-5.7	2.43	-2.8	2.62	-9.3	2.61
3	-8.0	2.14	-10.9	2.34	-6.4	2.45	-15.4	2.44
4	-9.5	2.12	-12.7	2.33	-9.0	2.38	-18.2	2.42
5=6	-6.6	2.18	-9.4	2.36	-6.0	2.47	-14.6	2.45
7=8	-8.7	2.13	-12.4	2.32	-7.0	2.43	-16.6	2.43
9	-9.3	2.12	-11.8	2.34	-7.2	2.42	-15.8	2.47

Table S6. Au_9 Lewis acidity details at the atomic sites: $V_{S,max}$ [kcal mol^{-1}] and $E_{S,min}$ [eV] as determined at the PBE0*/LACV3P*//PBE0*/LANL2-DZ level of theory with PBE0* indicating 10% HF admixture. $V_{S,max}$ and $E_{S,min}$ are reported at both the 0.001 and 0.004 a.u. isodensity surface.

Site	$V_{S,max}^{0.001}$	$V_{S,max}^{0.004}$	$E_{S,min}^{0.001}$	$E_{S,min}^{0.004}$
1	4.94	18.39	-6.85	-3.83
2	0.39	11.62	-4.17	-2.41
3	8.14	22.89	-8.04	-4.7
4	16.09	34.62	-11.38	-6.15
5=6	6.08	19.95	-7.39	-4.07
7=8	10.17	25.85	-8.87	-4.8
9	12.48	29.42	-9.70	-5.55

Table S7. Cu_9 Lewis acidity details at the atomic sites: $V_{S,max}$ [kcal mol^{-1}] and $E_{S,min}$ [eV] as determined at the PBE0*/LACV3P*//PBE0*/LANL2-DZ level of theory with PBE0* indicating 10% HF admixture. $V_{S,max}$ and $E_{S,min}$ are reported at both the 0.001 and 0.004 a.u. isodensity surface.

Site	$V_{S,max}^{0.001}$	$V_{S,max}^{0.004}$	$E_{S,min}^{0.001}$	$E_{S,min}^{0.004}$
1	8.44	25.52	-6.30	-2.86
2	3.30	16.31	-3.66	-2.01
3	13.11	31.82	-7.95	-4.11
4	21.04	41.6	-10.26	-4.82
5=6	9.72	27.15	-6.78	-3.69
7=8	16.46	36.1	-8.88	-4.29
9	16.98	36.2	-9.69	-4.87

Table S8. Ag_{11} Lewis acidity details at the atomic sites: $V_{S,max}$ [kcal mol^{-1}], $E_{S,min}$ [eV] and $\bar{I}_{S,ave}$ [eV] as determined at the PBE0*/LACV3P*//PBE0*/LANL2-DZ level of theory with PBE0* indicating 10% HF admixture and atomic partial charges (q_{NBO}, q_{Bader} and $q_{Mulliken}$) obtained at the PBE0-D3(BJ)/def2-TVZPP//PBE0-D3(BJ)/def2-TVZP level of theory. $V_{S,max}$ and $E_{S,min}$ are reported at both the 0.001 and 0.004 a.u. isodensity surface.

Site	$V_{S,max}^{0.001}$	$V_{S,max}^{0.004}$	$E_{S,min}^{0.001}$	$E_{S,min}^{0.004}$	$\bar{I}_{S,ave}$	q_{NBO}	q_{Bader}	$q_{Mulliken}$
1	13.24	32.19	-7.83	-3.8	6.55	0.031	0.044	-0.468
2=10	10.36	28.13	-7.78	-3.86	6.19	0.181	0.043	-0.133
3=11	15.14	34.56	-8.99	-4.43	6.4	0.255	0.054	-0.103
4=6	-0.71	14.45	-4.98	-2.64	6.19	-0.634	0.074	0.415
5=9	16.53	36.31	-8.9	-4.31	6.59	0.232	0.074	-0.282
7=8	13.03	33.02	-7.76	-3.83	6.44	-0.048	0.114	0.338

Table S9. Ag_{17} Lewis acidity details at the atomic sites: $V_{S,max}$ [kcal mol^{-1}], $E_{S,min}$ [eV] and $\bar{I}_{S,ave}$ [eV] as determined at the PBE0*/LACV3P*//PBE0*/LANL2-DZ level of theory with PBE0* indicating 10% HF admixture and atomic partial charges (q_{NBO}, q_{Bader} and $q_{Mulliken}$) obtained at the PBE0-D3(BJ)/def2-TVZPP//PBE0-D3(BJ)/def2-TVZP level of theory. $V_{S,max}$ and $E_{S,min}$ are reported at both the 0.001 and 0.004 a.u. isodensity surface.

Site	$V_{S,max}^{0.001}$	$V_{S,max}^{0.004}$	$E_{S,min}^{0.001}$	$E_{S,min}^{0.004}$	$\bar{I}_{S,ave}$	q_{NBO}	q_{Bader}	$q_{Mulliken}$
1=6	0.10	11.47	-4.83	-2.45	6.09	-0.393	0.037	-0.748
2=3	12.21	30.99	-8.12	-3.62	6.39	0.238	0.040	0.027
4=17	14.14	33.16	-8.49	-3.82	6.39	0.308	0.021	0.108
5=7	7.71	23.77	-8.14	-4.20	6.31	-0.164	0.075	-1.093
8=12	8.68	26.97	-7.07	-3.40	6.37	0.103	0.058	-1.260
9=14	21.45	44.82	-11.10	-5.20	6.73	0.336	0.043	-1.311
11=16	11.60	30.28	-8.02	-3.66	6.33	0.238	0.034	-1.208
13=15	14.79	34.97	-8.93	-4.31	6.48	0.322	0.046	-1.240

Table S10. Ag_{18} Lewis acidity details at the atomic sites: ($V_{S,max}$ [kcal mol^{-1}], $E_{S,min}$ [eV] and $\bar{I}_{S,ave}$ [eV] as determined at the PBE0*/LACV3P*//PBE0*/LANL2-DZ level of theory with PBE0* indicating 10% HF admixture and atomic partial charges (q_{NBO}, q_{Bader} and $q_{Mulliken}$) obtained at the PBE0-D3(BJ)/def2-TVZPP//PBE0-D3(BJ)/def2-TVZP level of theory. $V_{S,max}$ and $E_{S,min}$ are reported at both the 0.001 and 0.004 a.u. isodensity surface.

Site	$V_{S,max}^{0.001}$	$V_{S,max}^{0.004}$	$E_{S,min}^{0.001}$	$E_{S,min}^{0.004}$	$\bar{I}_{S,ave}$	q_{NBO}	q_{Bader}	$q_{Mulliken}$
1=5	3.77	15.21	-4.68	-2.62	6.21	-0.383	0.102	-0.759
2	11.75	30.25	-7.19	-3.36	6.44	0.261	0.038	0.081
3	11.55	29.75	-6.88	-3.82	6.41	0.208	0.027	0.071
4=18	18.00	38.13	-9.78	-4.71	6.60	0.328	0.044	0.195
6	0.85	13.59	-4.11	-2.30	6.14	-0.270	0.021	-0.857
7=12	6.26	23.24	-5.95	-3.09	6.38	-0.074	0.035	-1.108
8=13	9.40	27.46	-6.84	-3.46	6.46	0.110	0.090	-1.324
9	21.44	44.95	-11.05	-5.60	6.83	0.345	0.090	-1.313
11=15	11.40	30.10	-6.85	-3.56	6.37	0.274	-0.019	-1.196
14	21.26	44.91	-10.85	-5.36	6.75	0.262	0.055	-1.342
16	12.2	31.15	-6.96	-3.52	6.40	0.245	-0.010	-1.282

S4. Functional test

The tables S12 to S15 summarizes the evaluation of the $V_{S,max}$ and $E_{S,min}$ descriptors determined using different exchange-correlation functionals with respect to interactions energies of the H_2O, H_2S, NH_3 and CO molecules adsorbed on the Ag_9 nanoparticle. As can be seen from the tables the prediction quality of the $V_{S,max}$ and $E_{S,min}$ descriptors is general not largely affected by the choice of functional. However, there are some distinct features can be noted. First of all $V_{S,max}$ performs well when obtained with all functionals, with the clear exceptions of B3LYP, and to a smaller degree for PBE and HSE06. The $V_{S,max}$ gives good correlations when determined at both the 0.001 and 0.004 a.u. isodensity surfaces. Concerning $E_{S,min}$, the 0.001 a.u. isosurface generally gives better results. $E_{S,min}$ seems to be largely affected by the amount of HF admixture in the exchange-correlation functional, which can be traced back to the number of virtual orbitals with negative eigenvalues. The dependence on the amount of HF admixture is especially apparent when evaluated at the denser 0.004 a.u. isodensity surface. From the test we find that the PBE0 functional with very high amount of HF admixture (66.7%) yields poor results, while the long-range corrected functionals LC-ωPBE and CAM-B3LYP give the weakest correlations among the studied functionals (due to very few virtual orbitals with negative eigenvalues). The pure GGA functionals appears to provide slightly weaker correlations than the hybrid functionals, especially when evaluated on the 0.004 a.u isosurface. We have decided to use the PBE0-$\frac{1}{10}$ (i.e. with 10% HF admixture) in this study since it gives reliable results for both descriptors, for all adsorbents and on different isosurfaces.

