

Supplementary information

Systematic computational study of the structure crossover and coordination number distribution of metallic nanoparticles

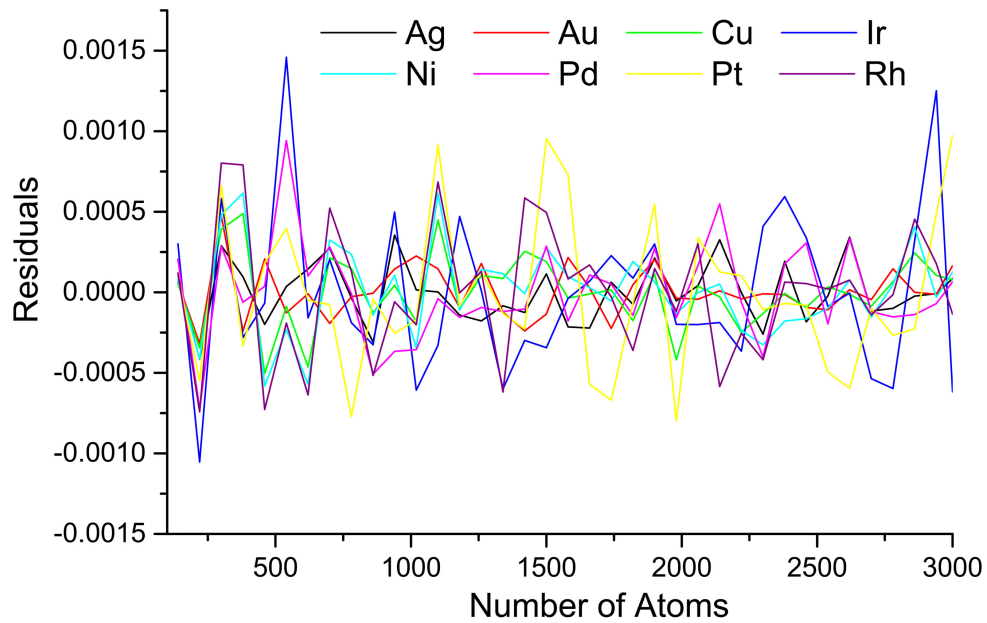
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Table S1 Approximation coefficients

Element	icosahedral				decahedral				cuboctahedral			
	e_c	e_f	e_e	e_v	e_c	e_f	e_e	e_v	e_c	e_f	e_e	e_v
Ag	-2.9912	1.7304	2.0181	-5.9351	-2.9828	1.3930	4.7231	-11.7567	-2.9993	1.8185	1.5863	-4.6228
Au	-3.8197	1.4928	0.4702	-0.8693	-3.8171	1.1933	2.4985	-5.6404	-3.8261	1.3705	1.3995	-3.2906
Cu	-3.6576	3.2388	0.6105	-6.1253	-3.6562	3.1123	1.9252	-8.6539	-3.6679	3.4489	-0.7110	-2.1156
Ir	-7.0074	4.3106	4.6913	-13.5736	-6.9679	2.9872	15.4022	-38.9537	-7.0175	4.2101	6.1074	-16.1670
Ni	-4.6510	4.1274	0.6586	-7.4223	-4.6426	3.8540	2.7985	-10.9699	-4.6641	4.3838	-0.8785	-2.7799
Pd	-3.9409	2.3573	2.6676	-7.7386	-3.9362	2.1031	4.3103	-9.7462	-3.9539	2.5032	1.9038	-5.4681
Pt	-5.8515	2.4982	4.3925	-11.5405	-5.8524	2.3292	4.9177	-10.7452	-5.8555	2.3258	5.4823	-13.0532
Rh	-5.9830	5.3364	2.1774	-12.5484	-6.0000	5.5521	1.2601	1.2601	-6.0050	5.7122	-0.0742	-5.7895

