Supporting Information for

The Influence of Force Field Parameters on the Atomistic Simulations of Metallic Surfaces and Nanoparticles

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Table S1. Simulation parameters for the cubic NCs.

NC size (nm)	Alcanethiols	number of gold atoms	number of thiolate molecules	total number of atoms	Size of simulation box (nm)	Simulation time (ns)
1.0	butane	14	25	139	5.4	300
2.0	butane	172	90	622	6.4	300
3.0	butane	666	210	1716	7.5	300
4.1	butane	1688	375	3563	8.5	300
5.1	butane	3430	600	6430	9.6	600
6.2	butane	6084	870	10434	10.6	300
7.2	butane	9842	1190	15792	11.7	600
8.3	butane	14896	1560	22696	12.7	300
8.8	butane	17969	1760	26769	13.3	300
9.8	butane	25327	2200	36327	14.3	300

Table S2. Simulation parameters for the octahedral NCs.

NC size (nm)	Alcanethiols	number of gold atoms	number of thiolate molecules	total number of atoms	Size of simulation box (nm)	Simulation time (ns)
1.0	butane	18	20	118	5.5	90
2.1	butane	230	100	730	6.6	90
3.0	butane	670	205	1695	7.5	90
4.1	butane	1834	400	3834	8.6	90
5.0	butane	3280	590	6230	9.5	90
6.1	butane	6180	900	10680	10.6	90
7.0	butane	9224	1170	15074	11.5	90
8.1	butane	14644	1590	22594	12.6	90
9.0	butane	19870	1950	29620	13.5	90
10.2	butane	28594	2500	41094	14.6	90

Table S3. Simulation parameters for the icosahedral NCs.

NC size (nm)	Alcanethiols	number of gold atoms	number of thiolate molecules	total number of atoms	Size of simulation box (nm)	Simulation time (ns)
0.9	butane	13	20	113	5.4	300
1.3	butane	55	45	280	5.8	300
1.8	butane	147	75	522	6.2	300
2.2	butane	309	115	884	6.7	300
2.7	butane	561	165	1386	7.1	300
3.1	butane	923	225	2048	7.6	300
3.6	butane	1415	290	2865	8.1	300
4.1	butane	2057	370	3907	8.5	300
4.5	butane	2869	455	5144	9	300
5.0	butane	3871	550	6621	9.5	300
5.5	butane	5083	655	8358	9.9	300
5.9	butane	6525	770	10375	10.4	300
6.4	butane	8217	890	12667	10.9	300
6.9	butane	10179	1020	15279	11.3	600
7.3	butane	12431	1160	18231	11.8	300
7.8	butane	14993	1310	21543	12.3	300
8.3	butane	17885	1470	25235	12.7	300
8.7	butane	21127	1640	29327	13.2	300
9.2	butane	24739	1815	33814	13.7	300
9.7	butane	28741	2000	38741	14.1	300
10.1	butane	33153	2200	44153	14.6	300

Table S4. Simulation results for the cubic NCs.

NC size (nm)	Alcanethiol	Number of adsorbed thiols			% SAM > 10 members	% SAM > 3 members			
		total	center	edge		total	center	edge	zigzag
Values for σ_{SS} = 4.25 Å									
1.0	butane	16.0	1.6	14.4	0.0	56.8	4.5	52.4	0.0
2.0	butane	73.3	12.0	61.3	52.8	93.6	99.8	92.4	0.0
3.0	butane	182.7	70.0	112.7	94.1	96.4	100.0	94.2	0.0
4.1	butane	329.8	164.0	165.8	27.5	96.4	100.0	92.9	0.0
5.1	butane	524.3	297.4	226.9	94.3	95.3	99.3	90.1	0.0
6.2	butane	756.0	466.0	290.0	92.8	95.6	99.9	88.5	0.0
7.2	butane	1014.5	692.8	321.7	94.5	97.0	99.7	91.2	0.0
8.3	butane	1316.9	940.0	376.9	94.9	97.2	99.8	90.8	0.0
8.8	butane	1492.3	1082.0	410.3	95.7	97.4	99.9	90.8	0.0
9.8	butane	1851.8	1398.0	453.8	96.4	97.4	99.8	90.1	0.0
Values for σ_{SS} = 4.98 Å									
1.0	butane	12.0	1.2	10.8	0.0	0.0	0.0	0.0	0.0
2.0	butane	65.4	6.0	59.4	0.0	6.8	16.7	5.8	0.0
3.0	butane	143.9	48.0	95.8	0.0	5.7	9.3	3.9	0.0
4.1	butane	262.2	125.0	137.1	0.0	6.9	6.8	6.9	0.0
5.1	butane	417.0	237.8	179.3	0.0	7.5	8.4	6.3	0.0
6.2	butane	586.3	373.6	212.7	0.0	5.1	5.9	3.8	0.0
7.2	butane	798.3	544.5	253.8	0.0	6.3	6.8	5.2	0.0
8.3	butane	1055.2	764.7	290.5	0.0	6.9	7.6	5.1	0.0
8.8	butane	1191.9	884.6	307.3	0.0	6.6	7.3	4.8	0.0
9.8	butane	1508.1	1150.1	358.0	0.0	5.9	6.0	5.6	0.0

