Supporting Information for

Atomistic Simulations of Self-Assembled Monolayers on Octahedral and Cubic Gold Nanocrystals

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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
1.0	octane	14	25	239	6.5	300
1.0	dodecane	14	25	339	7.5	300
1.0	hexadecane	14	25	439	8.5	300
2.0	butane	172	90	622	6.4	300
2.0	octane	172	90	982	7.5	300
2.0	dodecane	172	90	1342	8.5	300
2.0	hexadecane	172	90	1702	9.5	300
3.0	butane	666	210	1716	7.5	300
3.0	octane	666	210	2556	8.5	600
3.0	dodecane	666	210	3396	9.5	600
3.0	hexadecane	666	210	4236	10.5	300
4.1	butane	1688	375	3563	8.5	300
4.1	octane	1688	375	5063	9.5	600
4.1	dodecane	1688	375	6563	10.6	600
4.1	hexadecane	1688	375	8063	11.6	300
5.1	butane	3430	600	6430	9.6	600
5.1	octane	3430	600	8830	10.6	600
5.1	dodecane	3430	600	11230	11.6	600
5.1	hexadecane	3430	600	13630	12.6	600
6.2	butane	6084	870	10434	10.6	300
6.2	octane	6084	870	13914	11.6	600
6.2	dodecane	6084	870	17394	12.7	600
6.2	hexadecane	6084	870	20874	13.7	300
7.2	butane	9842	1190	15792	11.7	600
7.2	octane	9842	1190	20552	12.7	600
7.2	dodecane	9842	1190	25312	13.7	600
7.2	hexadecane	9842	1190	30072	14.7	600
8.3	butane	14896	1560	22696	12.7	300
8.3	octane	14896	1560	28936	13.7	600
8.3	dodecane	14896	1560	35176	14.8	600
8.3	hexadecane	14896	1560	41416	15.8	300
8.8	butane	17969	1760	26769	13.3	300
8.8	octane	17969	1760	33809	14.3	600
8.8	dodecane	17969	1760	40849	15.3	600
8.8	hexadecane	17969	1760	47889	16.3	300
9.8	butane	25327	2200	36327	14.3	300
9.8	octane	25327	2200	45127	15.3	600
9.8	dodecane	25327	2200	53927	16.3	600
9.8	hexadecane	25327	2200	62727	17.4	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
1.0	octane	18	20	198	6.5	90
1.0	dodecane	18	20	278	7.5	90
2.1	butane	230	100	730	6.6	90
2.1	octane	230	100	1130	7.6	90
2.1	dodecane	230	100	1530	8.6	90
3.0	butane	670	205	1695	7.5	90
3.0	octane	670	205	2515	8.5	90
3.0	dodecane	670	205	3335	9.5	90
4.1	butane	1834	400	3834	8.6	90
4.1	octane	1834	400	5434	9.6	90
4.1	dodecane	1834	400	7034	10.6	90
5.0	butane	3280	590	6230	9.5	90
5.0	octane	3280	590	8590	10.5	90
5.0	dodecane	3280	590	10950	11.5	90
6.1	butane	6180	900	10680	10.6	90
6.1	octane	6180	900	14280	11.6	90
6.1	dodecane	6180	900	17880	12.6	90
7.0	butane	9224	1170	15074	11.5	90
7.0	octane	9224	1170	19754	12.5	90
7.0	dodecane	9224	1170	24434	13.5	90
8.1	butane	14644	1590	22594	12.6	90
8.1	octane	14644	1590	28954	13.6	90
8.1	dodecane	14644	1590	35314	14.7	90
9.0	butane	19870	1950	29620	13.5	90
9.0	octane	19870	1950	37420	14.5	90
9.0	dodecane	19870	1950	45220	15.5	90
10.2	butane	28594	2500	41094	14.6	90
10.2	octane	28594	2500	51094	15.7	90
10.2	dodecane	28594	2500	61094	16.7	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
0.9	octane	13	20	193	6.4	300
0.9	dodecane	13	20	273	7.4	300
0.9	hexadecane	13	20	353	8.4	300
1.3	butane	55	45	280	5.8	300
1.3	octane	55	45	460	6.8	300
1.3	dodecane	55	45	640	7.8	300
1.3	hexadecane	55	45	820	8.8	300
1.8	butane	147	75	522	6.2	300
1.8	octane	147	75	822	7.3	300
1.8	dodecane	147	75	1122	8.3	300
1.8	hexadecane	147	75	1422	9.3	300
2.2	butane	309	115	884	6.7	300
2.2	octane	309	115	1344	7.7	300
2.2	dodecane	309	115	1804	8.7	300
2.2	hexadecane	309	115	2264	9.7	300
2.7	butane	561	165	1386	7.1	300
2.7	octane	561	165	2046	8.2	300
2.7	dodecane	561	165	2706	9.2	300
2.7	hexadecane	561	165	3366	10.2	300
3.1	butane	923	225	2048	7.6	300
3.1	octane	923	225	2948	8.6	300
3.1	dodecane	923	225	3848	9.6	300
3.1	hexadecane	923	225	4748	10.7	300
3.6	butane	1415	290	2865	8.1	300
3.6	octane	1415	290	4025	9.1	300
3.6	dodecane	1415	290	5185	10.1	300
3.6	hexadecane	1415	290	6345	11.1	300
4.1	butane	2057.0	370	3907	8.5	300
4.1	octane	2057.0	370	5387	9.6	300
4.1	dodecane	2057.0	370	6867	10.6	300
4.1	hexadecane	2057.0	370	8347	11.6	300
4.5	butane	2869	455	5144	9	300
4.5	octane	2869	455	6964	10	300
4.5	dodecane	2869	455	8784	11	300
4.5	hexadecane	2869	455	10604	12.1	300
5.0	butane	3871	550	6621	9.5	300
5.0	octane	3871	550	8821	10.5	300
5.0	dodecane	3871	550	11021	11.5	300
5.0	hexadecane	3871	550	13221	12.5	300
5.5	butane	5083	655	8358	9.9	300
5.5	octane	5083	655	10978	11	300
5.5	dodecane	5083	655	13598	12	300
5.5	hexadecane	5083	655	16218	13	300
5.9	butane	6525	770	10375	10.4	300
5.9	octane	6525	770	13455	11.4	300
5.9	dodecane	6525	770	16535	12.4	300
5.9	hexadecane	6525	770	19615	13.4	300
6.4	butane	8217	890	12667	10.9	300

6.4	octane	8217	890	16227	11.9	300
6.4	dodecane	8217	890	19787	12.9	300
6.4	hexadecane	8217	890	23347	13.9	300
6.9	butane	10179	1020	15279	11.3	600
6.9	octane	10179	1020	19359	12.3	600
6.9	dodecane	10179	1020	23439	13.4	600
6.9	hexadecane	10179	1020	27519	14.4	600
7.3	butane	12431	1160	18231	11.8	300
7.3	octane	12431	1160	22871	12.8	300
7.3	dodecane	12431	1160	27511	13.8	300
7.3	hexadecane	12431	1160	32151	14.8	300
7.8	butane	14993	1310	21543	12.3	300
7.8	octane	14993	1310	26783	13.3	300
7.8	dodecane	14993	1310	32023	14.3	300
7.8	hexadecane	14993	1310	37263	15.3	300
8.3	butane	17885	1470	25235	12.7	300
8.3	octane	17885	1470	31115	13.7	300
8.3	dodecane	17885	1470	36995	14.8	300
8.3	hexadecane	17885	1470	42875	15.8	300
8.7	butane	21127	1640	29327	13.2	300
8.7	octane	21127	1640	35887	14.2	300
8.7	dodecane	21127	1640	42447	15.2	300
9.2	butane	24739	1815	33814	13.7	300
9.2	octane	24739	1815	41074	14.7	300
9.2	dodecane	24739	1815	48334	15.7	300
9.7	butane	28741	2000	38741	14.1	300
9.7	octane	28741	2000	46741	15.1	300
9.7	dodecane	28741	2000	54741	16.2	300
10.1	butane	33153	2200	44153	14.6	300
10.1	octane	33153	2100	52053	15.6	300
10.1	dodecane	33153	2100	60453	16.6	300