**Fig. S1** Residuals plot for cuboctahedral (crystalline) structure motif of all metals.

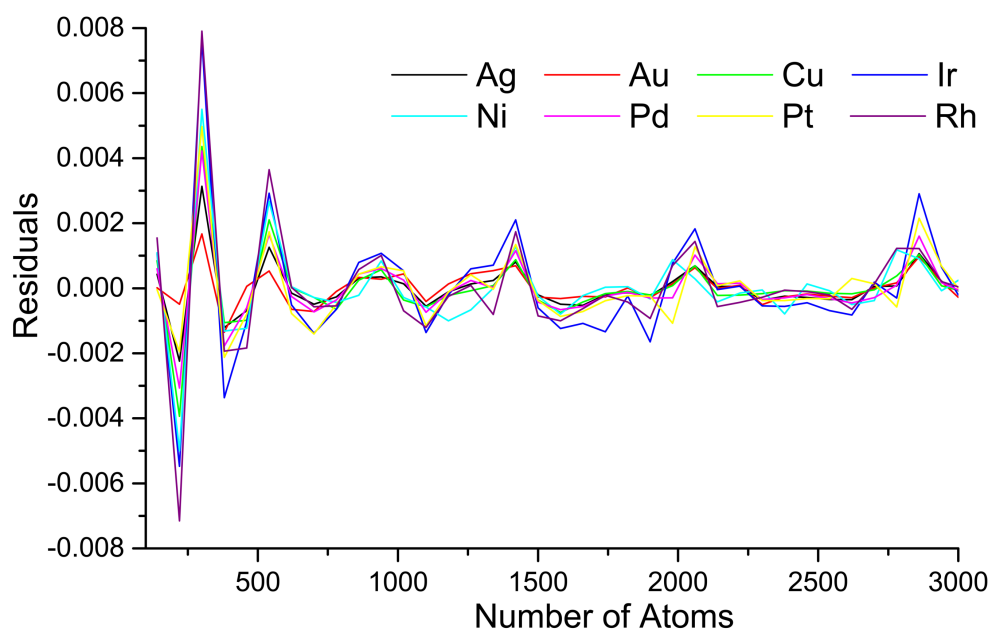


Fig. S2 Residuals plot for icosahedral structure motif of all metals.

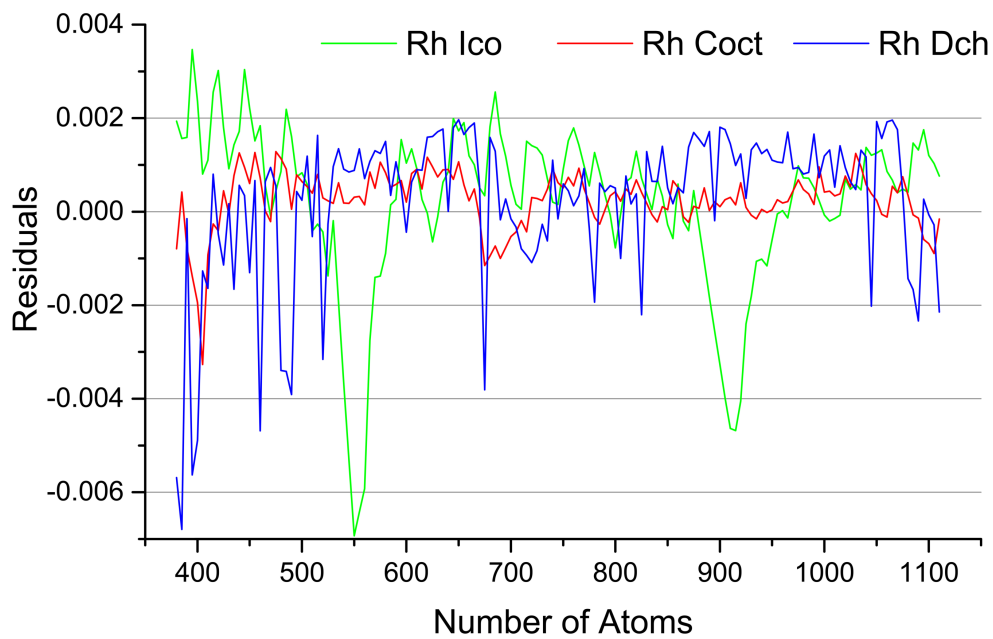


Fig. S3 Residuals plot for icosahedral, decahedral and cuboctahedral structure motifs of Rh nanoparticles.

Table S2 Simulated annealing schedule - change of temperature T with Monte Carlo (MC) steps. See graph in Fig. S11.