NC size (nm)	Alcane-thiol	S-S Distance		% Occupation of adsorption sites				R_{st}		
		center	edge	on top	bridge	3f-hollow	4f-hollow	total	center	edge
Values for σ_{SS} = 4.25 Å										
1.0	butane	0.60	3.68	19.6	52.6	27.7	0.0	0.06	0.00	0.06
2.0	butane	3.91	4.16	1.8	5.9	43.5	48.7	0.98	2.00	0.78
3.0	butane	4.11	4.13	2.4	8.4	25.3	63.9	1.31	2.06	0.85
4.1	butane	4.11	4.12	2.2	8.0	18.5	71.3	1.53	2.20	0.87
5.1	butane	4.11	4.12	3.2	8.1	13.7	75.1	1.65	2.26	0.85
6.2	butane	4.11	4.11	2.1	8.5	10.2	79.2	1.75	2.32	0.83
7.2	butane	4.11	4.11	1.3	5.7	11.0	82.0	1.85	2.29	0.90
8.3	butane	4.12	4.12	1.1	5.3	9.8	83.8	1.91	2.32	0.89
8.8	butane	4.12	4.11	1.2	5.4	8.9	84.5	1.93	2.33	0.88
9.8	butane	4.12	4.11	0.9	5.1	8.2	85.9	1.98	2.33	0.90
Values for σ_{SS} = 4.98 Å										
1.0	butane	0.60	3.68	6.6	38.3	55.1	0.0	0.08	0.00	0.08
2.0	butane	3.91	4.16	28.1	25.5	17.0	29.4	1.10	4.00	0.81
3.0	butane	4.11	4.13	11.5	38.1	17.6	32.8	1.67	3.00	1.00
4.1	butane	4.11	4.12	9.2	43.1	13.5	34.2	1.92	2.88	1.05
5.1	butane	4.11	4.12	8.1	44.0	12.1	35.8	2.07	2.83	1.07
6.2	butane	4.11	4.11	5.3	43.8	12.1	38.8	2.25	2.89	1.13
7.2	butane	4.11	4.11	4.4	43.3	11.6	40.8	2.35	2.91	1.13
8.3	butane	4.12	4.12	3.9	45.0	11.0	40.1	2.39	2.86	1.16
8.8	butane	4.12	4.11	3.5	45.3	11.0	40.2	2.42	2.85	1.17
9.8	butane	4.12	4.11	3.8	46.6	9.8	39.7	2.43	2.84	1.14

Table S5. Simulation results for the octahedral NCs.