Suite Table S3

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
1.0	butane	15.2	1.5	13.7	0.0	51.6	3.5	48.1	0.0
1.0	octane	15.1	1.5	13.6	0.0	48.6	3.0	45.6	0.0
1.0	dodecane	15.0	1.5	13.5	0.0	48.3	3.5	44.8	0.0
1.0	hexadecane	15.0	1.5	13.5	0.0	45.2	3.1	42.1	0.0
2.0	butane	76.0	12.0	64.0	11.2	89.2	99.7	87.3	0.0
2.0	octane	76.0	11.0	65.0	12.4	88.2	99.4	86.3	0.0
2.0	dodecane	76.6	12.0	64.6	14.3	92.4	99.6	91.0	0.0
2.0	hexadecane	71.0	12.0	59.0	12.9	93.2	99.9	91.8	0.0
3.0	butane	180.9	69.0	111.9	27.5	96.0	100.0	93.5	0.0
3.0	octane	180.8	66.0	114.8	25.3	93.8	100.0	90.3	0.0
3.0	dodecane	177.0	69.0	108.0	28.4	97.3	100.0	95.6	0.0
3.0	hexadecane	154.3	53.0	101.3	24.4	95.2	99.7	92.9	0.0
4.1	butane	325.4	162.0	163.4	25.7	95.6	99.8	91.5	0.0
4.1	octane	342.1	174.0	168.1	27.3	93.8	100.0	87.4	0.0
4.1	dodecane	314.7	151.0	163.7	27.3	96.1	99.2	93.2	0.0
4.1	hexadecane	246.5	115.0	131.5	21.3	93.3	94.7	92.1	0.0
5.1	butane	506.7	287.0	219.7	26.7	95.5	99.8	89.9	0.0
5.1	octane	521.8	310.0	211.8	27.7	96.1	99.9	90.5	0.0
5.1	dodecane	494.3	284.0	210.3	27.9	96.6	99.3	92.9	0.0
5.1	hexadecane	389.9	213.4	176.5	22.4	92.0	92.0	92.0	0.0
6.2	butane	739.8	457.0	282.8	27.3	96.0	99.9	89.7	0.0
6.2	octane	760.5	486.0	274.5	28.1	96.3	99.9	89.9	0.0
6.2	dodecane	716.4	457.0	259.4	28.1	97.2	99.6	93.0	0.0
6.2	hexadecane	528.2	317.9	210.3	20.1	88.7	87.0	91.2	0.0
7.2	butane	1008.5	694.0	314.5	27.6	96.9	99.8	90.5	0.0
7.2	octane	1035.1	719.0	316.1	28.1	97.0	99.9	90.4	0.0
7.2	dodecane	984.2	653.0	331.2	27.2	95.6	99.5	87.8	0.0
7.2	hexadecane	806.4	524.5	281.8	25.0	92.0	90.5	95.0	0.0
8.3	butane	1275.7	911.3	364.4	27.6	97.3	99.7	91.6	0.0
8.3	octane	1331.7	966.9	364.7	28.3	97.4	99.8	90.8	0.0
8.3	dodecane	1232.9	873.0	359.9	28.1	97.3	99.1	93.1	0.0
8.3	hexadecane	982.7	681.8	300.9	19.6	90.8	90.5	91.4	0.0
8.8	butane	1451.9	1036.2	415.7	27.6	96.4	99.4	89.0	0.0
8.8	octane	1489.4	1102.0	387.4	28.2	97.7	99.9	91.4	0.0
8.8	dodecane	1414.5	1009.0	405.5	27.9	96.3	98.9	89.7	0.0
8.8	hexadecane	1044.6	710.4	334.2	19.9	85.5	82.4	92.2	0.0
9.8	butane	1810.2	1351.9	458.3	28.0	97.4	99.7	90.5	0.0
9.8	octane	1885.1	1408.0	477.1	28.0	96.9	99.9	88.3	0.0
9.8	dodecane	1706.0	1254.0	452.0	27.7	96.6	98.6	91.0	0.0
9.8	hexadecane	1315.8	920.1	395.7	18.8	85.5	83.4	90.5	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
1.0	butane	0.59	3.61	16.8	57.5	25.8	0.0	0.06	0.00	0.07
1.0	octane	0.56	3.57	17.2	58.1	24.8	0.0	0.06	0.00	0.07
1.0	dodecane	0.58	3.56	17.5	57.1	25.5	0.0	0.06	0.00	0.07
1.0	hexadecane	0.56	3.49	15.5	59.8	24.6	0.0	0.06	0.00	0.07
2.0	butane	3.86	4.18	6.7	13.5	32.9	46.9	0.95	2.00	0.75
2.0	octane	3.11	4.17	7.7	14.5	32.4	45.4	0.95	2.18	0.74
2.0	dodecane	3.84	4.17	7.4	13.4	32.9	46.4	0.94	2.00	0.74
2.0	hexadecane	3.89	4.19	0.2	7.9	42.0	49.9	1.01	2.00	0.81
3.0	butane	4.12	4.15	2.6	9.7	23.8	63.8	1.33	2.09	0.86
3.0	octane	4.12	4.15	5.4	10.0	23.5	61.0	1.36	2.29	0.84
3.0	dodecane	4.12	4.15	0.1	7.6	27.2	65.0	1.36	2.09	0.89
3.0	hexadecane	4.13	4.16	0.5	9.3	24.7	65.4	1.56	2.72	0.95
4.1	butane	4.12	4.15	2.1	9.0	17.7	71.2	1.55	2.22	0.88
4.1	octane	4.11	4.14	3.7	10.7	14.9	70.8	1.50	2.16	0.85
4.1	dodecane	4.14	4.14	1.9	8.1	20.2	69.8	1.67	2.59	0.89
4.1	hexadecane	4.16	4.17	0.2	5.2	20.1	74.5	2.04	3.13	1.09
5.1	butane	4.13	4.14	2.3	8.1	14.5	75.1	1.71	2.34	0.87
5.1	octane	4.12	4.13	1.6	7.4	14.8	76.2	1.71	2.29	0.91
5.1	dodecane	4.13	4.13	0.9	6.8	16.9	75.4	1.77	2.44	0.91
5.1	hexadecane	4.15	4.16	0.5	5.3	17.5	76.7	2.22	3.15	1.09
6.2	butane	4.12	4.13	1.5	8.5	10.9	79.2	1.78	2.36	0.85
6.2	octane	4.13	4.13	2.8	7.2	11.6	78.5	1.82	2.36	0.90
6.2	dodecane	4.13	4.13	0.9	5.8	14.7	78.6	1.86	2.44	0.90
6.2	hexadecane	4.17	4.15	0.1	3.6	15.3	81.0	2.50	3.40	1.14
7.2	butane	4.13	4.13	1.2	6.2	10.9	81.7	1.88	2.33	0.92
7.2	octane	4.13	4.13	0.8	6.4	10.8	82.0	1.88	2.39	0.87
7.2	dodecane	4.14	4.13	2.6	7.1	10.8	79.5	1.94	2.49	0.87
7.2	hexadecane	4.17	4.14	0.4	4.4	13.0	82.1	2.65	3.62	1.07
8.3	butane	4.13	4.13	0.6	5.5	10.6	83.2	1.98	2.40	0.92
8.3	octane	4.14	4.13	1.2	5.5	10.4	82.9	2.00	2.40	0.95
8.3	dodecane	4.14	4.13	0.3	5.0	11.8	82.9	2.08	2.63	0.89
8.3	hexadecane	4.17	4.15	0.2	4.2	11.7	84.0	2.56	3.20	1.12
8.8	butane	4.14	4.13	1.3	6.5	8.7	83.5	1.98	2.43	0.87
8.8	octane	4.13	4.13	0.8	4.9	10.1	84.2	2.01	2.39	0.95
8.8	dodecane	4.14	4.13	2.0	5.8	10.0	82.1	2.10	2.63	0.86
8.8	hexadecane	4.17	4.14	0.3	3.6	11.2	84.9	2.76	3.55	1.08
9.8	butane	4.14	4.13	0.9	5.4	8.6	85.0	2.03	2.41	0.89
9.8	octane	4.14	4.13	1.2	6.3	7.5	85.0	2.07	2.47	0.90
9.8	dodecane	4.15	4.13	0.9	5.2	9.8	84.0	2.19	2.67	0.91
9.8	hexadecane	4.18	4.14	0.4	4.7	9.4	85.4	2.79	3.55	1.03