Table S11. Exchange-correlation functional test for the Ag_9-H_2O interactions. Reported are R^2 correlation constants for ΔE_{int} versus descriptor value ($V_{S,max}$ and $E_{S,min}$) at the 0.001 and 0.004 a.u. isodensity surfaces.

Functional[a]	$V_{S,max}^{0.001}$	$E_{S,max}^{0.001}$	$V_{S,min}^{0.004}$	$E_{S,min}^{0.004}$
PBE[6]	0.962	0.983	0.953	0.882
LC-ωPBE[7]	0.991	0.113	0.992	0.666
$\frac{1}{3}$	0.971	0.989	0.966	0.984
$\frac{1}{4}$	0.974	0.993	0.970	0.982
$\frac{1}{5}$	0.978	0.993	0.975	0.978
$\frac{1}{6}$	0.975	0.984	0.976	0.919
$\frac{1}{7}$	0.985	0.955	0.970	0.852
$\frac{1}{8}$	0.989	0.373	0.995	0.183
HSE06[8,9]	0.968	0.992	0.965	0.986
TPSSh[10,11]	0.979	0.984	0.975	0.966
B3LYP[12,13]	0.935	0.986	0.924	0.904
CAM-B3LYP[14]	0.980	0.943	0.976	0.862

[a] The amount of HF admixture used in the tested PBE0 functional family is given supplied as $\frac{X}{Y}$. [b] I.e. the original PBE0 functional of Adamo *et al*.[1]

Table S12. Exchange-correlation functional test for the Ag_9-H_2S interactions. Reported are R^2 correlation constants for ΔE_{int} versus descriptor value ($V_{S,max}$ and $E_{S,min}$) at the 0.001 and 0.004 a.u. isodensity surfaces.

Functional[a]	$V_{S,max}^{0.001}$	$E_{S,max}^{0.001}$	$V_{S,min}^{0.004}$	$E_{S,min}^{0.004}$
PBE[6]	0.968	0.965	0.974	0.808
LC-ωPBE[7]	0.951	0.757	0.965	0.740
$\frac{1}{3}$	0.971	0.968	0.979	0.939
$\frac{1}{4}$	0.971	0.972	0.980	0.937
$\frac{1}{5}$	0.972	0.971	0.982	0.932
$\frac{1}{6}$	0.966	0.945	0.980	0.868
$\frac{1}{7}$	0.973	0.867	0.977	0.758
$\frac{1}{8}$	0.951	0.552	0.982	0.340
HSE06[8,9]	0.969	0.973	0.978	0.945
TPSSh[10,11]	0.970	0.934	0.981	0.893
B3LYP[12,13]	0.962	0.972	0.962	0.826
CAM-B3LYP[14]	0.974	0.933	0.982	0.808

[a] The amount of HF admixture used in the tested PBE0 functional family is given supplied as $\frac{X}{Y}$. [b] I.e. the original PBE0 functional of Adamo *et al*.[1]

Table S13. Exchange-correlation functional test for the Ag_9-NH_3 interactions. Reported are R^2 correlation constants for ΔE_{int} versus descriptor value ($V_{S,max}$ and $E_{S,min}$) at the 0.001 and 0.004 a.u. isodensity surfaces.

Functional[a)]	$V_{S,max}^{0.001}$	$E_{S,max}^{0.001}$	$V_{S,min}^{0.004}$	$E_{S,min}^{0.004}$
PBE[6]	0.951	0.983	0.940	0.892
LC-ωPBE[7]	0.988	0.024	0.988	0.652
$\frac{1}{3}$	0.961	0.987	0.954	0.990
$\frac{1}{3}$	0.964	0.991	0.959	0.988
$\frac{1}{1}$	0.969	0.990	0.965	0.984
$\frac{1}{1}$	0.966	0.979	0.965	0.927
$\frac{1}{1}$	0.977	0.944	0.951	0.855
$\frac{1}{2}$	0.976	0.320	0.988	0.168
HSE06[8,9]	0.957	0.988	0.952	0.990
TPSSh[10,11]	0.971	0.986	0.965	0.976
B3LYP[12,13]	0.917	0.983	0.905	0.913
CAM-B3LYP[14]	0.969	0.935	0.963	0.855

a) The amount of HF admixture used in the tested PBE0 functional family is given supplied as $\frac{X}{Y}$. b) I.e. the original PBE0 functional of Adamo *et al*.[1]

Table S14. Exchange-correlation functional test for the Ag_9-CO interactions. Reported are R^2 correlation constants for ΔE_{int} versus descriptor value ($V_{S,max}$ and $E_{S,min}$) at the 0.001 and 0.004 a.u. isodensity surfaces.

Functional[a)]	$V_{S,max}^{0.001}$	$E_{S,max}^{0.001}$	$V_{S,min}^{0.004}$	$E_{S,min}^{0.004}$
PBE[6]	0.917	0.920	0.931	0.756
LC-ωPBE[7]	0.872	0.919	0.890	0.784
$\frac{1}{3}$	0.918	0.911	0.934	0.887
$\frac{1}{3}$	0.917	0.912	0.933	0.882
$\frac{1}{1}$	0.917	0.908	0.933	0.873
$\frac{1}{1}$	0.904	0.859	0.926	0.826
$\frac{1}{1}$	0.914	0.672	0.863	0.647
$\frac{1}{2}$	0.804	0.523	0.918	0.542
HSE06[8,9]	0.913	0.911	0.928	0.886
TPSSh[10,11]	0.913	0.866	0.932	0.828
B3LYP[12,13]	0.914	0.920	0.920	0.763
CAM-B3LYP[14]	0.910	0.855	0.924	0.710

a) The amount of HF admixture used in the tested PBE0 functional family is given supplied as $\frac{X}{Y}$. b) I.e. the original PBE0 functional of Adamo *et al*.[1]

S5. Distortion energy and geometries

The Table S15 shows the results of the analysis of the correlation between adsorbate-induced distortion and the corresponding R^2 values for the ΔE_{int} versus descriptor () trends. The distortion is here measured in two ways: first by the distortion energy, ΔE_{dist}, of the nanoparticle substrate upon adsorption by:

$$\Delta E_{dist} = E(distorted\ NP) - E(undistorted\ NP)$$

where the adsorbate molecule has been deleted from the NP structure. Table S15 reports the average distortion energy over the series, $\Delta \bar{E}_{dist}$. We also estimate the distortion by the root mean square deviation (RMSD) for the geometrical change of the particles.

Table S15. Displays data from the distortion analysis for a selection of nanoparticles and adsorbates including Ag: average distortion energy (in eV) and the corresponding standard deviation (St.dev.), as well as the RMSD of the geometric change of the NP upon interaction compared to the optimized NP structure, and the corresponding standard deviation (St.dev.).

Adsorbate	Particle	$\Delta \bar{E}_{dist}$	St.dev.	RMSD	St.dev.
H_2O	Ag_9	0.008	0.003	0.036	0.010
H_2S	Ag_9	0.018	0.008	0.056	0.018
NH_3	Ag_9	0.029	0.029	0.073	0.027
CO	Ag_9	0.032	0.022	0.077	0.041
H_2O	Cu_9	0.027	0.014	0.078	0.034
H_2O	Au_9	0.025	0.013	0.063	0.025
	R^2 vs. $V_{S,max}$	0.582	0.240	0.490	0.809
	R^2 vs. $E_{S,min}$	0.371	0.319	0.238	0.470

S6. References

(1) Adamo, C.; Barone, V. Toward Reliable Density Functional Methods without Adjustable Parameters: The PBE0 Model. *J. Chem. Phys.* **1999**, *110*, 6158–6170.

(2) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A Consistent and Accurate Ab Initio Parametrization of Density Functional Dispersion Correction (DFT-D) for the 94 Elements H-Pu. *J. Chem. Phys.* **2010**, *132*, 154104.

(3) Grimme, S.; Ehrlich, S.; Goerigk, L. Effect of the Damping Function in Dispersion Corrected Density Functional Theory. *J. Comput. Chem.* **2011**, *32*, 1456–1465.

(4) Weigend, F.; Ahlrichs, R. Balanced Basis Sets of Split Valence, Triple Zeta Valence and Quadruple Zeta Valence Quality for H to Rn: Design and Assessment of Accuracy. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297.