NC size (nm)	Alcanethiol	Number of adsorbed thiols			% SAM > 10 members	% SAM > 3 members			
		total	center	edge		total	center	edge	Zigzag
Values for σ_{SS} = 4.25 Å									
1.0	butane	19.0	0.0	19.0	0.0	0.0	0.0	0.0	0.0
2.1	butane	97.1	10.7	86.4	0.0	49.1	74.3	46.0	85.2
3.0	butane	195.0	52.9	142.1	1.0	60.8	81.8	52.9	77.8
4.1	butane	360.3	147.3	213.0	2.4	68.9	85.0	57.7	75.6
5.0	butane	521.0	261.6	259.5	4.3	73.3	85.7	60.8	70.6
6.1	butane	785.9	452.0	333.9	4.3	76.5	86.9	62.4	72.0
7.0	butane	1009.0	625.7	383.2	6.9	78.2	87.8	62.6	70.7
8.1	butane	1356.5	906.2	450.3	7.7	79.9	87.7	64.1	72.3
9.0	butane	1648.2	1142.9	505.3	9.5	81.2	88.7	64.2	72.1
10.2	butane	2088.3	1516.0	572.3	10.3	82.1	88.7	64.6	70.8
Values for σ_{SS} = 4.98 Å									
1.0	butane	14.8	0.0	14.8	0.0	0.0	0.0	0.0	0.0
2.1	butane	74.0	12.0	62.0	3.3	88.4	99.7	86.2	15.0
3.0	butane	142.8	46.2	96.5	23.3	89.4	99.8	84.5	18.1
4.1	butane	275.5	131.0	144.5	28.0	95.9	99.9	92.3	12.5
5.0	butane	416.3	232.0	184.3	28.6	97.8	100.0	95.1	10.0
6.1	butane	612.3	385.4	226.9	28.3	98.1	100.0	94.9	12.1
7.0	butane	802.1	542.8	259.3	28.8	98.6	100.0	95.6	11.6
8.1	butane	1073.7	767.0	306.8	28.8	98.5	100.0	94.9	9.7
9.0	butane	1338.9	988.0	350.9	29.1	99.3	100.0	97.3	7.8
10.2	butane	1686.0	1290.0	396.0	29.0	99.1	100.0	96.0	10.0

NC size (nm)	Alcane-thiol	S-S Distance		% Occupation of adsorption sites			R_{st}		
		center	edge	on top	bridge	3f-hollow	total	center	edge
Values for σ_{SS} = 4.25 Å									
1.0	butane	0.00	0.00	32.2	38.4	29.4	1.48	0.00	1.48
2.1	butane	1.59	4.42	17.0	36.5	46.5	2.96	6.73	2.50
3.0	butane	4.48	4.38	15.8	43.3	40.9	3.32	5.44	2.53
4.1	butane	4.54	4.39	13.0	38.3	48.7	3.75	5.43	2.59
5.0	butane	4.53	4.40	11.8	38.4	49.9	3.93	5.17	2.68
6.1	butane	4.53	4.39	10.1	39.9	50.0	4.07	5.12	2.66
7.0	butane	4.54	4.39	9.3	38.2	52.5	4.19	5.11	2.69
8.1	butane	4.54	4.40	8.3	38.1	53.6	4.30	5.09	2.72
9.0	butane	4.55	4.40	7.4	38.3	54.3	4.37	5.10	2.71
10.2	butane	4.55	4.40	7.0	38.2	54.8	4.43	5.07	2.73
Values for σ_{SS} = 4.98 Å									
1.0	butane	0.00	0.00	32.1	31.3	36.6	1.89	0.00	1.89
2.1	butane	2.48	4.88	10.8	28.9	60.3	3.89	6.00	3.49
3.0	butane	4.98	4.90	6.7	20.7	72.6	4.54	6.23	3.73
4.1	butane	4.98	4.92	4.2	17.6	78.2	4.91	6.11	3.82
5.0	butane	4.98	4.95	10.1	8.8	81.1	4.92	5.83	3.78
6.1	butane	4.98	4.93	3.7	11.4	84.9	5.23	6.00	3.91
7.0	butane	4.98	4.95	5.3	7.6	87.1	5.28	5.90	3.98
8.1	butane	4.99	4.94	2.5	8.6	88.9	5.43	6.01	3.99
9.0	butane	4.97	4.97	5.5	6.1	88.4	5.38	5.90	3.90
10.2	butane	4.99	4.94	3.1	6.5	90.4	5.49	5.96	3.94

Table S6. Simulation results for the icosahedral NCs.