MC Step	T, K	MC Step	T, K	MC Step	T, K	MC Step	T, K
5	3000	315	1830	625	1140	935	500
10	2900	320	1820	630	1130	940	490
15	2850	325	1810	635	1120	945	490
20	2800	330	1800	640	1110	950	480
25	2750	335	1790	645	1100	955	480
30	2700	340	1770	650	1090	960	470
35	2650	345	1760	655	1070	965	470
40	2600	350	1750	660	1060	970	460
45	2550	355	1740	665	1050	975	460
50	2500	360	1730	670	1040	980	450
55	2450	365	1720	675	1030	985	450
60	2400	370	1710	680	1020	990	440
65	2390	375	1700	685	1010	995	440
70	2370	380	1690	690	1000	1000	430
75	2360	385	1670	695	990	1005	2450
80	2350	390	1660	700	980	1010	2400
85	2340	395	1650	705	970	1015	2390
90	2330	400	1640	710	960	1020	2370
95	2320	405	1630	715	950	1025	2360
100	2310	410	1620	720	940	1030	2350
105	2300	415	1610	725	930	1035	2340
110	2290	420	1600	730	920	1040	2330
115	2270	425	1590	735	910	1045	2320
120	2260	430	1570	740	900	1050	2310
125	2250	435	1560	745	890	1055	430
130	2240	440	1550	750	870	1060	420
135	2230	445	1540	755	860	1065	420
140	2220	450	1530	760	850	1070	410
145	2210	455	1520	765	840	1075	410
150	2200	460	1510	770	830	1080	400
155	2190	465	1500	775	820	1085	400
160	2170	470	1490	780	810	1090	390
165	2160	475	1470	785	800	1095	390
170	2150	480	1460	790	790	1100	380
175	2140	485	1450	795	770	1105	380
180	2130	490	1440	800	760	1110	370
185	2120	495	1430	805	750	1115	370
190	2110	500	1420	810	740	1120	360
195	2100	505	1410	815	730	1125	360
200	2090	510	1400	820	720	1130	350
205	2070	515	1390	825	710	1135	350
210	2060	520	1370	830	700	1140	340
215	2050	525	1360	835	690	1145	340
220	2040	530	1350	840	670	1150	330
225	2030	535	1340	845	660	1155	380
230	2020	540	1330	850	650	1160	370
235	2010	545	1320	855	640	1165	370
240	2000	550	1310	860	630	1170	360
245	1980	555	1300	865	620	1175	360
250	1970	560	1290	870	610	1180	350
255	1960	565	1270	875	600	1185	350
260	1950	570	1260	880	590	1190	340
265	1940	575	1250	885	570	1195	340
270	1930	580	1240	890	560	1200	330
275	1920	585	1230	895	550	1205	330
280	1910	590	1220	900	540	1210	320
285	1900	595	1210	905	530	1215	320
290	1890	600	1200	910	520	1220	310
295	1870	605	1190	915	520	1225	310
300	1860	610	1170	920	510	1230	300
305	1850	615	1160	925	510		
310	1840	620	1150	930	500		

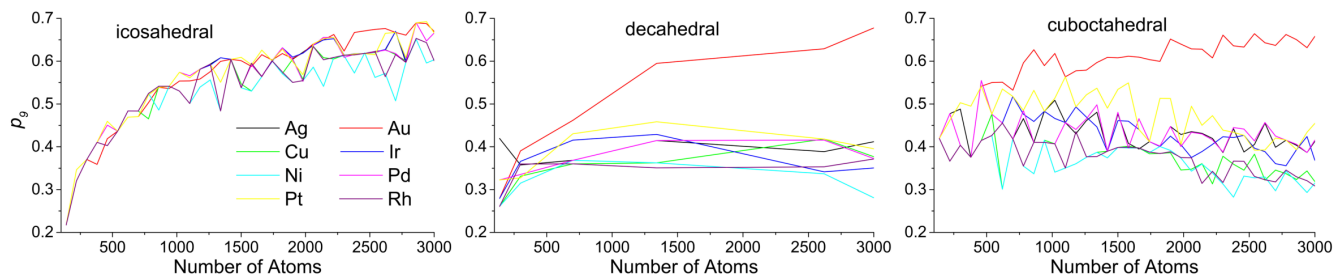


Fig. S4 Ratio of number of atoms with coordination numbers equal to 9 to number of all surface atoms (p_9) as a function of nanoparticle size