Suite Table S4

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
1.0	butane	18.8	0.0	18.8	0.0	0.0	0.0	0.0	0.0
1.0	octane	18.7	0.0	18.7	0.0	0.0	0.0	0.0	0.0
1.0	dodecane	18.8	0.0	18.8	0.0	0.0	0.0	0.0	0.0
2.1	butane	86.1	8.0	78.1	0.0	56.7	77.6	54.6	95.2
2.1	octane	83.9	8.0	75.9	0.0	42.0	66.5	39.4	96.0
2.1	dodecane	84.3	8.0	76.3	0.0	42.3	67.1	39.7	95.6
3.0	butane	179.2	48.3	130.8	4.9	66.1	80.7	60.7	83.2
3.0	octane	180.9	48.0	132.8	4.8	67.3	84.2	61.2	83.5
3.0	dodecane	176.6	46.1	130.5	7.1	64.7	81.2	58.9	87.4
4.1	butane	344.8	145.0	199.8	6.7	75.0	87.8	65.7	79.0
4.1	octane	347.3	144.2	203.2	5.7	72.5	86.2	62.8	78.9
4.1	dodecane	346.1	143.8	202.3	6.6	75.2	88.3	65.9	78.2
5.0	butane	498.6	245.3	253.2	11.9	77.4	89.0	66.2	78.4
5.0	octane	501.2	246.9	254.3	11.1	77.3	89.1	65.8	77.0
5.0	dodecane	498.9	246.2	252.7	10.1	76.9	88.6	65.5	77.6
6.1	butane	734.5	424.6	309.9	15.7	80.8	90.2	68.0	78.6
6.1	octane	759.1	436.1	323.0	10.5	79.7	89.3	66.8	76.9
6.1	dodecane	750.2	433.6	316.7	11.6	79.6	88.8	67.1	74.5
7.0	butane	962.0	599.0	363.0	15.4	82.4	91.1	67.9	75.6
7.0	octane	981.7	610.4	371.2	12.1	81.1	89.6	67.1	74.2
7.0	dodecane	972.0	608.6	363.4	10.8	80.4	89.0	66.0	74.5
8.1	butane	1286.0	853.8	432.2	18.2	83.5	91.2	68.3	76.8
8.1	octane	1321.5	880.2	441.3	12.7	82.3	90.1	66.9	73.5
8.1	dodecane	1304.1	871.2	432.8	13.2	81.4	88.5	67.1	74.0
9.0	butane	1568.9	1089.3	479.6	17.7	84.0	90.7	68.6	78.1
9.0	octane	1619.7	1126.2	493.5	12.4	82.9	89.4	68.2	73.7
9.0	dodecane	1587.3	1102.3	485.0	14.6	82.8	89.3	68.1	75.0
10.2	butane	1988.5	1440.1	548.4	19.0	84.9	91.1	68.8	75.4
10.2	octane	2035.8	1478.8	557.0	15.2	84.1	90.5	67.1	74.0
10.2	dodecane	1981.6	1444.2	537.3	16.2	83.9	89.7	68.2	74.7

NC size (nm)	Alcane-thiol	S-S Distance		% Occupation of adsorption sites			R_{st}		
		center	edge	on top	bridge	3f-hollow	total	center	edge
1.0	butane	0.00	0.00	35.7	32.7	31.6	1.49	0.00	1.49
1.0	octane	0.00	0.00	36.2	33.0	30.9	1.50	0.00	1.50
1.0	dodecane	0.00	0.00	35.6	34.4	30.0	1.49	0.00	1.49
2.1	butane	0.01	4.53	4.2	38.1	57.7	3.34	8.98	2.76
2.1	octane	0.00	4.50	14.3	6.9	78.7	3.43	9.00	2.85
2.1	dodecane	0.00	4.51	14.8	7.6	77.6	3.42	9.00	2.83
3.0	butane	4.55	4.50	10.9	37.8	51.3	3.62	5.96	2.75
3.0	octane	4.55	4.48	10.0	41.2	48.8	3.58	6.00	2.71
3.0	dodecane	4.57	4.49	9.7	36.4	53.9	3.67	6.25	2.76
4.1	butane	4.59	4.47	9.0	40.2	50.8	3.92	5.52	2.76
4.1	octane	4.57	4.47	10.4	38.0	51.6	3.89	5.55	2.72
4.1	dodecane	4.58	4.47	10.1	38.7	51.1	3.91	5.57	2.73
5.0	butane	4.62	4.47	8.9	37.3	53.8	4.11	5.51	2.75
5.0	octane	4.60	4.46	9.2	37.6	53.2	4.09	5.48	2.74
5.0	dodecane	4.60	4.46	8.7	38.1	53.3	4.10	5.49	2.75
6.1	butane	4.63	4.50	6.1	36.5	57.4	4.36	5.45	2.87
6.1	octane	4.59	4.45	8.8	37.7	53.5	4.22	5.30	2.75
6.1	dodecane	4.60	4.46	8.2	37.4	54.4	4.27	5.33	2.80
7.0	butane	4.63	4.49	6.7	36.7	56.6	4.40	5.34	2.84
7.0	octane	4.59	4.46	8.1	37.6	54.3	4.31	5.24	2.78
7.0	dodecane	4.58	4.46	7.6	37.0	55.4	4.35	5.26	2.84
8.1	butane	4.65	4.48	5.6	35.4	58.9	4.54	5.40	2.83
8.1	octane	4.59	4.45	7.3	37.5	55.2	4.41	5.24	2.77
8.1	dodecane	4.60	4.46	6.8	36.1	57.1	4.47	5.29	2.83
9.0	butane	4.64	4.49	5.0	35.7	59.3	4.59	5.35	2.85
9.0	octane	4.58	4.45	7.5	37.3	55.2	4.45	5.18	2.77
9.0	dodecane	4.61	4.45	5.9	36.5	57.6	4.54	5.29	2.82
10.2	butane	4.65	4.48	5.1	35.0	59.9	4.65	5.34	2.84
10.2	octane	4.60	4.45	6.1	37.2	56.7	4.54	5.20	2.80
10.2	dodecane	4.62	4.48	4.6	35.6	59.8	4.67	5.32	2.90