NC size (nm)	Alcanethiol	Number of adsorbed thiols			% SAM > 10 members	% SAM > 3 members			
		total	center	edge		total	total	center	edge
Values for σ_{SS} = 4.25 Å									
1.8	butane	69.9	0.0	69.9	0.0	0.2	0.0	0.2	40.9
2.2	butane	105.8	0.0	105.8	0.0	10.8	0.0	10.8	58.1
2.7	butane	144.0	0.0	144.0	0.0	37.9	0.1	37.9	77.7
3.1	butane	208.0	20.0	188.0	0.0	17.2	31.5	15.7	79.8
3.6	butane	271.4	49.5	221.9	0.0	37.6	49.8	34.9	75.8
4.1	butane	328.0	61.4	266.6	1.2	48.0	65.1	44.1	91.1
4.5	butane	422.2	117.2	305.0	1.2	35.3	49.7	29.7	92.6
5.0	butane	503.1	167.0	336.2	3.2	56.4	71.9	48.7	80.1
5.5	butane	587.4	211.8	375.7	3.7	53.9	70.1	44.8	85.6
5.9	butane	698.5	295.4	403.1	3.8	63.8	78.6	52.9	75.5
6.4	butane	807.8	364.3	443.5	4.7	64.3	78.7	52.5	76.6
6.9	butane	921.2	440.4	480.7	6.3	67.6	81.7	54.7	79.6
7.3	butane	1045.2	530.6	514.5	6.7	69.3	82.2	56.0	78.5
7.8	butane	1179.7	622.5	557.2	7.3	70.1	83.4	55.3	79.3
8.3	butane	1327.6	742.3	585.4	7.1	72.1	84.3	56.6	72.9
8.7	butane	1465.9	840.6	625.2	8.8	71.8	83.8	55.7	76.6
9.2	butane	1622.3	957.7	664.6	9.4	72.9	84.5	56.2	78.9
9.7	butane	1780.8	1082.0	698.8	10.3	74.0	84.9	57.2	78.5
10.1	butane	1959.1	1218.1	741.1	10.5	74.2	85.1	56.4	79.1
Values for σ_{SS} = 4.98 Å									
1.8	butane	48.5	0.0	48.5	0.0	26.0	0.0	26.0	0.1
2.2	butane	78.0	0.0	78.0	0.0	73.8	0.0	73.8	27.8
2.7	butane	121.4	20.0	101.4	0.0	99.8	100.0	99.7	7.9
3.1	butane	158.9	22.3	136.6	0.3	92.4	99.8	91.1	15.2
3.6	butane	203.8	44.4	159.4	6.7	91.3	99.5	89.0	9.0
4.1	butane	242.0	99.9	142.1	27.9	97.2	99.8	95.5	0.4
4.5	butane	309.7	128.4	181.3	25.1	93.7	99.6	89.6	6.6
5.0	butane	385.3	159.3	226.0	24.8	94.1	99.9	90.0	5.8
5.5	butane	481.3	200.0	281.3	29.3	99.9	100.0	99.8	5.2
5.9	butane	539.3	269.3	269.9	26.4	96.4	99.9	93.0	9.8
6.4	butane	633.1	328.9	304.2	26.9	97.0	99.9	93.8	7.8
6.9	butane	751.3	380.0	371.3	29.3	99.9	100.0	99.8	4.9
7.3	butane	811.2	508.7	302.4	28.3	98.6	99.9	96.5	3.6
7.8	butane	949.8	528.2	421.6	28.9	99.1	99.9	98.1	7.4
8.3	butane	1041.2	642.5	398.7	26.9	97.2	99.7	93.2	7.6
8.7	butane	1187.6	723.7	463.9	28.1	98.9	99.8	97.4	8.2
9.2	butane	1302.2	853.8	448.4	27.9	98.1	99.9	94.7	7.7
9.7	butane	1450.4	956.8	493.5	28.1	98.0	99.9	94.4	9.0
10.1	butane	1574.7	1072.2	502.5	27.9	98.4	99.9	95.2	7.7