(5) Duanmu, K.; Truhlar, D. G. Partial Ionic Character beyond the Pauling Paradigm: Metal Nanoparticles. *J. Phys. Chem. C* **2014**, *118*, 28069–28074.
(6) Perdew, J. P.; Burke, K.; Ernzerhof, M. Generalized Gradient Approximation Made Simple. *Phys. Rev. Lett.* **1996**, *77*, 3865–3868.
(7) Vydrov, O. A.; Scuseria, G. E. Assessment of a Long-Range Corrected Hybrid Functional. *J. Chem. Phys.* **2006**, *125*, 234109.
(8) Heyd, J.; Scuseria, G. E.; Ernzerhof, M. Hybrid Functionals Based on a Screened Coulomb Potential. *J. Chem. Phys.* **2003**, *118*, 8207–8215.
(9) Heyd, J.; Scuseria, G. E.; Ernzerhof, M. Erratum: “Hybrid Functionals Based on a Screened Coulomb Potential” [J. Chem. Phys.118, 8207 (2003)]. *J. Chem. Phys.* **2006**, *124*, 219906.
(10) Staroverov, V. N.; Scuseria, G. E.; Tao, J.; Perdew, J. P. Comparative Assessment of a New Nonempirical Density Functional: Molecules and Hydrogen-Bonded Complexes. *J. Chem. Phys.* **2003**, *119*, 12129–12137.
(11) Staroverov, V. N.; Scuseria, G. E.; Tao, J.; Perdew, J. P. Erratum: “Comparative Assessment of a New Nonempirical Density Functional: Molecules and Hydrogen-Bonded Complexes” [J. Chem. Phys. 119, 12129 (2003)]. *J. Chem. Phys.* **2004**, *121*, 11507–11507.
(12) Becke, A. D. Density-functional Thermochemistry. III. The Role of Exact Exchange. *J. Chem. Phys.* **1993**, *98*, 5648–5652.
(13) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. Ab Initio Calculation of Vibrational Absorption and Circular Dichroism Spectra Using Density Functional Force Fields. *J. Phys. Chem.* **1994**, *98*, 11623–11627.
(14) Yanai, T.; Tew, D. P.; Handy, N. C. A New Hybrid Exchange–correlation Functional Using the Coulomb-Attenuating Method (CAM-B3LYP). *Chem. Phys. Lett.* **2004**, *393*, 51–57.

S7. Appendix. Optimized structures (xyz-coordinates)

Optimized structures at the Ag, Cu and Au particles with and without adsorbates. All structures are optimized at the PBE0-D3(BJ)/def2-TVZP level of theory.

Ag_9

Ag9 – ground state

Ag	-2.059981	0.197135	0.000000
Ag	1.605696	0.217540	-0.000000
Ag	-1.627231	-2.578373	0.000000
Ag	1.234049	-2.480577	-0.000000
Ag	-0.243045	-0.943107	1.840258
Ag	-0.243045	-0.943107	-1.840258
Ag	-0.241248	1.766243	-1.463614
Ag	-0.241247	1.766243	1.463614
Ag	1.814063	2.996995	-0.000000

H_2O

Ag9-H2O site=1

Ag	-1.901931	0.591155	0.041239
Ag	1.840496	0.097795	-0.027797
Ag	-1.746526	-2.260862	0.057950
Ag	1.120468	-2.523883	0.006264
Ag	-0.161317	-0.782955	1.820462
Ag	-0.229703	-0.808883	-1.783491
Ag	0.138773	1.865149	-1.447328
Ag	0.194665	1.885599	1.430984
Ag	2.397091	2.813204	-0.057969
O	-4.448863	0.645724	0.088949
H	-4.673304	0.101531	0.849780
H	-4.707998	0.127235	-0.678721

Ag9-H2O site=2

Ag	-2.292664	0.039436	-0.000527
Ag	1.439076	0.496241	0.000727
Ag	-1.550371	-2.652738	-0.000860
Ag	1.305370	-2.258868	0.000085
Ag	-0.313678	-0.882225	1.808001
Ag	-0.312605	-0.881478	-1.808239
Ag	-0.617328	1.800610	-1.449829
Ag	-0.618241	1.800030	1.450540
Ag	1.223521	3.313942	0.001226
O	4.051561	0.803325	0.001258
H	4.275995	0.264009	0.765639
H	4.276615	0.262594	-0.761941

Ag9-H2O site=3

Ag	-1.910546	-0.065422	-0.002530
Ag	1.738723	0.471170	0.001167
Ag	-1.108219	-2.789922	-0.005678

Ag	1.683452	-2.275719	-0.001867
Ag	0.029103	-0.949349	1.817243
Ag	0.031898	-0.945681	-1.820551
Ag	-0.311787	1.743744	-1.457648
Ag	-0.313995	1.740839	1.459476
Ag	1.520205	3.278512	0.003920
O	-3.043923	-4.363405	0.001636
H	-3.587894	-4.170399	0.771649
H	-3.598875	-4.171366	-0.760724

Ag9-H2O site=4

Ag	-1.970702	-0.143220	0.007241
Ag	1.553346	0.995633	-0.006344
Ag	-0.674552	-2.634578	0.001672
Ag	2.082675	-1.667861	-0.009776
Ag	0.167671	-0.663069	1.812096
Ag	0.153008	-0.662285	-1.814747
Ag	-0.727022	1.907441	-1.443026
Ag	-0.715772	1.906621	1.449062
Ag	0.889301	3.692169	-0.002563
O	3.136724	-3.892621	-0.010547
H	2.802331	-4.371013	0.754636
H	2.799422	-4.366996	-0.776964

Ag9-H2O site=5

Ag	-1.945535	0.341533	-0.066699
Ag	1.586768	0.349034	-0.348539
Ag	-1.551257	-2.411440	0.112762
Ag	1.278373	-2.332781	-0.108803
Ag	-0.035130	-0.652571	1.775813
Ag	-0.335843	-0.957353	-1.987990
Ag	-0.317654	1.777286	-1.862339
Ag	-0.077332	2.033034	1.113583
Ag	1.830329	3.105301	-0.653178
O	0.056317	-1.527400	4.146706
H	-0.630238	-1.085414	4.654393
H	0.889301	-1.242539	4.533410

Ag9-H2O site=8

Ag	-1.846521	0.229733	0.331911
Ag	1.660863	-0.073566	-0.205608
Ag	-1.734608	-2.534331	-0.045667
Ag	1.050240	-2.706503	-0.521162
Ag	0.051867	-1.272594	1.756480
Ag	-0.493216	-0.831093	-1.932235
Ag	-0.152370	1.808939	-1.225587
Ag	0.297510	1.482052	1.681222
Ag	2.244532	2.636479	-0.038745
O	-0.329321	3.479846	2.975910
H	-0.185410	4.261807	2.435020
H	-1.270046	3.464021	3.174549

Ag9-H2O site=9

Ag	-2.248853	-0.280563	-0.010683
Ag	1.330733	0.550582	0.007969

Ag	-1.203360	-2.902309	0.000569
Ag	1.541134	-2.164624	0.015557
Ag	-0.241368	-0.972635	1.839566
Ag	-0.219485	-0.980515	-1.834907
Ag	-0.791855	1.675194	-1.444848
Ag	-0.807859	1.681706	1.431569
Ag	0.940770	3.326827	-0.000043
O	2.768017	4.988502	-0.006443
H	3.314397	4.927336	-0.795960
H	3.367309	4.868608	0.736584

H_2S

Ag9-H2S site=1

Ag	-1.990065	-0.092313	-0.029913
Ag	1.848469	0.265253	-0.017346
Ag	-1.184634	-2.842978	0.087618
Ag	1.718033	-2.452285	0.087363
Ag	0.010080	-0.992990	1.780117
Ag	0.032006	-1.131836	-1.734416
Ag	-0.201616	1.557321	-1.517950
Ag	-0.218493	1.670411	1.349894
Ag	1.745312	3.036197	-0.128252
S	-4.651058	0.316361	-0.025496
H	-4.674685	0.947222	1.159137
H	-4.611518	1.470446	-0.710457

Ag9-H2S site=2

Ag	-2.360260	0.176583	0.001479
Ag	1.484145	0.165212	-0.002310
Ag	-1.941603	-2.584867	0.001237
Ag	0.962109	-2.573294	-0.001483
Ag	-0.467770	-0.989188	1.773179
Ag	-0.471204	-0.989521	-1.773743
Ag	-0.454173	1.697446	-1.447082
Ag	-0.451326	1.697743	1.445997
Ag	1.523701	3.017176	-0.002713
S	4.253630	0.217952	-0.001716
H	4.394019	1.126134	0.976565
H	4.395973	1.143514	-0.963310

Ag9-H2S site=3

Ag	-1.984853	0.593379	-0.000157
Ag	1.707441	0.257470	-0.002341
Ag	-1.876546	-2.232993	-0.009239
Ag	1.005766	-2.396189	-0.010727
Ag	-0.302861	-0.729331	1.797795
Ag	-0.304111	-0.717821	-1.807598
Ag	0.015755	1.976174	-1.451130
Ag	0.016609	1.966865	1.458492
Ag	2.159149	3.047751	0.006583
S	-3.530328	-4.306819	-0.010523
H	-2.911913	-4.959167	0.987711
H	-2.865969	-4.996311	-0.952767