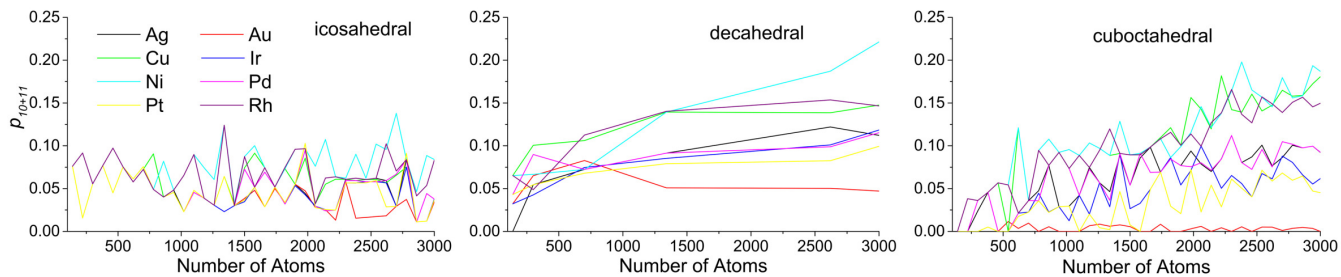


Fig. S5 Ratio of number of atoms with coordination numbers equal to 10 or 11 to number of all surface atoms (p_{10+11}) as a function of nanoparticle size

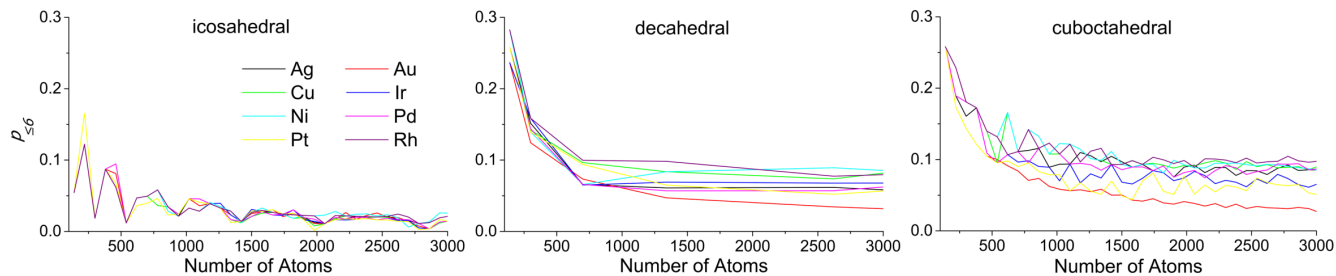


Fig. S6 Ratio of number of atoms with coordination numbers less or equal to 6 to number of all surface atoms ($p_{\leq 6}$) as a function of nanoparticle size

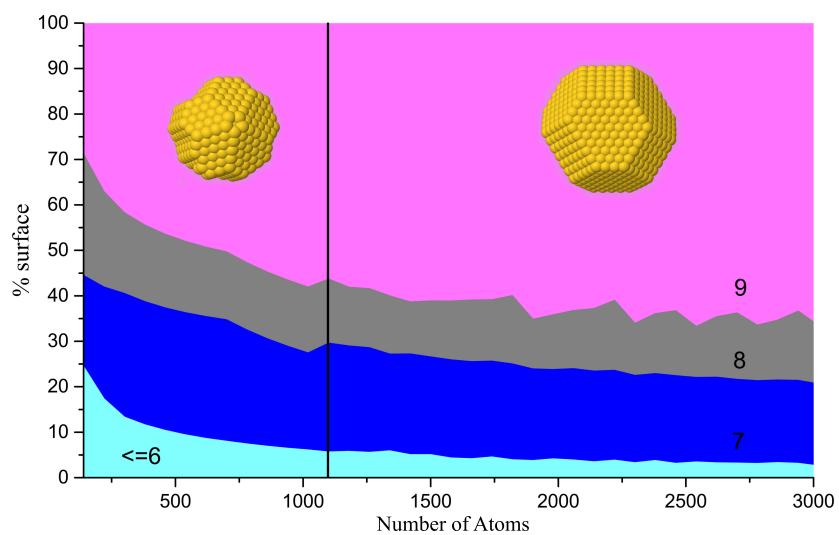


Fig. S7 Distribution of the coordination numbers of surface atoms of Au NPs in the vicinity of decahedral-cuboctahedral transition