Suite Table S6

NC size (nm)	Alcane-thiol	S-S Distance		% Occupation of adsorption sites			R_{st}		
		center	edge	on top	bridge	3f-hollow	total	center	edge
Values for σ_{SS} = 4.25 Å									
1.8	Butane	0.00	4.22	14.5	68.3	17.2	2.57	0.00	2.57
2.2	Butane	0.00	4.36	11.0	34.4	54.6	3.03	2.00	2.84
2.7	Butane	0.00	4.44	4.2	29.2	66.7	3.47	8.00	2.92
3.1	Butane	0.00	4.36	15.5	29.5	55.0	3.46	9.00	2.87
3.6	Butane	4.27	4.41	12.8	29.1	58.1	3.61	6.47	2.97
4.1	Butane	4.28	4.42	6.1	24.6	69.3	3.90	8.15	2.93
4.5	Butane	4.35	4.37	14.6	26.3	59.1	3.84	6.14	2.95
5.0	Butane	4.46	4.40	8.1	30.7	61.2	3.98	5.87	3.03
5.5	Butane	4.47	4.42	9.3	25.9	64.8	4.12	6.04	3.03
5.9	Butane	4.50	4.41	7.9	31.8	60.3	4.12	5.48	3.13
6.4	Butane	4.51	4.41	6.7	32.0	61.3	4.18	5.49	3.11
6.9	Butane	4.53	4.41	6.3	31.6	62.0	4.26	5.49	3.12
7.3	Butane	4.53	4.42	6.0	32.3	61.7	4.31	5.43	3.15
7.8	Butane	4.54	4.42	5.2	32.5	62.3	4.34	5.43	3.12
8.3	Butane	4.54	4.40	6.1	33.5	60.4	4.35	5.28	3.18
8.7	Butane	4.55	4.42	5.0	32.3	62.7	4.42	5.35	3.17
9.2	butane	4.56	4.42	4.8	32.3	62.8	4.45	5.35	3.16
9.7	butane	4.56	4.44	4.6	32.4	63.1	4.49	5.34	3.18
10.1	butane	4.56	4.43	4.7	32.2	63.2	4.50	5.32	3.16
Values for σ_{SS} = 4.98 Å									
1.8	Butane	0.00	4.32	8.2	39.6	52.2	3.71	0.00	3.71
2.2	Butane	0.00	4.92	12.3	31.1	56.6	4.10	0.00	3.85
2.7	Butane	0.00	4.65	9.5	25.1	65.4	4.12	4.00	4.14
3.1	Butane	0.74	4.88	3.6	31.1	65.3	4.53	8.07	3.95
3.6	Butane	4.95	4.66	3.3	24.6	72.1	4.81	7.21	4.14
4.1	Butane	5.05	4.85	0.9	7.8	91.2	5.29	5.01	5.49
4.5	Butane	5.00	4.85	1.5	11.1	87.4	5.23	5.61	4.96
5.0	Butane	4.99	4.88	2.4	16.3	81.3	5.19	6.15	4.51
5.5	Butane	4.99	4.96	2.4	19.0	78.6	5.03	6.40	4.05
5.9	Butane	4.98	4.88	1.4	12.5	86.1	5.34	6.01	4.67
6.4	Butane	4.98	4.40	1.3	13.6	85.1	5.34	6.08	4.54
6.9	Butane	4.99	4.97	1.6	16.2	82.2	5.22	6.37	4.04
7.3	Butane	4.99	4.84	0.6	5.3	94.1	5.55	5.66	5.36
7.8	Butane	4.99	4.68	0.8	15.7	83.5	5.39	6.40	4.13
8.3	Butane	4.97	4.87	0.6	10.1	89.4	5.55	6.10	4.66
8.7	Butane	4.97	4.91	0.7	14.0	85.3	5.46	6.22	4.27
9.2	butane	4.97	4.61	0.6	9.4	90.0	5.54	6.00	4.68
9.7	butane	4.97	4.87	0.9	11.6	87.5	5.52	6.04	4.50
10.1	butane	4.97	4.88	0.5	9.2	90.3	5.60	6.04	4.66