Suite Table S5

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
0.9	butane	14.0	0.0	14.0	0.0	0.0	0.0	0.0	0.0
0.9	octane	14.0	0.0	14.0	0.0	0.0	0.0	0.0	0.0
0.9	dodecane	14.0	0.0	14.0	0.0	0.0	0.0	0.0	0.0
0.9	hexadecane	14.0	0.0	14.0	0.0	0.0	0.0	0.0	0.0
1.3	butane	36.1	0.0	36.1	0.0	0.0	0.0	0.0	0.0
1.3	octane	35.9	0.0	35.9	0.0	0.0	0.0	0.0	0.0
1.3	dodecane	35.9	0.0	35.9	0.0	0.0	0.0	0.0	0.0
1.3	hexadecane	35.9	0.0	35.9	0.0	0.0	0.0	0.0	0.0
1.8	butane	61.8	0.0	61.8	0.0	10.3	0.0	10.3	17.7
1.8	octane	61.8	0.0	61.8	0.0	10.6	0.0	10.6	17.4
1.8	dodecane	61.7	0.0	61.7	0.0	10.3	0.0	10.3	17.0
1.8	hexadecane	61.6	0.0	61.6	0.0	9.2	0.0	9.2	16.2
2.2	butane	102.0	0.0	102.0	0.0	11.6	0.0	11.6	74.0
2.2	octane	102.0	0.0	102.0	0.0	11.2	0.0	11.2	75.4
2.2	dodecane	102.0	0.0	102.0	0.0	11.4	0.0	11.4	75.6
2.2	hexadecane	97.9	0.1	97.9	0.0	17.3	5.2	17.3	71.6
2.7	butane	140.9	0.0	140.9	0.0	33.9	0.0	33.9	82.7
2.7	octane	140.9	0.0	140.9	0.0	33.6	0.2	33.6	81.4
2.7	dodecane	139.9	0.0	139.9	0.0	32.9	0.1	32.9	84.5
2.7	hexadecane	138.9	0.0	138.9	0.0	32.4	0.3	32.4	80.8
3.1	butane	197.0	20.0	177.0	0.0	30.8	50.0	28.6	81.4
3.1	octane	197.7	20.0	177.7	0.0	31.5	48.7	29.6	83.3
3.1	dodecane	194.7	20.0	174.7	0.0	31.2	57.0	28.2	80.4
3.1	hexadecane	192.0	20.0	172.0	0.0	33.5	53.6	31.2	76.0
3.6	butane	252.6	43.1	209.5	0.0	44.0	58.7	41.0	77.2
3.6	octane	262.7	45.8	216.9	0.0	36.2	48.7	33.6	83.3
3.6	dodecane	257.9	47.5	210.5	0.0	42.5	55.3	39.7	77.7
3.6	hexadecane	249.9	39.6	210.3	0.0	40.4	57.8	37.1	81.4
4.1	butane	314.5	60.1	254.4	0.6	42.9	60.8	38.6	90.7
4.1	octane	318.9	60.7	258.3	1.3	46.6	65.9	42.1	90.7
4.1	dodecane	315.9	60.1	255.8	1.0	47.1	63.0	43.3	91.4
4.1	hexadecane	312.0	63.2	248.8	0.8	46.3	65.6	41.4	85.9
4.5	butane	397.9	110.1	287.8	2.1	51.1	68.6	44.4	84.2
4.5	octane	408.0	114.6	293.4	1.0	42.8	60.0	36.0	87.9
4.5	dodecane	400.5	111.4	289.1	1.7	46.4	65.5	39.0	84.4
4.5	hexadecane	392.6	113.9	278.8	2.7	56.7	74.2	49.6	76.0
5.0	butane	481.7	160.4	321.4	7.0	62.5	81.5	53.0	80.7
5.0	octane	482.5	154.2	328.3	5.9	59.0	77.1	50.5	84.0
5.0	dodecane	484.3	158.3	326.0	4.8	58.2	74.9	50.1	80.4
5.0	hexadecane	462.6	141.5	321.1	2.4	51.1	67.5	43.9	84.1
5.5	butane	570.1	202.9	367.2	5.9	56.5	74.3	46.8	88.2
5.5	octane	573.8	201.8	372.0	7.1	58.3	76.6	48.4	91.2
5.5	dodecane	571.5	210.4	361.2	7.4	63.1	81.0	52.7	84.1
5.5	hexadecane	546.1	198.2	347.9	5.4	58.3	74.9	48.9	79.3
5.9	butane	668.4	264.7	403.6	11.5	65.2	84.1	52.7	86.4
5.9	octane	685.4	288.4	397.0	5.6	66.2	82.0	54.7	76.8
5.9	dodecane	676.4	290.6	385.8	7.0	67.8	82.7	56.5	69.5
5.9	hexadecane	627.0	249.6	377.3	6.9	60.4	75.7	50.3	80.8
6.4	butane	771.0	333.7	437.3	12.3	67.7	84.8	54.6	87.2
6.4	octane	787.6	353.2	434.4	7.1	67.7	82.9	55.3	77.3
6.4	dodecane	779.3	359.1	420.2	6.0	70.0	83.8	58.1	69.3

6.4	hexadecane	716.0	328.3	387.7	9.5	67.2	82.0	54.6	67.6
6.9	butane	883.4	407.5	475.8	12.4	70.1	85.3	57.1	89.1
6.9	octane	906.2	433.2	473.0	7.8	70.4	84.9	57.2	80.7
6.9	dodecane	898.9	440.5	458.4	6.6	71.7	84.6	59.3	70.4
6.9	hexadecane	832.1	404.9	427.2	10.2	70.1	84.3	56.6	71.2
7.3	butane	1007.4	501.8	505.6	11.5	71.6	85.8	57.5	82.9
7.3	octane	1036.7	536.7	500.1	6.8	71.9	85.2	57.7	69.2
7.3	dodecane	1021.0	525.3	495.7	8.7	73.3	86.0	59.8	72.1
7.3	hexadecane	933.1	481.3	451.8	14.3	72.3	87.3	56.4	72.3
7.8	butane	1136.3	591.5	544.7	13.1	73.3	87.2	58.1	84.8
7.8	octane	1171.0	631.7	539.3	8.0	72.2	85.6	56.6	72.3
7.8	dodecane	1140.7	610.1	530.6	8.8	72.2	84.5	57.9	75.0
7.8	hexadecane	959.0	549.4	409.6	16.2	76.9	89.5	60.2	47.1
8.3	butane	1267.3	693.0	574.3	14.1	74.0	87.4	57.9	81.6
8.3	octane	1307.6	730.8	576.8	8.9	73.5	86.4	57.3	72.5
8.3	dodecane	1272.2	716.3	555.9	11.0	75.7	86.8	61.4	70.6
8.3	hexadecane	1101.8	635.9	465.9	13.6	73.8	86.2	56.9	59.2
8.7	butane	1410.8	800.7	610.1	15.0	75.7	88.5	59.0	82.8
8.7	octane	1449.3	830.2	619.0	10.7	74.7	86.5	58.8	78.1
8.7	dodecane	1427.0	827.7	599.3	10.2	74.4	85.6	59.0	72.0
9.2	butane	1558.5	913.0	645.5	15.6	76.8	88.6	60.2	82.5
9.2	octane	1604.5	950.8	653.6	11.0	75.5	86.6	59.3	76.2
9.2	dodecane	1636.4	988.8	647.5	7.1	75.9	86.5	59.7	66.4
9.7	butane	1719.4	1035.2	684.2	15.0	76.8	88.3	59.3	81.9
9.7	octane	1769.4	1078.8	690.6	11.5	77.0	87.5	60.5	78.4
9.7	dodecane	1808.2	1119.8	688.4	6.2	75.2	85.7	58.0	72.0
10.1	butane	1878.8	1157.6	721.3	16.4	77.1	88.7	58.6	82.8
10.1	octane	1952.8	1227.6	725.2	10.2	76.8	86.9	59.6	73.1
10.1	dodecane	1915.1	1212.5	702.6	11.9	78.5	87.6	62.8	71.3