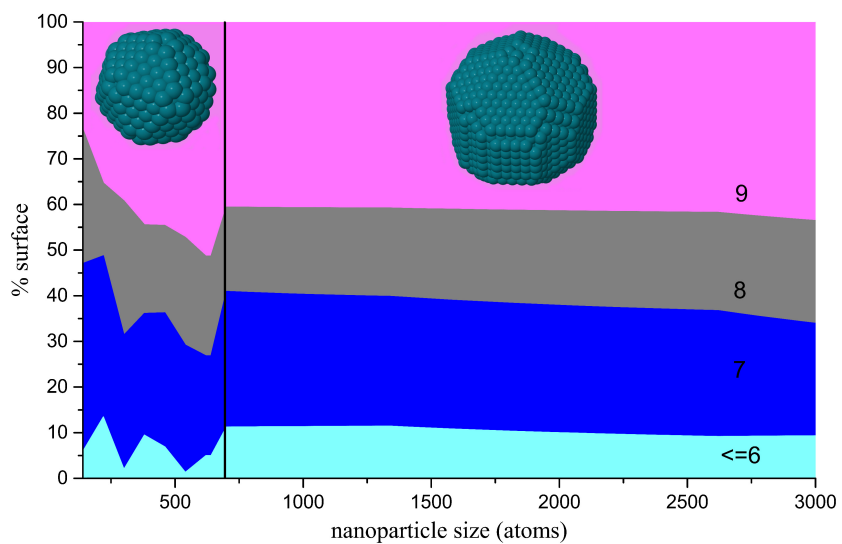


Fig. S8 Distribution of the coordination numbers of surface atoms of Rh NPs in the vicinity of icosahedral-decahedral transition.

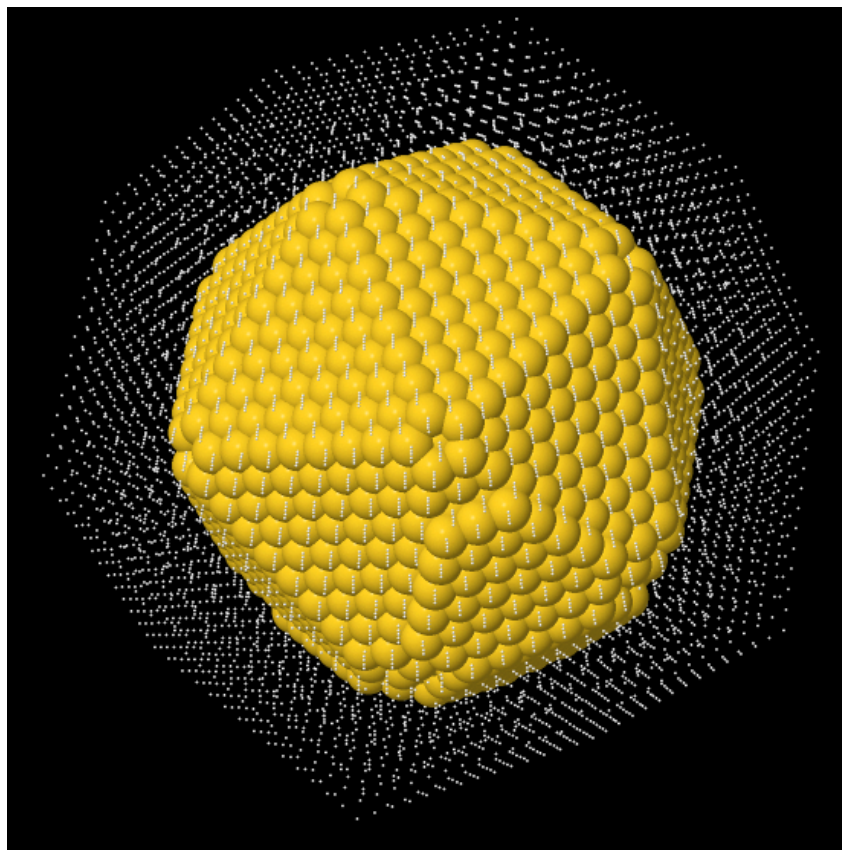


Fig. S9 Au NP of 3000 atom in icosahedral lattice. Small white dots indicate free lattice vacancies.