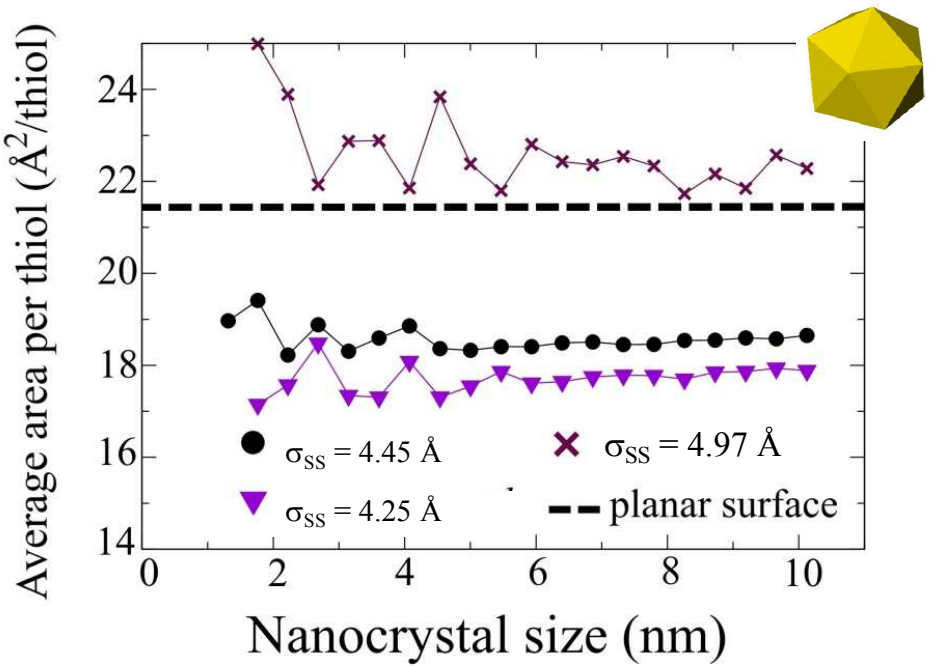

Figure S1. *Average surface area per adsorbed thiolate as a function of the NC diameter for icosahedral NCs. The results using three different values for σ_{SS} are shown. The details of the determination of the NC surface are explained in our previous papers[21]. The results for the planar surface are those obtained by experiments.*

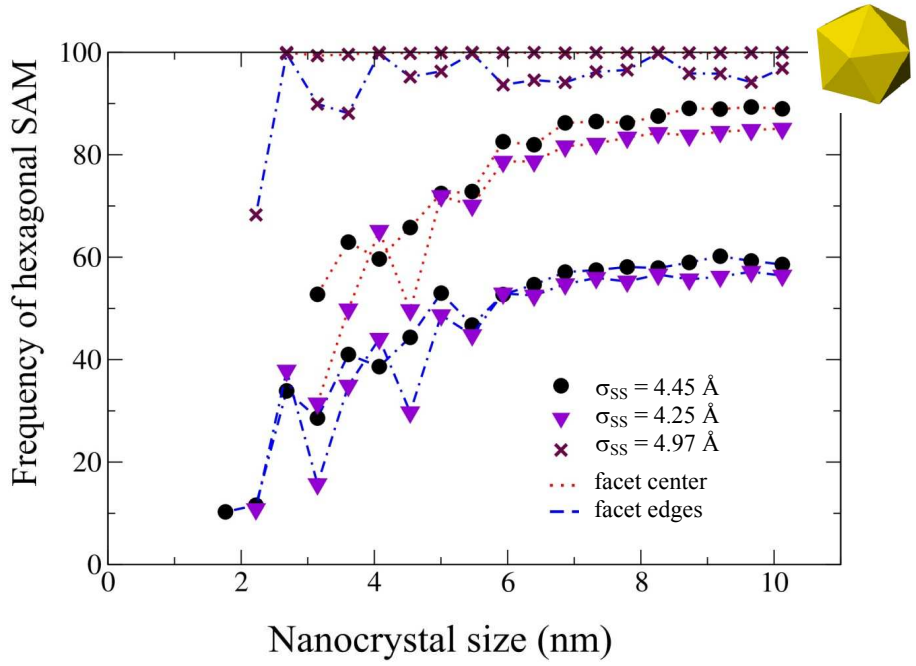

Figure S2. *Frequencies of S atoms participating in the formation of a SAM of at least 3 members for icosahedral nanocrystals using three different values for σ_{SS}.*