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
0.9	butane	0.00	0.00	0.0	42.9	57.1	1.43	0.00	1.43
0.9	octane	0.00	0.00	1.7	45.3	53.0	1.43	0.00	1.43
0.9	dodecane	0.00	0.00	1.9	45.7	52.4	1.43	0.00	1.43
0.9	hexadecane	0.00	0.00	1.8	45.3	53.0	1.43	0.00	1.43
1.3	butane	0.00	0.00	29.7	23.3	47.0	2.22	0.00	2.22
1.3	octane	0.00	0.00	29.1	23.5	47.4	2.23	0.00	2.23
1.3	dodecane	0.00	0.00	29.9	23.2	46.9	2.23	0.00	2.23
1.3	hexadecane	0.00	0.00	32.0	22.6	45.4	2.23	0.00	2.23
1.8	butane	0.00	4.40	3.7	29.4	67.0	2.91	0.00	2.91
1.8	octane	0.00	4.41	3.7	29.5	66.8	2.91	0.00	2.91
1.8	dodecane	0.00	4.41	3.7	29.4	66.8	2.92	0.00	2.92
1.8	hexadecane	0.00	4.41	3.6	29.6	66.8	2.92	0.00	2.92
2.2	butane	0.00	4.45	15.5	28.6	55.9	3.14	0.00	2.94
2.2	octane	0.00	4.45	15.5	28.9	55.6	3.14	0.00	2.94
2.2	dodecane	0.00	4.45	15.7	28.5	55.8	3.14	0.00	2.94
2.2	hexadecane	0.00	4.46	13.1	25.4	61.5	3.27	82.50	3.07
2.7	butane	0.00	4.47	5.5	24.1	70.4	3.55	8.00	2.98
2.7	octane	0.00	4.47	5.5	23.9	70.5	3.55	24.00	2.98
2.7	dodecane	0.00	4.48	4.8	23.4	71.7	3.57	16.00	3.00
2.7	hexadecane	0.00	4.49	5.3	22.9	71.8	3.60	72.67	3.02
3.1	butane	0.00	4.46	8.4	21.8	69.8	3.65	8.99	3.05
3.1	octane	0.00	4.45	8.4	22.1	69.5	3.64	9.00	3.04
3.1	dodecane	0.00	4.46	8.3	20.2	71.5	3.70	9.00	3.09
3.1	hexadecane	0.00	4.47	7.2	19.4	73.5	3.75	8.99	3.14
3.6	butane	3.93	4.47	7.8	24.3	67.9	3.88	7.43	3.15
3.6	octane	3.86	4.46	13.6	26.3	60.1	3.73	6.99	3.04
3.6	dodecane	4.09	4.47	10.9	26.3	62.8	3.80	6.74	3.14
3.6	hexadecane	3.11	4.49	9.2	22.4	68.4	3.92	8.08	3.14
4.1	butane	4.36	4.45	5.6	16.8	77.6	4.07	8.32	3.07
4.1	octane	4.36	4.45	6.5	19.1	74.3	4.01	8.24	3.02
4.1	dodecane	4.37	4.47	6.4	18.1	75.5	4.05	8.31	3.05
4.1	hexadecane	4.42	4.47	6.0	18.2	75.8	4.10	7.91	3.14
4.5	butane	4.48	4.47	7.9	24.9	67.2	4.07	6.54	3.13
4.5	octane	4.42	4.44	11.0	23.9	65.1	3.97	6.28	3.07
4.5	dodecane	4.47	4.45	8.7	25.0	66.3	4.05	6.47	3.11
4.5	hexadecane	4.53	4.48	7.5	25.9	66.6	4.13	6.32	3.23
5.0	butane	4.55	4.45	6.1	30.5	63.4	4.15	6.11	3.17
5.0	octane	4.52	4.46	5.3	29.1	65.6	4.15	6.35	3.11
5.0	dodecane	4.52	4.47	7.1	29.4	63.5	4.13	6.19	3.13
5.0	hexadecane	4.52	4.47	4.7	19.8	75.5	4.32	6.93	3.18
5.5	butane	4.52	4.45	7.5	23.1	69.4	4.25	6.31	3.10
5.5	octane	4.52	4.45	7.1	24.9	68.0	4.22	6.34	3.06
5.5	dodecane	4.56	4.46	5.9	28.7	65.4	4.23	6.09	3.16
5.5	hexadecane	4.56	4.49	4.5	21.6	73.9	4.43	6.46	3.28
5.9	butane	4.59	4.45	5.0	28.7	66.2	4.31	6.12	3.12
5.9	octane	4.54	4.45	6.7	33.1	60.2	4.20	5.62	3.17
5.9	dodecane	4.59	4.45	6.6	33.0	60.4	4.26	5.57	3.27
5.9	hexadecane	4.60	4.49	2.2	21.1	76.6	4.59	6.49	3.34
6.4	butane	4.61	4.46	4.4	29.1	66.4	4.38	5.99	3.16
6.4	octane	4.56	4.46	5.5	32.1	62.4	4.29	5.66	3.18
6.4	dodecane	4.57	4.46	4.9	34.2	60.8	4.34	5.57	3.28
6.4	hexadecane	4.64	4.50	1.6	23.2	75.2	4.72	6.09	3.56
6.9	butane	4.61	4.47	3.3	30.0	66.7	4.44	5.94	3.15
6.9	octane	4.56	4.45	5.5	32.7	61.9	4.33	5.59	3.17

6.9	dodecane	4.57	4.47	5.4	34.4	60.2	4.36	5.49	3.27
6.9	hexadecane	4.64	4.50	1.6	26.6	71.8	4.71	5.98	3.51
7.3	butane	4.60	4.47	4.0	30.3	65.8	4.47	5.74	3.20
7.3	octane	4.57	4.43	6.0	35.0	59.0	4.34	5.37	3.24
7.3	dodecane	4.59	4.45	4.8	34.5	60.8	4.41	5.48	3.27
7.3	hexadecane	4.69	4.50	1.0	24.5	74.5	4.82	5.98	3.59
7.8	butane	4.62	4.47	3.6	31.3	65.1	4.51	5.71	3.19
7.8	octane	4.57	4.44	6.1	34.0	59.9	4.37	5.35	3.23
7.8	dodecane	4.58	4.47	4.1	32.9	63.0	4.49	5.54	3.28
7.8	hexadecane	4.78	4.53	0.1	14.9	85.0	5.34	6.15	4.25
8.3	butane	4.63	4.47	3.5	30.9	65.6	4.56	5.66	3.24
8.3	octane	4.57	4.44	6.0	33.8	60.2	4.42	5.36	3.22
8.3	dodecane	4.60	4.48	3.7	34.1	62.1	4.54	5.47	3.35
8.3	hexadecane	4.74	4.51	0.3	16.3	83.4	5.25	6.16	3.99
8.7	butane	4.63	4.47	3.2	31.4	65.4	4.59	5.62	3.25
8.7	octane	4.58	4.45	4.8	33.5	61.8	4.47	5.42	3.20
8.7	dodecane	4.59	4.45	4.0	33.9	62.1	4.54	5.44	3.30
9.2	butane	4.64	4.48	3.0	31.4	65.7	4.63	5.61	3.25
9.2	octane	4.58	4.45	4.8	33.3	61.8	4.50	5.38	3.21
9.2	dodecane	4.55	4.41	6.6	36.3	57.2	4.41	5.18	3.24
9.7	butane	4.63	4.47	2.8	31.2	66.0	4.65	5.58	3.24
9.7	octane	4.58	4.45	4.5	34.0	61.5	4.52	5.36	3.21
9.7	dodecane	4.53	4.43	6.7	35.6	57.7	4.42	5.16	3.22
10.1	butane	4.65	4.47	2.7	30.6	66.7	4.69	5.60	3.24
10.1	octane	4.57	4.44	5.1	34.5	60.4	4.52	5.28	3.23
10.1	dodecane	4.60	4.46	3.6	34.8	61.6	4.61	5.34	3.33