Ag9-H2S site=4

Ag	-2.214230	0.228816	-0.012898
Ag	1.484168	0.628964	0.014186
Ag	-1.436820	-2.475610	-0.000981
Ag	1.461383	-2.118888	0.020315
Ag	-0.222019	-0.709964	1.798656
Ag	-0.195333	-0.718285	-1.790009
Ag	-0.566143	1.980862	-1.446267
Ag	-0.588333	1.987647	1.436996
Ag	1.364639	3.404956	0.007035
S	2.908406	-4.293870	0.016444
H	3.803906	-3.878519	0.928119
H	3.696825	-3.935941	-1.010837

Ag9-H2S site=5

Ag	-1.858612	0.411918	0.051078
Ag	1.561298	0.323494	-0.474070
Ag	-1.558921	-2.343845	0.222553
Ag	1.244509	-2.347398	-0.199453
Ag	0.125987	-0.622539	1.803279
Ag	-0.467269	-0.953502	-1.991071
Ag	-0.377389	1.780567	-1.921368
Ag	0.106091	2.064106	1.095223
Ag	1.865873	3.063527	-0.869453
S	0.164522	-1.820270	4.180110
H	-0.977471	-1.251865	4.598572
H	0.919483	-0.907513	4.813701

Ag9-H2S site=8

Ag	-1.810873	0.327579	0.242700
Ag	1.666685	-0.162123	-0.171870
Ag	-1.830481	-2.443530	-0.113161
Ag	0.942150	-2.764249	-0.518149
Ag	-0.048116	-1.246642	1.743432
Ag	-0.456944	-0.830775	-1.982622
Ag	-0.001152	1.801357	-1.276074
Ag	0.350005	1.512625	1.645623
Ag	2.417085	2.499883	-0.040763
S	-0.134684	3.530995	3.220737
H	-0.355207	4.430840	2.248799
H	-1.444957	3.288849	3.387438

Ag9-H2S site=9

Ag	-2.241171	-0.147179	0.070877
Ag	1.435649	0.240219	0.069059
Ag	-1.509715	-2.869909	-0.183587
Ag	1.300238	-2.472929	-0.166303
Ag	-0.299324	-1.234805	1.791115
Ag	-0.327589	-0.915247	-1.854106
Ag	-0.556938	1.741146	-1.214355
Ag	-0.523545	1.498634	1.628508
Ag	1.398679	3.053757	0.316967
S	3.316706	4.861189	0.184024
H	3.210845	5.032319	-1.144448

H	2.545732	5.930896	0.441158

$\underline{NH_3}$

Ag9-NH3 site=1

Ag	-1.992414	0.028023	0.095341
Ag	1.923345	0.245794	-0.041302
Ag	-1.263400	-2.772730	-0.073341
Ag	1.698443	-2.466719	-0.164591
Ag	0.079728	-1.105103	1.676694
Ag	-0.044770	-0.935733	-1.740945
Ag	-0.162542	1.725493	-1.324529
Ag	-0.053832	1.583493	1.535139
Ag	1.895583	3.013336	0.095972
N	-4.340288	0.398730	0.188417
H	-4.560046	1.382262	0.284340
H	-4.785066	0.060675	-0.655834
H	-4.749811	-0.090680	0.974230

Ag9-NH3 site=2

Ag	-2.378677	0.159056	0.000223
Ag	1.527280	0.276565	-0.000158
Ag	-1.875122	-2.589344	-0.000400
Ag	1.040494	-2.504569	-0.000652
Ag	-0.431341	-0.949630	1.745760
Ag	-0.431677	-0.948901	-1.746151
Ag	-0.492835	1.732246	-1.438819
Ag	-0.492563	1.731634	1.439555
Ag	1.415176	3.146102	0.000489
N	3.937070	0.355742	-0.000038
H	4.297665	0.826018	0.821321
H	4.298091	0.831012	-0.818327
H	4.295247	-0.591583	-0.002804

Ag9-NH3 site=3

Ag	-1.951405	0.405116	0.002929
Ag	1.776604	0.363861	-0.001891
Ag	-1.606402	-2.441189	0.000451
Ag	1.265520	-2.348715	-0.003142
Ag	-0.165747	-0.781284	1.783110
Ag	-0.170203	-0.778623	-1.783597
Ag	-0.058779	1.929515	-1.454657
Ag	-0.054944	1.927327	1.457958
Ag	1.966432	3.197303	-0.000111
N	-3.255641	-4.108179	-0.000203
H	-3.194303	-4.689259	0.827552
H	-3.172437	-4.710845	-0.810418
H	-4.177533	-3.688367	-0.017960

Ag9-NH3 site=4

Ag	-2.132624	0.106029	-0.028749
Ag	1.541581	0.766923	0.023619
Ag	-1.163871	-2.535258	-0.038466
Ag	1.725467	-1.975667	0.006863

Ag	-0.077228	-0.703866	1.774194
Ag	-0.028999	-0.677386	-1.790458
Ag	-0.603409	1.982497	-1.436835
Ag	-0.639436	1.961919	1.445964
Ag	1.217657	3.522149	0.039049
N	2.918318	-3.974360	0.002797
H	3.650650	-3.983229	0.702623
H	3.347807	-4.144461	-0.898728
H	2.291007	-4.745340	0.198137

Ag9-NH3 site=5

Ag	-1.868679	0.359315	-0.090884
Ag	1.512895	0.462515	-0.296463
Ag	-1.444002	-2.355069	0.268203
Ag	1.367140	-2.201312	0.104742
Ag	-0.028040	-0.436277	1.927639
Ag	-0.247967	-1.027272	-1.937080
Ag	-0.323884	1.710714	-2.021689
Ag	-0.146898	2.204845	1.036211
Ag	1.726374	3.183390	-0.837869
N	-0.106993	-1.456615	4.058785
H	-0.197503	-0.768817	4.796795
H	0.726868	-2.003022	4.237814
H	-0.905243	-2.078224	4.109146

Ag9-NH3 site=8

Ag	-1.865268	0.059564	0.303508
Ag	1.582388	0.002640	-0.278830
Ag	-1.568206	-2.692281	-0.010758
Ag	1.198432	-2.676883	-0.565076
Ag	0.142225	-1.257256	1.739489
Ag	-0.507950	-0.966319	-1.984529
Ag	-0.354804	1.719895	-1.337983
Ag	0.187371	1.541401	1.586533
Ag	2.014993	2.738444	-0.246179
N	-0.374729	3.258183	3.061912
H	0.433403	3.609234	3.560844
H	-0.789826	4.032588	2.558427
H	-1.048048	2.931139	3.743952

Ag9-NH3 site=9

Ag	-2.235167	-0.133775	-0.005676
Ag	1.437324	0.290140	0.002748
Ag	-1.494577	-2.868247	0.001730
Ag	1.317575	-2.430606	0.007742
Ag	-0.314732	-1.046327	1.828757
Ag	-0.305668	-1.053537	-1.826783
Ag	-0.543798	1.649611	-1.430960
Ag	-0.551014	1.655147	1.421310
Ag	1.367328	3.117326	-0.003080
N	3.018268	4.770726	0.000579
H	2.973364	5.345552	-0.832775
H	2.933582	5.382522	0.803966
H	3.936983	4.344140	0.032440

CO

Ag9-CO site=1

Ag	-2.053160	-0.187514	0.143059
Ag	1.834648	0.286911	-0.062430
Ag	-1.205236	-2.922208	0.028540
Ag	1.812231	-2.434409	-0.127627
Ag	0.110436	-1.156704	1.698842
Ag	-0.079548	-1.072063	-1.685601
Ag	-0.367392	1.594788	-1.344317
Ag	-0.207259	1.522923	1.521185
Ag	1.622061	3.048280	0.019070
C	-4.046847	0.685387	0.347767
O	-4.743414	1.559538	0.489464

Ag9-CO site=2

Ag	-2.391024	0.055228	-0.005581
Ag	1.523340	0.480594	-0.029475
Ag	-1.671889	-2.639378	0.021410
Ag	1.268560	-2.323184	0.002783
Ag	-0.332056	-0.874901	1.720869
Ag	-0.346962	-0.912085	-1.729219
Ag	-0.612685	1.758900	-1.468257
Ag	-0.603721	1.791636	1.404250
Ag	1.189778	3.329328	-0.055863
C	3.712180	0.585215	0.266465
O	4.708399	0.261437	0.682206

Ag9-CO site=3

Ag	-1.966592	0.363762	-0.073316
Ag	1.723266	0.350668	0.031614
Ag	-1.594018	-2.442398	-0.137480
Ag	1.270549	-2.357669	-0.058619
Ag	-0.236022	-0.858910	1.750647
Ag	-0.114393	-0.747656	-1.871726
Ag	-0.084816	1.957685	-1.436212
Ag	-0.127798	1.865974	1.479936
Ag	1.927734	3.163706	0.057116
C	-2.936915	-4.138367	0.148034
O	-3.403896	-4.818634	0.918174