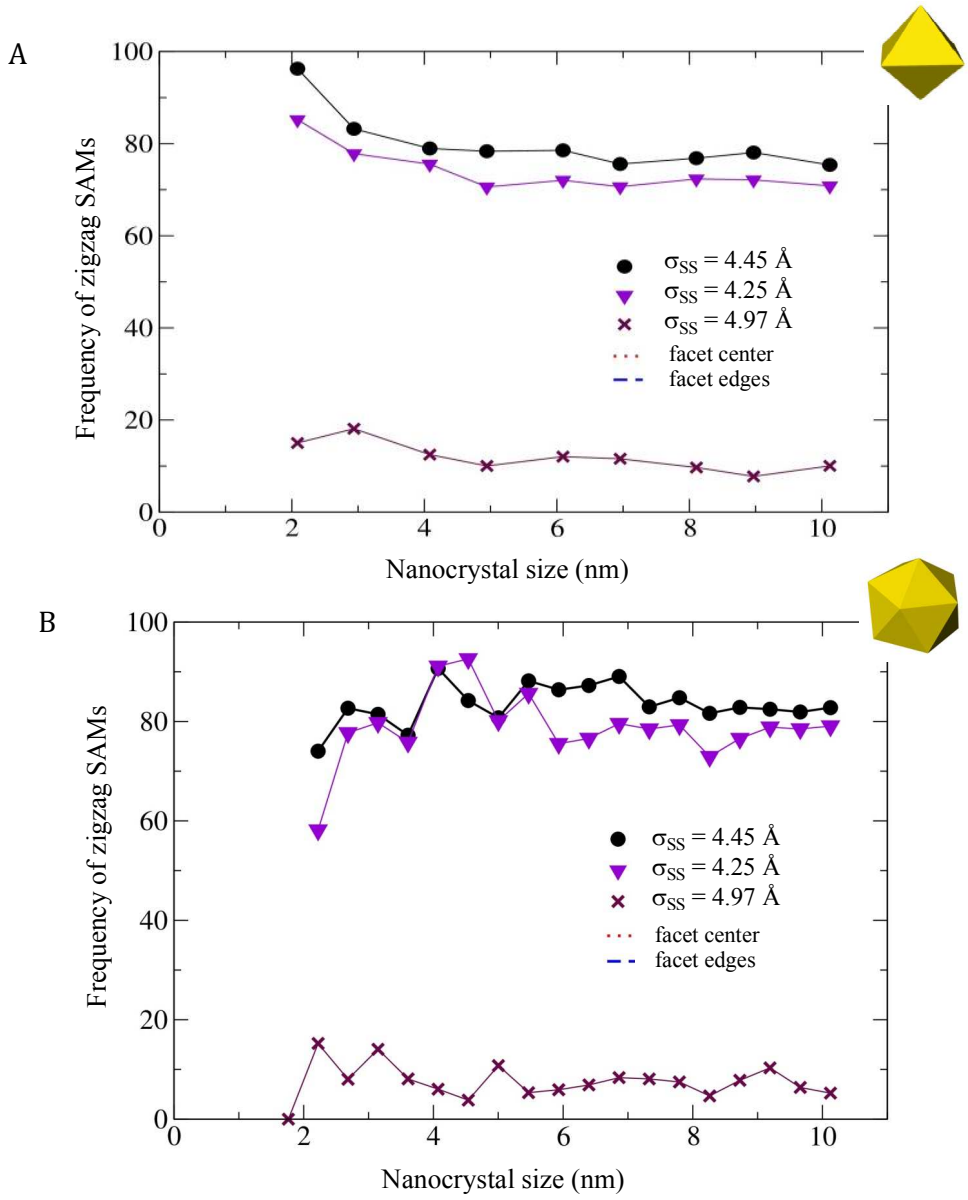

Figure S3. *Frequencies of S atoms participating in the formation of a zigzag SAM of at least 3 members for octahedral and icosahedral nanocrystals using three different values for* σ_{SS}.