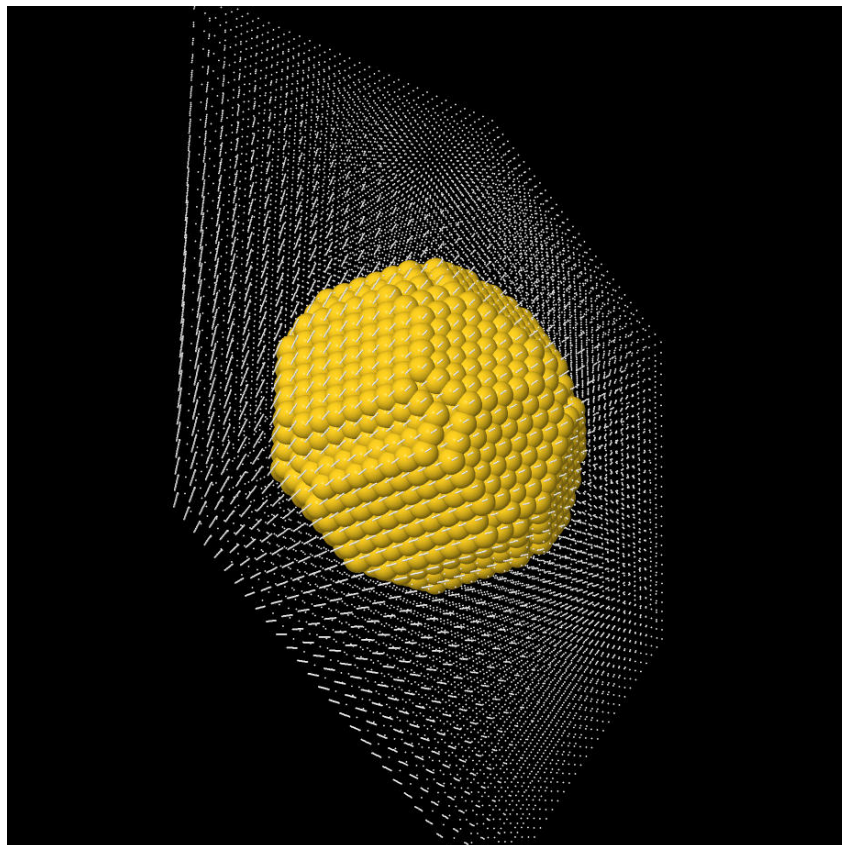


Fig. S10 Au NP of 3000 atom in decahedral lattice. Small white dots indicate free lattice vacancies.

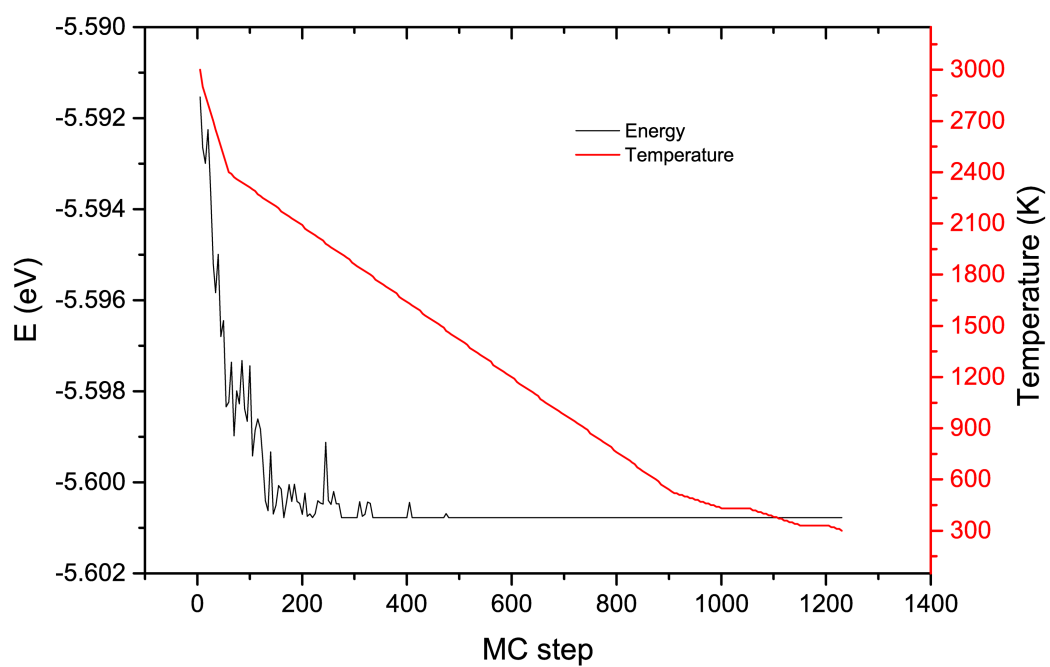


Fig. S11 Energy (E) and temperature change during simulated annealing optimization of decahedral Pt NP of 1340 atoms. See temperature values in Table S2.