Ag9-CO site=4

Ag	-2.156108	0.121853	-0.059026
Ag	1.509941	0.797086	0.069560
Ag	-1.149144	-2.508097	0.061377
Ag	1.696228	-1.936644	0.163375
Ag	-0.143842	-0.600472	1.846195
Ag	0.007441	-0.713878	-1.746037
Ag	-0.611346	1.955054	-1.490988
Ag	-0.722094	2.047251	1.371075
Ag	1.172885	3.551620	-0.041602
C	2.917770	-3.685870	0.272525
O	3.565030	-4.602503	0.332796

Ag9-CO site=5

Ag	-1.848620	0.363944	-0.170687
Ag	1.473579	0.374122	-0.295683
Ag	-1.551456	-2.379102	0.051684
Ag	1.279291	-2.311439	-0.040577
Ag	-0.119667	-0.647751	1.837426
Ag	-0.260566	-0.986800	-2.062187
Ag	-0.245917	1.752961	-2.050671
Ag	-0.126639	2.065897	1.158794
Ag	1.745689	3.123384	-0.668153
C	-0.200168	-1.210510	3.914132
O	-0.256825	-1.127925	5.035763

Ag9-CO site=8

Ag	-1.790911	0.327595	0.158440
Ag	1.628571	-0.108869	-0.241500
Ag	-1.747305	-2.467343	0.108099
Ag	1.009166	-2.757197	-0.336285
Ag	0.009421	-1.011096	1.818046
Ag	-0.465864	-1.032565	-1.968643
Ag	-0.070372	1.688624	-1.552327
Ag	0.334736	1.742919	1.374158
Ag	2.367489	2.544728	-0.430395
C	-0.192162	3.386761	2.614537
O	-0.620441	4.131112	3.341052

Ag9-CO site=9

Ag	-2.185840	-0.009121	-0.011001
Ag	1.492716	0.084148	-0.052376
Ag	-1.665287	-2.776322	0.113147
Ag	1.165329	-2.621376	0.079166
Ag	-0.317629	-1.005936	1.855592
Ag	-0.351148	-1.181450	-1.811920
Ag	-0.377076	1.546526	-1.544227
Ag	-0.350599	1.684562	1.327610
Ag	1.677896	2.893925	-0.183572
C	2.813269	4.763685	-0.284588
O	2.724967	5.887218	-0.339380

$\underline{BH_3}$

Ag	-1.87928	-0.68213	-0.18610
Ag	1.62173	0.28385	-0.05670
Ag	-0.69006	-3.28882	-0.37184
Ag	1.98483	-2.41089	-0.12537
Ag	0.07763	-1.40351	1.66601
Ag	0.15540	-1.22991	-2.03226
Ag	-0.48762	1.37820	-1.56151
Ag	-0.57139	1.30057	1.37208
Ag	1.13277	3.02413	0.05236
B	-2.03159	-0.33788	2.25328
H	-2.08823	0.79705	2.73835
H	-1.69201	-1.16264	3.08158
H	-3.07277	-0.63542	1.68971

Ag9-BH3 site=h178

Ag	-1.82415	-0.82715	-0.02941
Ag	1.65139	0.24497	0.11864
Ag	-0.61804	-3.30025	-0.22430
Ag	2.07707	-2.41650	-0.10525
Ag	0.23888	-1.53420	1.84143
Ag	0.29902	-1.20619	-1.92678
Ag	-0.55015	1.35866	-1.24816
Ag	-0.59112	1.11283	1.58839
Ag	1.25585	2.91661	0.33898
B	-2.64927	1.40166	0.16268
H	-2.51433	1.95993	1.24497
H	-3.60845	0.66759	0.08258
H	-2.48091	2.14354	-0.79738

Ag9-BH3 site=h245/h258

Ag	-2.12016	-0.82249	-0.19727
Ag	1.33735	0.41860	0.15370
Ag	-0.83092	-3.27563	-0.39167
Ag	1.82804	-2.28924	-0.10148
Ag	-0.13164	-1.39605	1.70687
Ag	0.07820	-1.18310	-1.99879
Ag	-0.75543	1.35082	-1.47088
Ag	-1.11396	1.18495	1.40949
Ag	0.56863	3.10301	0.22090
B	2.38019	-1.05319	1.85486
H	2.87093	0.05733	1.82247
H	3.16926	-1.93566	1.51733
H	1.79839	-1.31485	2.89066

Ag9-BH3 site=h345

Ag	-2.00672	-0.45583	0.13790
Ag	1.50491	0.41655	-0.23624
Ag	-0.90965	-3.02729	0.12636
Ag	1.82883	-2.29910	-0.12347
Ag	0.18960	-1.12479	1.87663
Ag	-0.11413	-1.19068	-1.88038
Ag	-0.81313	1.43261	-1.53694
Ag	-0.48056	1.48886	1.43674
Ag	0.95823	3.15571	-0.32332
B	0.82200	-3.63952	1.65570
H	-0.02271	-4.50757	1.50547
H	0.79416	-3.07071	2.73197
H	1.93669	-3.95465	1.26406

Ag9-BH3 site=h789

Ag	-1.85516	-1.04812	-0.31530
Ag	1.38454	0.08505	0.09597
Ag	-0.48741	-3.47417	-0.12019
Ag	2.07633	-2.52268	0.20980
Ag	-0.11026	-1.46904	1.86461
Ag	0.38586	-1.49386	-1.96996
Ag	-0.58571	1.08576	-1.64071
Ag	-0.96701	1.10209	1.26764

Ag	0.97987	2.82070	0.03798
B	-1.26437	3.16968	-0.27963
H	-0.83696	4.30195	-0.22485
H	-1.97599	2.84107	0.66192
H	-1.69343	2.83756	-1.38030

BF_3

Ag9-BF3 site=h135/h158

Ag	-1.63590	-0.58328	-0.49606
Ag	1.92302	0.27747	-0.35831
Ag	-0.57718	-3.18661	-0.54209
Ag	2.17769	-2.43805	-0.42203
Ag	0.32795	-1.32964	1.38345
Ag	0.44758	-1.22625	-2.29042
Ag	-0.18338	1.40505	-1.85886
Ag	-0.27763	1.31802	1.06307
Ag	1.48401	3.02883	-0.28722
B	-2.78571	-0.40916	3.06028
F	-2.56626	0.85294	3.36058
F	-2.14714	-1.35636	3.70798
F	-3.72761	-0.72037	2.19926

Ag9-BF3 site=h178

Ag	-1.49093	-0.98719	0.19638
Ag	1.97697	0.05972	-0.25456
Ag	-0.28952	-3.51927	0.32083
Ag	2.39816	-2.62245	-0.03137
Ag	0.74271	-1.39273	1.88186
Ag	0.37187	-1.75101	-1.78421
Ag	-0.37050	0.88235	-1.57568
Ag	-0.08467	1.16091	1.31808
Ag	1.38041	2.77045	-0.45583
B	-3.47469	1.96730	0.35713
F	-4.29636	0.96614	0.56079
F	-3.22517	2.37799	-0.86556
F	-2.95247	2.60930	1.37855

Ag9-BF3 site=h245/h258

Ag	-2.27023	-1.12898	-0.47895
Ag	1.08406	0.35174	-0.43495
Ag	-0.75791	-3.49625	-0.58126
Ag	1.82773	-2.26689	-0.54585
Ag	-0.13321	-1.52093	1.33020
Ag	-0.15147	-1.37271	-2.34105
Ag	-1.23482	1.10107	-1.85432
Ag	-1.21297	0.97483	1.06792
Ag	0.17457	2.97824	-0.31830
B	2.09812	0.85331	3.06354
F	2.98306	1.31224	2.20851
F	2.20724	-0.36931	3.53052
F	1.15933	1.64972	3.52339

Ag9-BF3 site=h345

Ag	-2.04688	-0.42430	-0.59530
Ag	1.33914	0.86267	-0.03477
Ag	-0.65541	-2.86414	-0.61471
Ag	1.95108	-1.79148	-0.18441
Ag	-0.19910	-1.02533	1.45990
Ag	0.28444	-0.70223	-2.17953
Ag	-0.73229	1.79667	-1.70369
Ag	-1.11356	1.54374	1.18478
Ag	0.54094	3.53192	0.09317
B	1.07404	-4.41534	2.29344
F	0.62779	-3.71742	3.31100
F	2.32149	-4.27921	1.90099
F	0.29582	-5.29193	1.70363