Suite Table S6

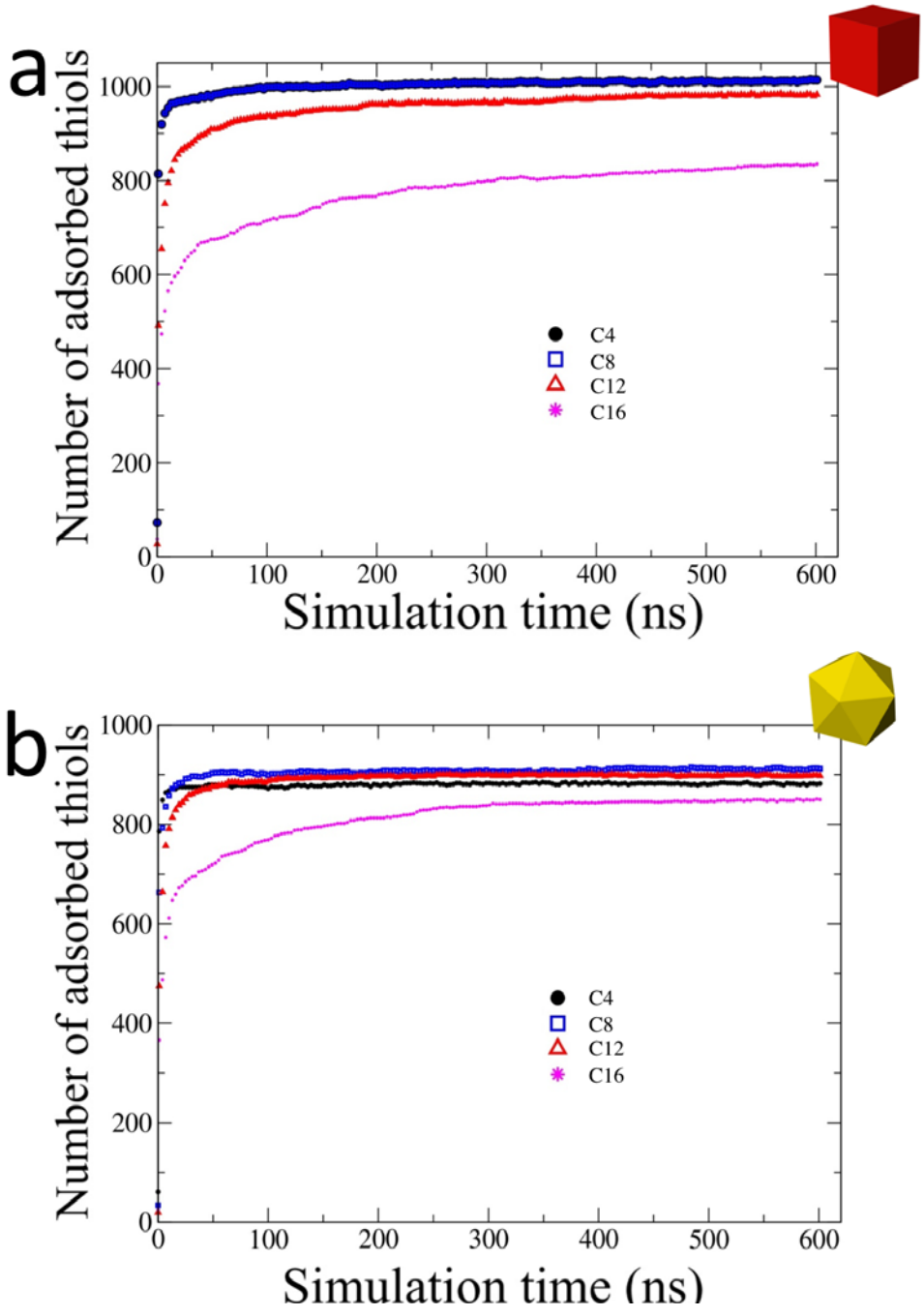

Figure S1. Time evolution of the number of adsorbed thiolate molecules for different alkane chain lengths for the following NCs. (a) octahedron of 7.0 nm, (b) icosahedra of 6.9 nm.

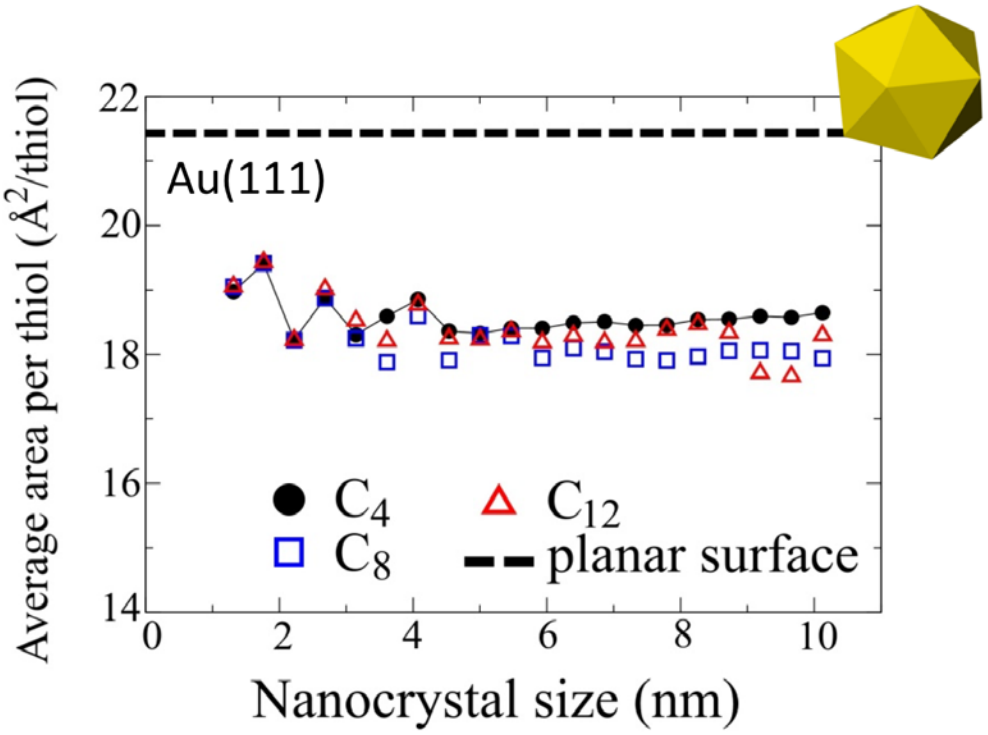

Figure S2. Average surface area per adsorbed thiolate as a function of the NC diameter for icosahedral NCs. The NC surface is described as an icosahedron (see main text for details).