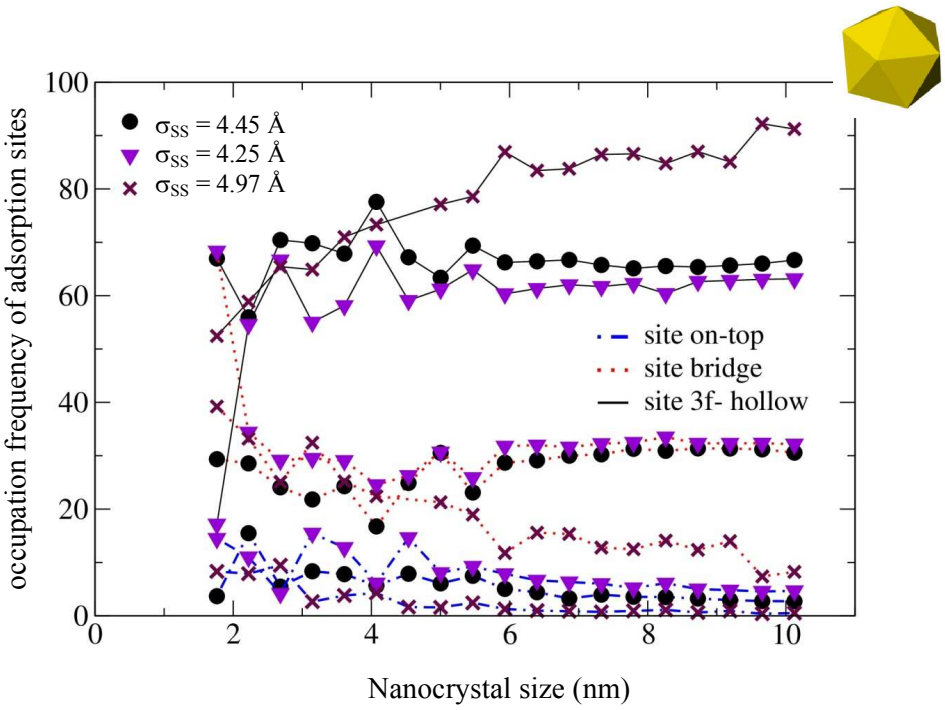

Figure S4. *Occupation frequencies of the different adsorption sites for icosahedral NCs for different interaction models. The results are shown for three different* σ_{SS} *values.*

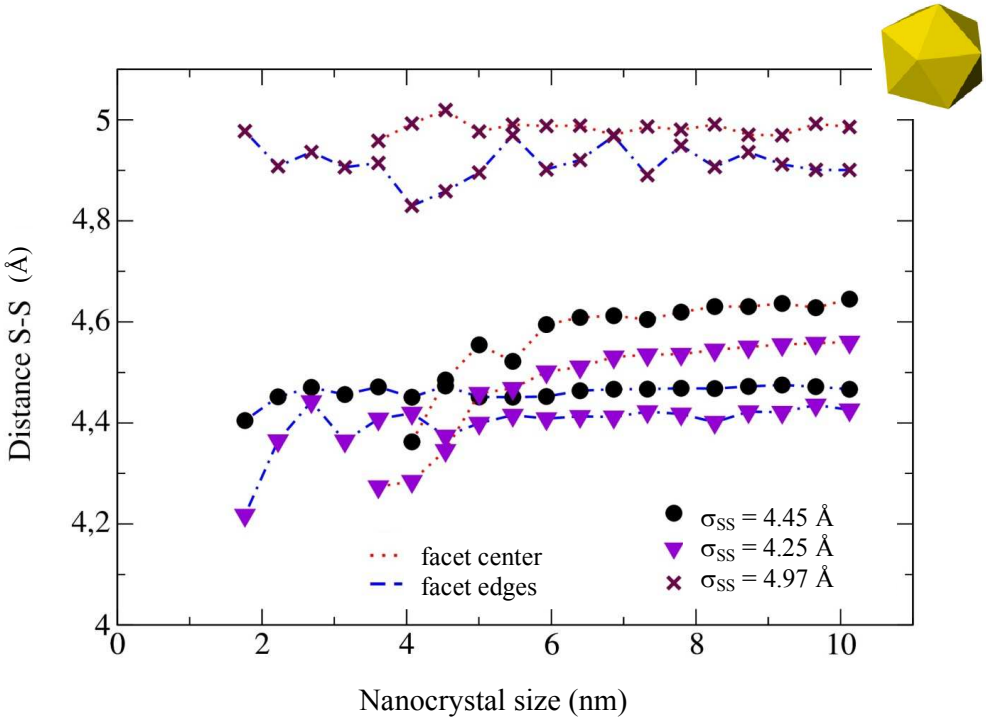

Figure S5. *Average distances between neighboring S groups on the edge and in the center of the NC facets for icosahedral NCs for the interaction models.*