Ag9-BF3 site=h789

Ag	-1.72786	-1.22545	-0.01102
Ag	1.77770	-0.21646	0.01629
Ag	-0.54298	-3.76575	0.12336
Ag	2.16986	-2.90711	0.14636
Ag	0.29256	-1.74319	1.90412
Ag	0.36993	-1.90775	-1.79034
Ag	-0.37878	0.71440	-1.53762
Ag	-0.44376	0.84582	1.38976
Ag	1.23942	2.51882	-0.11092
B	-1.91276	3.97111	-0.47840
F	-1.54691	4.69103	0.55682
F	-2.74912	2.97013	-0.31883
F	-1.49699	4.29042	-1.68259

HCl

Ag9-HCl site=h135/h158

Ag	-1.87908	-0.70889	-0.16032
Ag	1.63634	0.34494	-0.10240
Ag	-0.68256	-3.25587	-0.10406
Ag	2.03244	-2.35532	-0.04906
Ag	0.14627	-1.26816	1.72287
Ag	0.21552	-1.31983	-1.94367
Ag	-0.54317	1.29478	-1.62108
Ag	-0.60606	1.32779	1.30090
Ag	1.04864	3.07028	-0.13857
H	-2.37671	-0.43303	2.63519
Cl	-3.33144	-0.45436	3.52141

Ag9-HCl site=h178

Ag	-1.84066	-0.87957	0.06591
Ag	1.59618	0.27682	-0.02641
Ag	-0.58478	-3.38733	-0.00569
Ag	2.08482	-2.40082	-0.07649
Ag	0.27351	-1.42564	1.85262
Ag	0.15957	-1.37894	-1.86200
Ag	-0.67014	1.20091	-1.41338
Ag	-0.57491	1.16518	1.52239
Ag	0.96543	2.97937	0.02541

H	-2.99100	1.49594	0.18819
Cl	-3.63604	2.62466	0.24180

Ag9-HCl site=h245/h258

Ag	-2.10540	-0.81504	-0.15085
Ag	1.38427	0.30276	-0.17608
Ag	-0.84935	-3.32954	-0.12164
Ag	1.85059	-2.38043	-0.13384
Ag	-0.01943	-1.33371	1.68656
Ag	-0.02621	-1.38049	-1.98436
Ag	-0.83827	1.22112	-1.63388
Ag	-0.83271	1.24934	1.28357
Ag	0.76650	3.01676	-0.19947
H	1.81463	0.61603	2.54494
Cl	2.57888	1.16901	3.43787

Ag9-HCl site=h345

Ag	-2.01915	-0.61650	-0.06543
Ag	1.48109	0.47179	-0.09984
Ag	-0.78225	-3.14020	-0.11572
Ag	1.91948	-2.21681	-0.15534
Ag	0.08219	-1.21727	1.73492
Ag	0.02994	-1.14137	-1.95342
Ag	-0.76389	1.43879	-1.50498
Ag	-0.71227	1.38384	1.42206
Ag	0.86423	3.19036	-0.04165
H	0.89212	-4.02134	1.77439
Cl	1.49510	-4.90693	2.51068

Ag9-HCl site=h789

Ag	-1.90693	-0.70702	-0.07750
Ag	1.62068	0.15591	0.02200
Ag	-0.82016	-3.29131	0.01734
Ag	1.91938	-2.55130	0.10151
Ag	0.05900	-1.34733	1.86030
Ag	0.18987	-1.43463	-1.84527
Ag	-0.47031	1.21065	-1.54403
Ag	-0.56969	1.28170	1.38878
Ag	1.20822	2.91392	-0.05713
H	-1.27217	3.56350	-0.20516
Cl	-2.49261	4.00306	-0.30950

Na^+

Ag9-Na+ site=h135/h158

Ag	-1.94175	-0.67509	-0.16080
Ag	1.66031	0.38253	-0.09711
Ag	-0.79141	-3.25654	-0.00152
Ag	2.01553	-2.36815	0.01044
Ag	0.15103	-1.22861	1.67986
Ag	0.15277	-1.33079	-1.85091
Ag	-0.56845	1.33426	-1.59550
Ag	-0.61765	1.36004	1.29445
Ag	1.04509	3.11652	-0.10975

Na	-2.54358	-0.68180	2.88556

Ag9-Na+ site=h178

Ag	-1.64826	-0.72625	0.06696
Ag	1.63332	0.27258	-0.02939
Ag	-0.80738	-3.34470	0.01943
Ag	1.82380	-2.43694	-0.05427
Ag	0.24566	-1.34219	1.99335
Ag	0.11966	-1.31268	-1.98416
Ag	-0.54756	1.34453	-1.41449
Ag	-0.45484	1.32312	1.50645
Ag	1.21055	3.02156	0.00431
Na	-3.46382	1.48031	0.15402

Ag9-Na+ site=h245/h258

Ag	-2.11621	-0.81122	-0.10100
Ag	1.42524	0.33764	-0.14848
Ag	-0.79922	-3.37024	-0.06031
Ag	1.94885	-2.34111	-0.02681
Ag	-0.02128	-1.32091	1.68296
Ag	0.04370	-1.37326	-1.86141
Ag	-0.79332	1.26483	-1.57970
Ag	-0.82248	1.26463	1.31371
Ag	0.87192	3.03980	-0.05449
Na	1.94670	0.77143	2.76881

Ag9-Na+ site=h345

Ag	-2.04114	-0.70063	-0.05428
Ag	1.53680	0.45514	-0.13136
Ag	-0.71491	-3.19375	-0.10665
Ag	1.97697	-2.25428	-0.18345
Ag	0.12633	-1.25184	1.66465
Ag	0.05657	-1.18352	-1.97007
Ag	-0.75269	1.39854	-1.42399
Ag	-0.70076	1.34137	1.44136
Ag	0.87231	3.16583	-0.00376
Na	0.84602	-4.12507	2.35314

Ag9-Na+ site=h789

Ag	-1.89622	-0.70116	-0.04492
Ag	1.52135	0.10603	-0.00758
Ag	-0.73145	-3.27138	0.03190
Ag	1.99200	-2.56053	0.06725
Ag	0.09485	-1.34712	1.91280
Ag	0.16185	-1.43709	-1.90520
Ag	-0.53085	1.20754	-1.55660
Ag	-0.57934	1.27961	1.41832
Ag	1.18245	2.89145	-0.08292
Na	-1.57448	3.98779	-0.15582

Cu_9

Cu9 – ground state

Cu	-1.578757	-0.048767	-0.180944

Cu	1.564325	0.234200	0.168642
Cu	-1.025103	-2.471214	-0.034111
Cu	1.459580	-2.190607	0.237932
Cu	-0.111824	-0.870892	1.630556
Cu	0.249737	-0.978550	-1.556389
Cu	0.042541	1.449260	-1.333201
Cu	-0.248828	1.535043	1.204176
Cu	1.637559	2.701598	0.095149

H_2O

Cu9-H2O site=1

Cu	-1.743887	0.218296	-0.206556
Cu	1.683272	0.200298	0.180396
Cu	-1.265396	-2.322078	-0.056721
Cu	1.335964	-2.240499	0.229132
Cu	-0.194022	-0.768661	1.461956
Cu	0.126798	-0.872134	-1.409593
Cu	0.166078	1.525299	-1.298661
Cu	-0.117788	1.615593	1.186669
Cu	1.865271	2.654284	0.114935
O	-3.898911	0.542202	-0.400073
H	-4.326316	0.130020	0.358164
H	-4.200133	0.052818	-1.173018

Cu9-H2O site=2

Cu	-2.055953	0.107341	-0.209751
Cu	1.348337	0.384377	0.137590
Cu	-1.486467	-2.336866	-0.113271
Cu	1.075096	-2.127574	0.145631
Cu	-0.451633	-0.763004	1.456142
Cu	-0.150557	-0.805096	-1.486065
Cu	-0.315414	1.586552	-1.314022
Cu	-0.576171	1.621298	1.182452
Cu	1.217043	2.900479	0.090481
O	3.615926	0.484730	0.379305
H	3.910586	-0.039523	-0.373269
H	3.735017	-0.083894	1.147797

Cu9-H2O site=3

Cu	-1.729274	-0.104949	-0.139273
Cu	1.488704	0.481437	0.020398
Cu	-0.931004	-2.523696	-0.373118
Cu	1.553672	-1.975322	-0.220993
Cu	-0.012749	-0.979587	1.363317
Cu	0.077707	-0.689854	-1.673518
Cu	-0.297463	1.666412	-1.196546
Cu	-0.386945	1.421399	1.331444
Cu	1.225257	2.958311	0.260333
O	-2.211971	-4.200567	-0.046626
H	-3.130415	-3.911189	-0.082739
H	-2.074746	-4.535926	0.846221

Cu9-H2O site=4

Cu	-1.888875	0.031952	-0.088334
Cu	1.332215	0.613600	0.082342
Cu	-1.056684	-2.332355	0.162760
Cu	1.485921	-1.845076	0.295858
Cu	-0.179404	-0.560323	1.613681
Cu	0.023205	-0.810468	-1.422051
Cu	-0.436375	1.582259	-1.388124
Cu	-0.602993	1.789460	1.123360
Cu	1.114702	3.057093	-0.136107
O	2.789849	-3.518100	0.184722
H	2.336915	-4.268794	-0.212846
H	3.558453	-3.343517	-0.367591