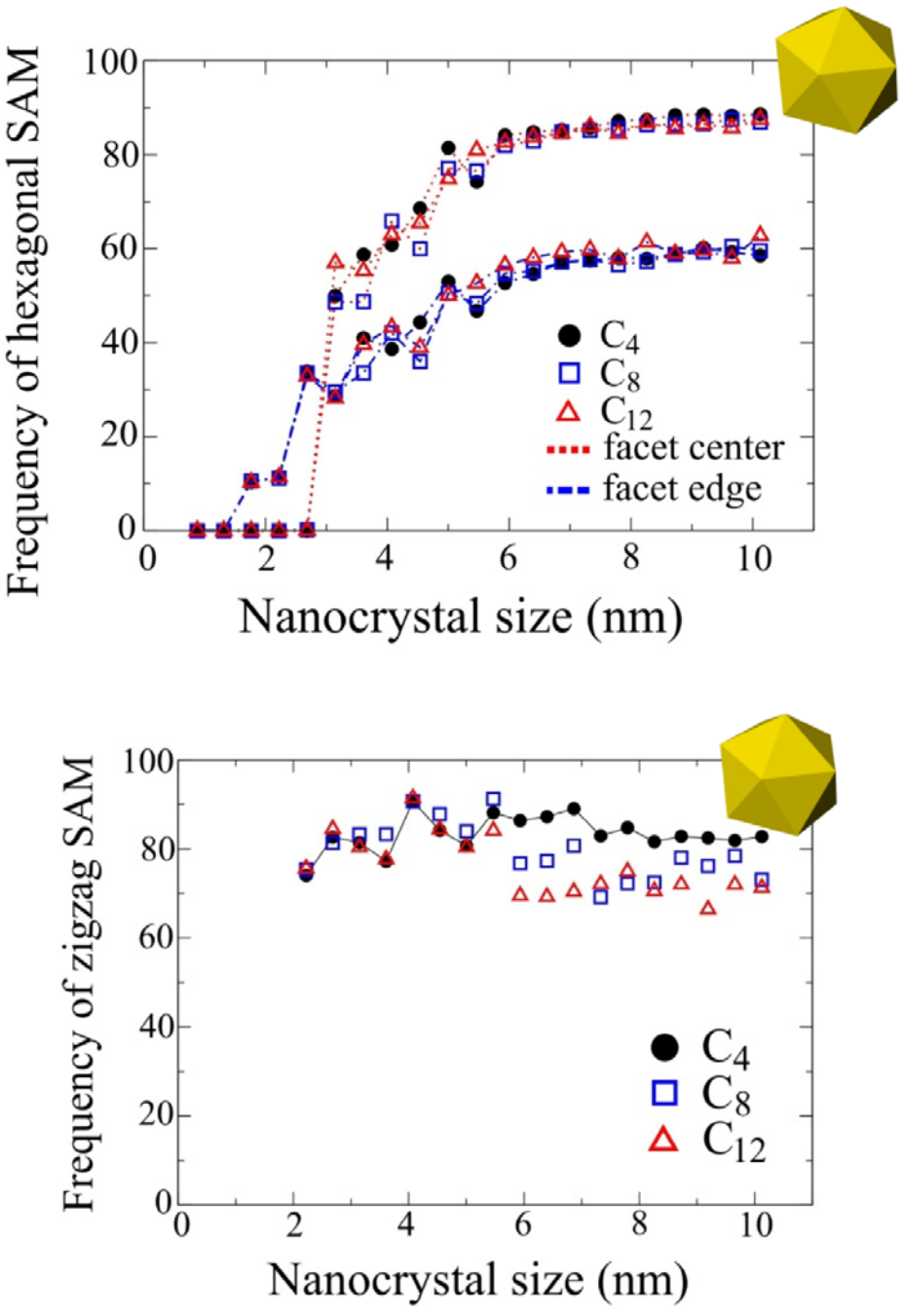

Figure S3. Frequencies of S groups participating in the formation of hexagonal (a) and zigzag (b) SAMs of at least 3 members for icosahedral nanocrystals.

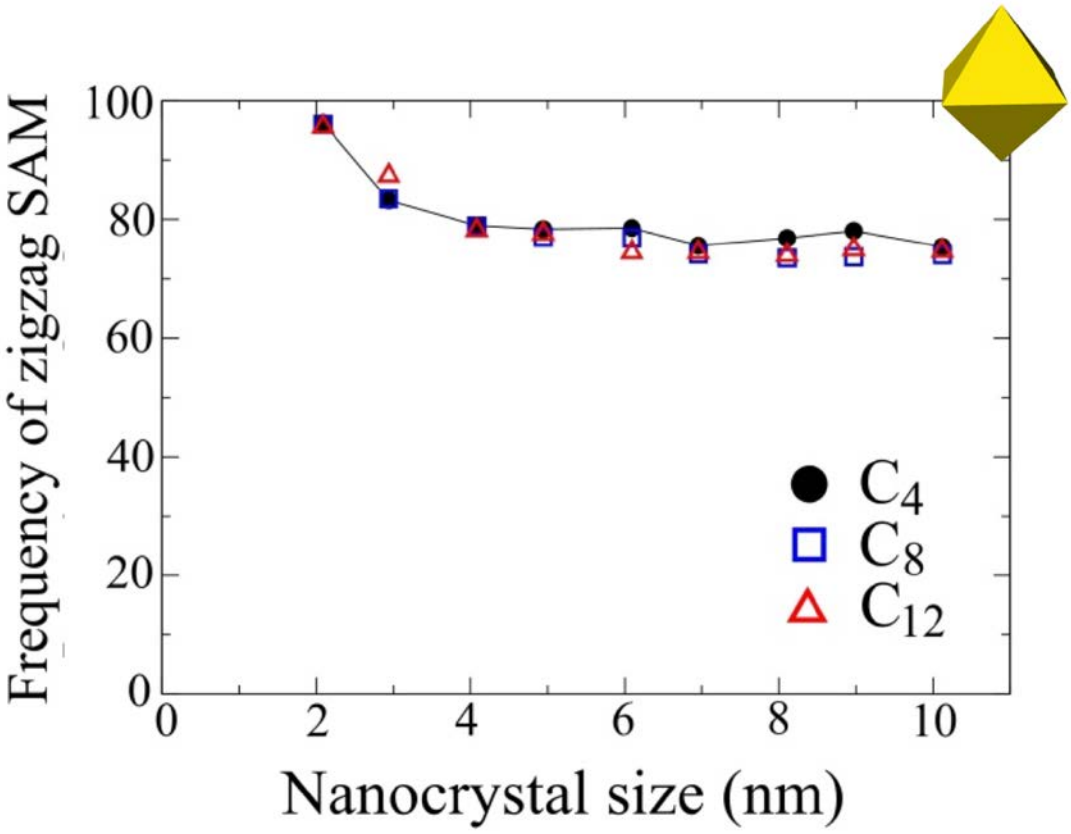

Figure S4. Frequencies of S groups belonging to a zigzag SAM (with at least 3 members) on the edges of the NCs facets for octahedral NCs.

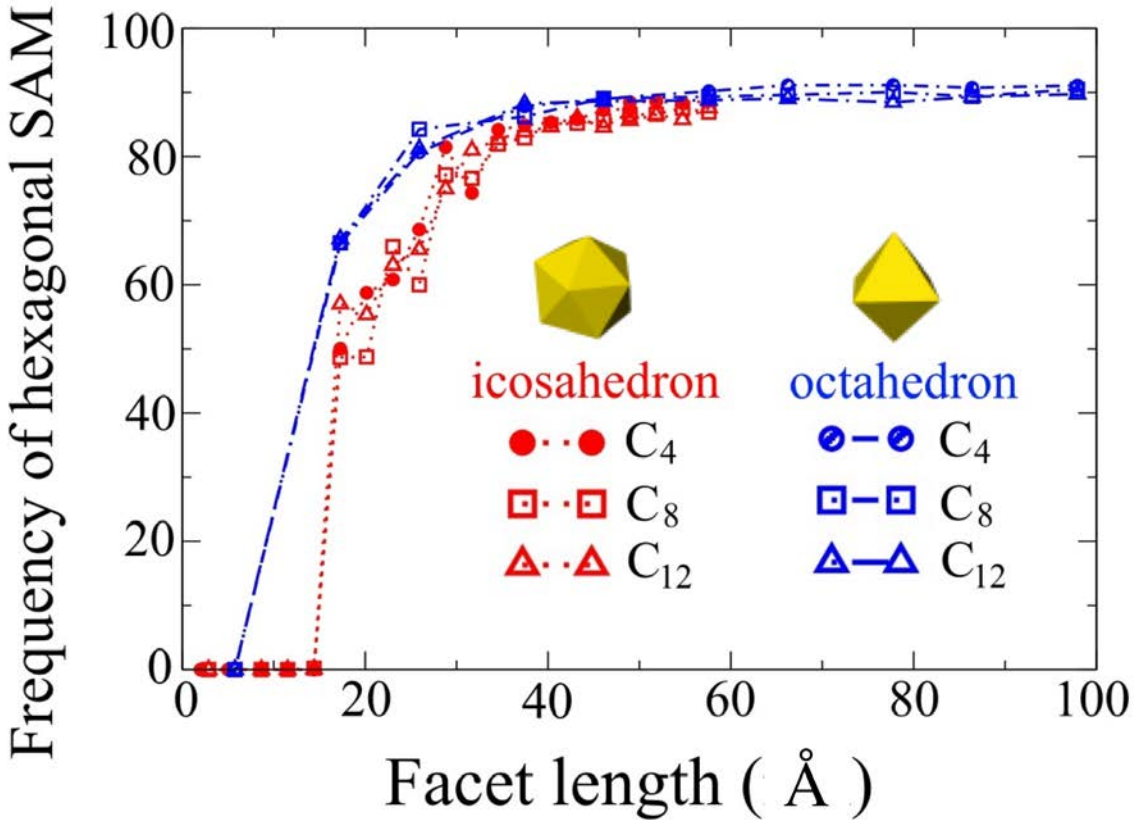

Figure S5. Frequencies of S groups participating in the formation of hexagonal SAMs of at least 3 members for octahedral and icosahedral nanocrystals. The frequency is plotted as a function of the facet length.