Cu9-H2O site=5

Cu	-1.587108	0.325012	-0.145318
Cu	1.239287	0.215453	-0.094509
Cu	-1.445733	-2.110120	-0.143414
Cu	1.013167	-2.161034	-0.076041
Cu	-0.222911	-0.726760	1.657062
Cu	-0.175225	-0.770184	-1.847560
Cu	-0.062277	1.687022	-1.529465
Cu	-0.097276	1.755420	1.157659
Cu	1.807890	2.608326	-0.207885
O	-0.900324	-1.845786	3.395560
H	-1.032096	-2.739614	3.059415
H	-1.782624	-1.510846	3.588497

Cu9-H2O site=8

Cu	-1.643023	0.134374	0.018391
Cu	1.266701	0.009212	-0.070423
Cu	-1.481613	-2.306043	-0.154606
Cu	0.987408	-2.365888	-0.281802
Cu	-0.173862	-1.049203	1.575932
Cu	-0.284819	-0.847441	-1.801369
Cu	-0.137299	1.583097	-1.257686
Cu	-0.025949	1.475675	1.365370
Cu	1.848744	2.395551	-0.028829
O	-0.869299	2.922154	2.674071
H	-1.757155	2.623148	2.896516
H	-0.973104	3.776214	2.242795

Cu9-H2O site=9

Cu	-1.941876	-0.058475	-0.037400
Cu	1.227983	0.399202	0.033381
Cu	-1.231154	-2.460313	0.074820
Cu	1.237703	-2.030146	0.124786
Cu	-0.273196	-0.769839	1.628349
Cu	-0.184963	-0.891557	-1.548664
Cu	-0.479658	1.533059	-1.310658
Cu	-0.547223	1.626774	1.186999
Cu	1.180350	2.892172	-0.064069
O	2.896781	4.131774	-0.066848
H	3.444065	3.968996	0.709140
H	3.456408	3.952983	-0.830385

H_2S

Cu9-H2S site=1

Cu	-1.72333	0.18769	-0.21329
Cu	1.75057	0.18288	0.19336
Cu	-1.18231	-2.38897	-0.05302
Cu	1.41847	-2.25247	0.24321
Cu	-0.14917	-0.79800	1.44832
Cu	0.17935	-0.90199	-1.38906
Cu	0.20869	1.48586	-1.29171
Cu	-0.08256	1.57634	1.18620
Cu	1.89353	2.63781	0.12073
S	-3.97769	0.86722	-0.43288
H	-4.51483	0.13169	0.55653
H	-4.38978	0.00738	-1.38176

Cu9-H2S site=2

Cu	-2.15565	0.08173	-0.21131
Cu	1.35786	0.41775	0.13165
Cu	-1.54178	-2.34961	-0.12435
Cu	1.04790	-2.13495	0.12650
Cu	-0.48044	-0.76739	1.39940
Cu	-0.20233	-0.79636	-1.44617
Cu	-0.40660	1.57318	-1.30904
Cu	-0.64881	1.59796	1.17750
Cu	1.07465	2.94536	0.07591
S	3.75454	0.70834	0.36408
H	4.13958	-0.21201	-0.53686
H	3.92689	-0.13517	1.39571

Cu9-H2S site=3

Cu	-1.71920	0.05129	-0.15314
Cu	1.52057	0.51116	0.07032
Cu	-1.03599	-2.41789	-0.25271
Cu	1.48006	-1.96505	-0.07136
Cu	-0.08015	-0.83906	1.42106
Cu	0.10252	-0.67252	-1.60604
Cu	-0.18255	1.71476	-1.24767
Cu	-0.34012	1.57324	1.29760
Cu	1.33005	3.01799	0.20161
S	-2.38476	-4.31485	-0.44842
H	-3.35361	-3.96515	0.41618
H	-1.76606	-5.08746	0.46145

Cu9-H2S site=4

Cu	-1.93549	0.11630	0.10612
Cu	1.30103	0.58543	-0.16159
Cu	-1.17757	-2.27607	-0.11289
Cu	1.38327	-1.89280	-0.32382
Cu	-0.00865	-0.75595	1.40660
Cu	-0.28425	-0.56620	-1.62007
Cu	-0.63670	1.80526	-1.17235
Cu	-0.40792	1.64817	1.32834
Cu	1.16383	3.03552	0.00716

S	2.77794	-3.75083	-0.43652
H	2.41226	-4.33124	0.71917
H	3.88919	-3.22186	0.10754

Cu9-H2S site=5

Cu	-1.57171	0.35982	-0.28132
Cu	1.21857	0.23150	-0.12542
Cu	-1.47468	-2.07133	-0.27063
Cu	0.97987	-2.13831	-0.10573
Cu	-0.32084	-0.71561	1.59660
Cu	-0.12410	-0.75341	-1.93466
Cu	0.00517	1.69745	-1.64335
Cu	-0.14683	1.78134	1.08157
Cu	1.79838	2.62552	-0.22285
S	-0.72875	-1.71731	3.69189
H	-0.81614	-3.00694	3.32302
H	-2.06418	-1.56585	3.70489

Cu9-H2S site=8

Cu	-1.63386	0.08116	0.00645
Cu	1.26087	-0.03703	-0.10330
Cu	-1.46631	-2.35434	-0.23720
Cu	0.99691	-2.40824	-0.39778
Cu	-0.15857	-1.13559	1.52714
Cu	-0.28888	-0.85304	-1.85747
Cu	-0.13969	1.57112	-1.23905
Cu	-0.02139	1.41789	1.38493
Cu	1.86875	2.33657	0.00282
S	-0.69176	3.01631	2.92185
H	-1.98432	2.67922	3.07265
H	-0.98502	4.03682	2.09732

Cu9-H2S site=9

Cu	-1.96030	-0.14086	-0.09012
Cu	1.18777	0.43539	0.09412
Cu	-1.15582	-2.51551	0.06607
Cu	1.28416	-1.99318	0.20593
Cu	-0.32791	-0.77186	1.63741
Cu	-0.11409	-0.90973	-1.52584
Cu	-0.50828	1.50375	-1.31487
Cu	-0.66970	1.61263	1.16725
Cu	1.07075	2.93966	-0.02131
S	2.85967	4.44268	-0.02343
H	3.65105	3.75175	0.81713
H	3.46791	3.93992	-1.11289

Au_9

Au9 – ground state

Au	-1.729947	0.182253	0.200992
Au	1.963257	0.278135	-0.028962
Au	-1.254736	-2.559345	0.010964
Au	1.643672	-2.366322	-0.153892
Au	0.208169	-1.035735	1.850680

Au	-0.019530	-0.828719	-1.806126
Au	-0.065579	1.819673	-1.324135
Au	0.123700	1.649281	1.680901
Au	1.973095	2.989979	0.128018

H_2O

Au9-H2O site=1

Au	-1.853812	0.463121	0.432646
Au	1.957690	0.219947	-0.109927
Au	-1.517958	-2.381343	0.081552
Au	1.396083	-2.377294	-0.217387
Au	0.129290	-0.941792	1.808940
Au	-0.302253	-0.681413	-1.713793
Au	-0.066008	1.928841	-1.241198
Au	0.249884	1.734686	1.676596
Au	2.182823	2.900564	0.090769
O	-4.220610	0.280414	-0.390516
H	-4.041168	0.188893	-1.332752
H	-4.483052	-0.599194	-0.098300

Au9-H2O site=2

Au	-2.234799	0.219667	-0.000000
Au	1.561735	0.228325	-0.000000
Au	-1.832115	-2.518633	0.000000
Au	1.126407	-2.445955	0.000000
Au	-0.372430	-0.952516	1.789972
Au	-0.372430	-0.952517	-1.789972
Au	-0.391379	1.708634	-1.495792
Au	-0.391379	1.708634	1.495792
Au	1.526658	2.989707	0.000000
O	4.182227	0.247973	-0.000000
H	4.721323	-0.546438	-0.000000
H	4.784242	0.995810	0.000000

Au9-H2O site=3

Au	-1.919057	0.272192	0.061195
Au	1.800639	0.555069	0.037467
Au	-1.375777	-2.425837	0.409299
Au	1.583454	-2.096292	0.301764
Au	-0.060445	-0.569871	1.964661
Au	-0.043204	-0.934901	-1.621957
Au	-0.228217	1.755204	-1.589676
Au	-0.192433	2.064234	1.383868
Au	1.683238	3.263894	-0.272378
O	-2.262405	-4.684706	0.040435
H	-3.195997	-4.703990	0.273397
H	-2.219017	-4.888546	-0.899165

Au9-H2O site=4

Au	-1.663064	-0.117059	0.185540
Au	1.906025	1.080510	-0.123671
Au	-0.474384	-2.611572	0.245505
Au	2.571285	-1.451055	-0.005841

Au	0.618586	-0.582268	1.810307
Au	0.393616	-0.787401	-1.663798
Au	-0.531350	1.753026	-1.516883
Au	-0.333525	1.931394	1.493189
Au	1.001398	3.632932	-0.212784
O	3.153132	-3.750188	0.124709
H	3.248835	-3.990631	1.051989
H	2.344736	-4.185188	-0.172320

Au9-H2O site=5

Au	-1.851587	0.601113	-0.495572
Au	1.591876	0.296975	0.066901
Au	-1.800938	-2.154815	-0.158144
Au	1.018069	-2.284216	0.275756
Au	-0.634776	-0.423170	1.809566
Au	-0.023144	-0.951948	-1.966020
Au	0.210868	1.720298	-2.021525
Au	-0.221784	2.146653	1.107342
Au	1.991571	2.963303	-0.336831
O	-0.973568	-2.078136	3.607872
H	-0.629788	-2.894139	3.230351
H	-1.922020	-2.215038	3.694323

Au9-H2O site=8

Au	-1.958934	-0.174857	0.094012
Au	1.643543	0.085416	-0.077548
Au	-1.352733	-2.865012	-0.322728
Au	1.478611	-2.541853	-0.568903
Au	0.026330	-1.420585	1.645656
Au	-0.247176	-0.933027	-2.031929
Au	-0.419864	1.658333	-1.295090
Au	-0.173204	1.267095	1.736968
Au	1.631567	2.788708	0.129652
O	-1.047092	3.265285	2.813900
H	-0.815956	3.998751	2.235305
H	-2.008352	3.222596	2.819066

Au9-H2O site=9

Au	-2.035247	0.310882	0.004200
Au	1.668782	-0.289666	0.042093
Au	-2.116421	-2.494219	0.040260
Au	0.849893	-2.826581	0.068149
Au	-0.464069	-1.126420	1.841703
Au	-0.435649	-1.177383	-1.771313
Au	0.028945	1.459492	-1.490616
Au	0.011018	1.502649	1.490319
Au	2.219047	2.324396	0.004687
O	3.208370	4.534365	-0.116383
H	2.997263	5.064718	0.658775
H	2.853277	5.012410	-0.872415

H_2S

Au9-H2S site=1

Au	-1.85567	0.46555	0.44096
Au	1.95463	0.21919	-0.11324
Au	-1.52063	-2.37822	0.08707
Au	1.39127	-2.37719	-0.22104
Au	0.13196	-0.94193	1.81017
Au	-0.30947	-0.68000	-1.71167
Au	-0.06941	1.92913	-1.23870
Au	0.25278	1.73428	1.67764
Au	2.18220	2.90042	0.08915
S	-4.28405	0.96742	0.26128
H	-4.50226	0.37034	-0.92268
H	-4.79302	-0.06982	0.94861

Au9-H2S site=2

Au	-2.28052	0.14789	0.06516
Au	1.47392	0.29816	-0.07530
Au	-1.77349	-2.56357	-0.00319
Au	1.11604	-2.38065	-0.10506
Au	-0.33816	-0.96408	1.80556
Au	-0.48035	-0.90552	-1.85430
Au	-0.56227	1.74558	-1.46751
Au	-0.45595	1.69947	1.51764
Au	1.35468	3.06975	-0.02774
S	4.06897	0.47762	-0.32934
H	4.30294	-0.81120	-0.62748
H	4.06139	0.83749	-1.62298

Au9-H2S site=3

Au	-1.95842	0.37255	0.01454
Au	1.80983	0.54795	0.03565
Au	-1.53965	-2.37982	0.23120
Au	1.53439	-2.13776	0.18031
Au	-0.11919	-0.62740	1.87152
Au	-0.08577	-0.83149	-1.68624
Au	-0.16842	1.89567	-1.55351
Au	-0.15861	2.07027	1.42590
Au	1.82085	3.30318	-0.15371
S	-2.38006	-4.66007	0.05741
H	-3.68906	-4.40231	-0.11716
H	-2.18249	-4.86712	-1.25708

Au9-H2S site=4

Au	-1.77062	-0.01476	0.14753
Au	1.85174	1.02117	-0.06815
Au	-0.56999	-2.55235	0.27648
Au	2.35443	-1.58512	0.12423
Au	0.44109	-0.48015	1.89481
Au	0.30380	-0.75127	-1.68323
Au	-0.51948	1.85106	-1.53440
Au	-0.42491	2.07341	1.43277
Au	1.14098	3.67407	-0.23240
S	3.37624	-3.77783	0.26239
H	2.69473	-4.26722	1.31370
H	2.59959	-4.43077	-0.62127

Au9-H2S site=5

Au	-1.84384	0.60142	-0.60070
Au	1.52736	0.22989	0.04967
Au	-1.86398	-2.19313	-0.47037
Au	0.93822	-2.37600	0.07751
Au	-0.77405	-0.57140	1.70248
Au	-0.00280	-0.86455	-2.15916
Au	0.28712	1.82946	-1.99808
Au	-0.28186	2.07081	1.14695
Au	2.04677	2.93589	-0.14105
S	-1.21802	-1.94970	3.67559
H	-1.02419	-3.17134	3.14863
H	-2.55499	-2.05361	3.57438

Au9-H2S site=8

Au	-1.92581	-0.09388	-0.06387
Au	1.63815	0.04974	-0.09800
Au	-1.40863	-2.85373	-0.22585
Au	1.45375	-2.63042	-0.42720
Au	-0.07363	-1.26541	1.69692
Au	-0.17561	-1.07996	-2.08441
Au	-0.29940	1.60150	-1.55155
Au	-0.12972	1.49358	1.50692
Au	1.78834	2.80169	-0.15396
S	-1.08123	3.28859	2.83356
H	-1.35458	4.18114	1.86571
H	-2.35729	2.86937	2.89663

Au9-H2S site=9

Au	-2.03525	0.31088	0.00420
Au	1.66877	-0.28967	0.04231
Au	-2.11642	-2.49422	0.04026
Au	0.84989	-2.82658	0.06804
Au	-0.46407	-1.12642	1.84170
Au	-0.43565	-1.17738	-1.77131
Au	0.02893	1.45949	-1.49062
Au	0.01102	1.50265	1.49032
Au	2.21906	2.32440	0.00458
S	4.03169	4.00656	0.03814
H	4.81635	3.39614	0.94410
H	4.74956	3.53685	-0.99777

Ag_{11}

Ag11 – ground state

Ag	-4.898884	2.454301	1.187046
Ag	-2.638632	3.867149	1.977048
Ag	-0.290012	2.628579	0.371641
Ag	-2.840828	2.659304	-0.693120
Ag	-2.383177	1.037872	1.538807
Ag	-4.383782	4.940944	0.024576
Ag	-1.532521	5.073256	-0.318528
Ag	-0.675630	2.414065	3.275156
Ag	0.428889	0.335589	1.768934

Ag	1.920446	2.670294	2.136958
Ag	0.017252	4.828298	2.106241

Ag_{17}

Ag17 – ground state

Ag	0.735534	1.558593	-1.576899
Ag	-1.280096	0.622541	-3.271210
Ag	1.280153	-0.622503	-3.271215
Ag	3.384566	0.738789	-1.866369
Ag	-1.979675	1.350514	-0.666219
Ag	-0.735480	-1.558557	-1.576966
Ag	1.979621	-1.350515	-0.666206
Ag	2.496807	1.246611	0.736591
Ag	0.000165	2.742356	0.850826
Ag	-0.000100	-0.000013	0.782981
Ag	-0.783257	-1.257952	3.143414
Ag	-2.496850	-1.246649	0.736615
Ag	-1.997152	1.207607	2.257992
Ag	-0.000233	-2.742356	0.850823
Ag	1.997120	-1.207622	2.257940
Ag	0.783411	1.258005	3.143309
Ag	-3.384535	-0.738848	-1.866407

Ag_{18}

Ag18 – ground state

Ag	-1.259105	-1.558227	1.399834
Ag	-3.433376	-0.501720	0.000000
Ag	-2.630449	0.735854	2.422647
Ag	-0.765202	-0.761296	3.961268
Ag	-1.259148	-1.558238	-1.399774
Ag	-1.659445	1.728752	-0.000006
Ag	0.052620	1.459666	2.345740
Ag	1.486572	-1.215842	2.358482
Ag	0.875699	-2.724810	-0.000031
Ag	0.714721	0.051918	-0.000071
Ag	2.790160	1.254786	-1.470992
Ag	0.052663	1.459670	-2.345791
Ag	1.486584	-1.215797	-2.358547
Ag	0.918414	2.795066	-0.000010
Ag	2.790041	1.254765	1.471128
Ag	3.235980	-1.180062	0.000001
Ag	-2.630430	0.735899	-2.422640
Ag	-0.765298	-0.761383	-3.961239