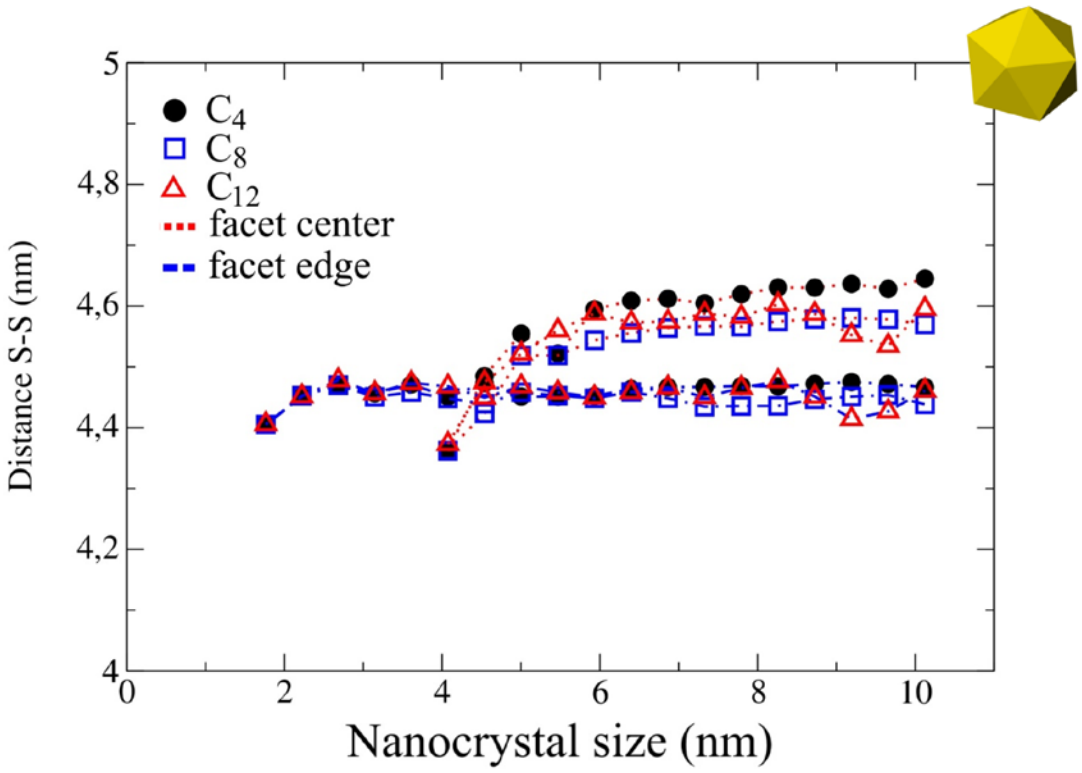

Figure S6. Average distances between the neighboring S groups on the edge and in the center of the facets of icosahedral NCs.

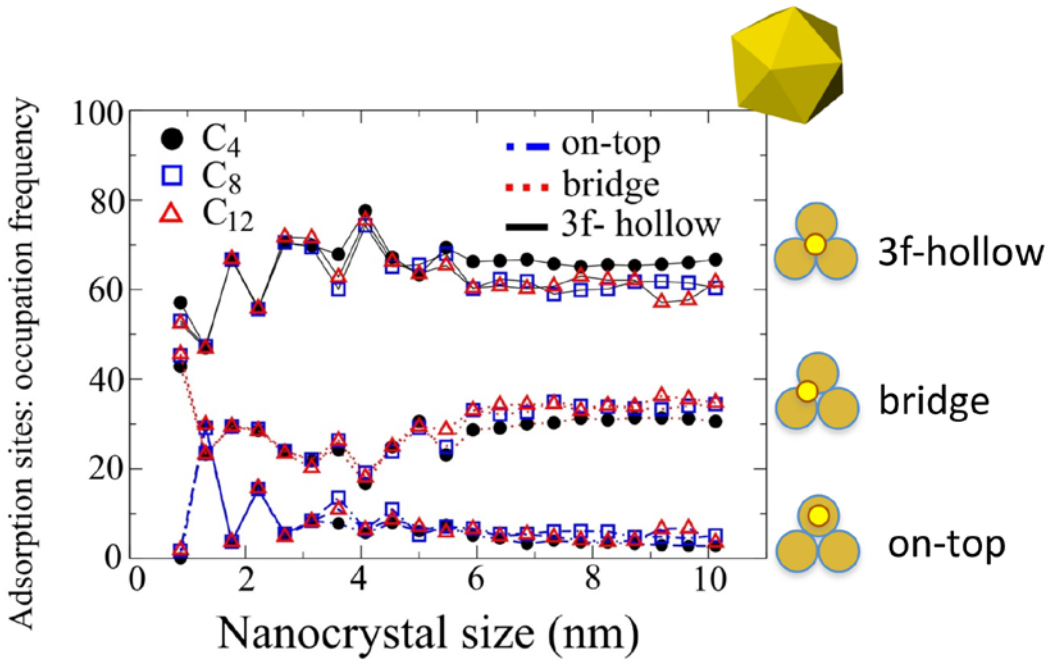

Figure S7. Frequency of occupation of the different adsorption sites for icosahedral NCs and different alkane thiolates.

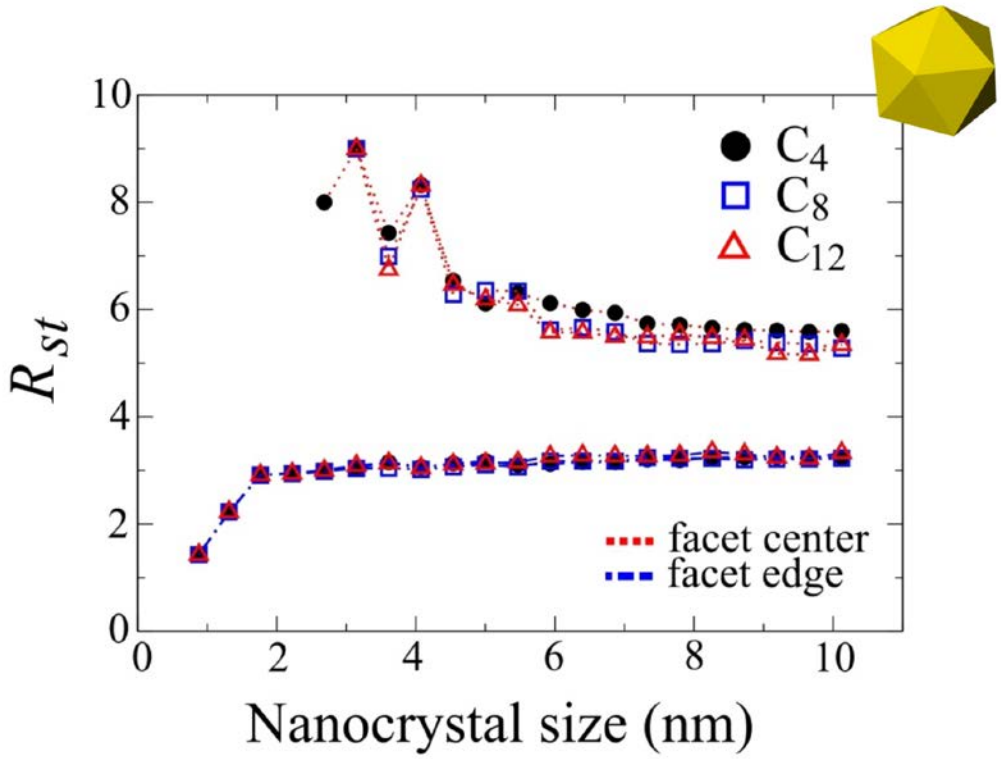

Figure S8. Ratio between the number of adsorption sites and adsorbed thiolates for icosahedral NCs and different alkane thiolates.