Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

First-Principles Database Driven Computational Neural Network Approach to the Discovery of Active Ternary Nanocatalysts for Oxygen Reduction Reaction

*Joonhee Kang, Seung Hyo Noh, Jeemin Hwang, Hoje Chun, Hansung Kim and Byungchan Han**

Department of Chemical and Biomolecular Engineering, Yonsei University, Seoul 03722, Korea

Table S1. List of the radial symmetry function (G^2) describing the atomic environments of transition metals in the binary nanoparticles within the cutoff radius R_c = 6.5 Å and R_{shift} = 0.

Symmetry functions (G^2)					
No.	Neighboring element	η ($Å^{-2}$)	No.	Neighboring element	η ($Å^{-2}$)
1	Pt	0.001	9	Pt	0.050
2	Ni	0.001	10	Ni	0.050
3	Pt	0.005	11	Pt	0.100
4	Ni	0.005	12	Ni	0.100
5	Pt	0.010	13	Pt	0.200
6	Ni	0.010	14	Ni	0.200
7	Pt	0.020	15	Pt	0.400
8	Ni	0.020	16	Ni	0.400

*Same symmetry functions (G^2) are utilized in PtCu and CuNi systems.

Table S2. List of the angular symmetry function (G^4) describing the atomic environments of transition metals in the binary nanoparticles within the cutoff radius R_c = 6.5 Å.

Symmetry functions (G^4)				
No.	Neighbors	η ($Å^{-2}$)	λ	ζ
17-19	Pt-Pt, Ni-Pt, Ni-Ni	0.005	1.0	1.0
20-22		0.005	-1.0	1.0
23-25		0.005	1.0	4.0
26-28		0.005	-1.0	4.0
29-31		0.010	1.0	1.0
32-34		0.010	-1.0	1.0
35-37		0.010	1.0	4.0
38-40		0.010	-1.0	4.0
41-43		0.020	1.0	1.0
44-46		0.020	-1.0	1.0
47-49		0.020	1.0	4.0
50-52		0.020	-1.0	4.0

*Same symmetry functions (G^4) are utilized in PtCu and CuNi systems.

Table S3. List of the radial symmetry function (G^2) describing the atomic environments of transition metals in the ternary nanoparticles within the cutoff radius R_c = 6.5 Å and R_{shift} = 0.

Symmetry functions (G^2)					
No.	Neighboring element	η ($Å^{-2}$)	No.	Neighboring element	η ($Å^{-2}$)
1	Pt	0.001	13	Pt	0.050
2	Ni	0.001	14	Ni	0.050
3	Cu	0.001	15	Cu	0.050
4	Pt	0.005	16	Pt	0.100
5	Ni	0.005	17	Ni	0.100
6	Cu	0.005	18	Cu	0.100
7	Pt	0.010	19	Pt	0.200
8	Ni	0.010	20	Ni	0.200
9	Cu	0.010	21	Cu	0.200
10	Pt	0.020	22	Pt	0.400
11	Ni	0.020	23	Ni	0.400
12	Cu	0.020	24	Cu	0.400

Table S4. List of the angular symmetry function (G^4) describing the atomic environments of transition metals in the ternary nanoparticles within the cutoff radius R_c = 6.5 Å.

Symmetry functions (G^4)				
No.	Neighbors	η ($Å^{-2}$)	λ	ζ
25-30		0.005	1.0	1.0
31-36		0.005	-1.0	1.0
37-42		0.005	1.0	4.0
43-48	Pt-Pt,	0.005	-1.0	4.0
49-54	Cu-Pt,	0.010	1.0	1.0
55-60	Ni-Pt,	0.010	-1.0	1.0
61-66	Cu-Cu,	0.010	1.0	4.0
67-72	Cu-Ni,	0.010	-1.0	4.0
73-78	Ni-Ni	0.020	1.0	1.0
79-84		0.020	-1.0	1.0
85-90		0.020	1.0	4.0
91-96		0.020	-1.0	4.0

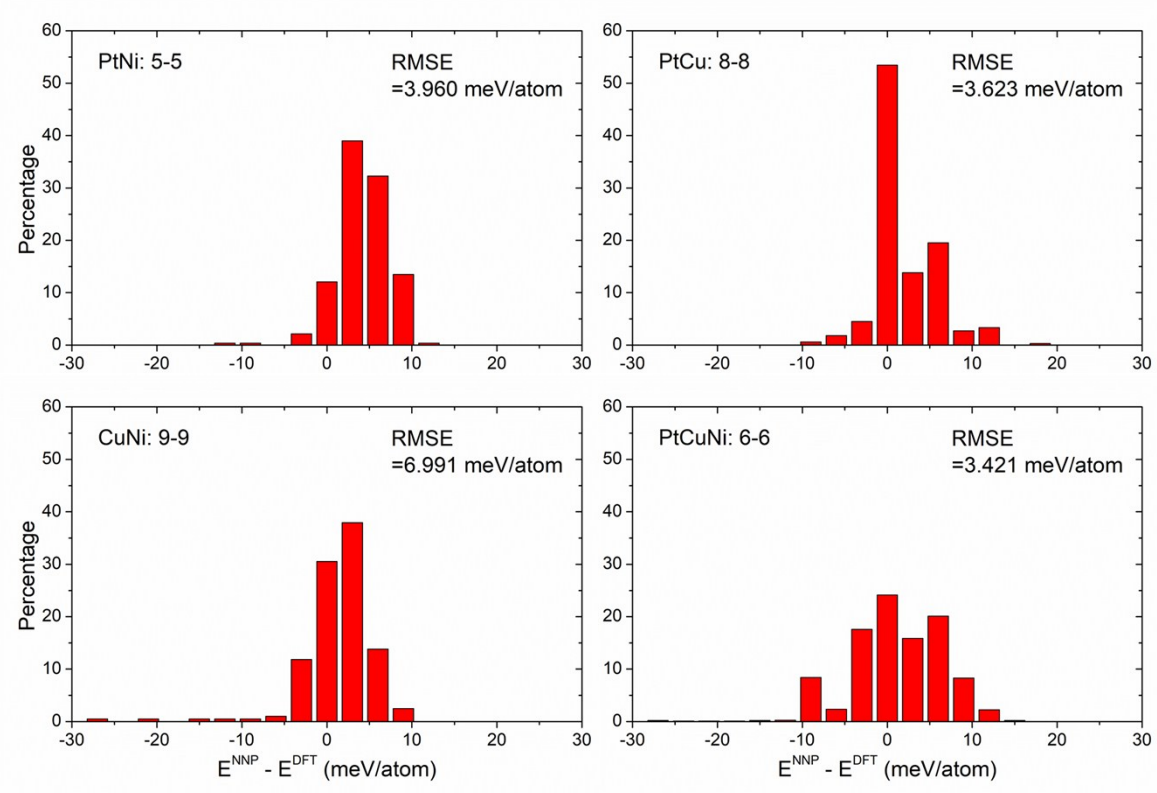

Figure S1. Distribution of the energy difference between NNP and DFT energies for binary and ternary nanoparticles.

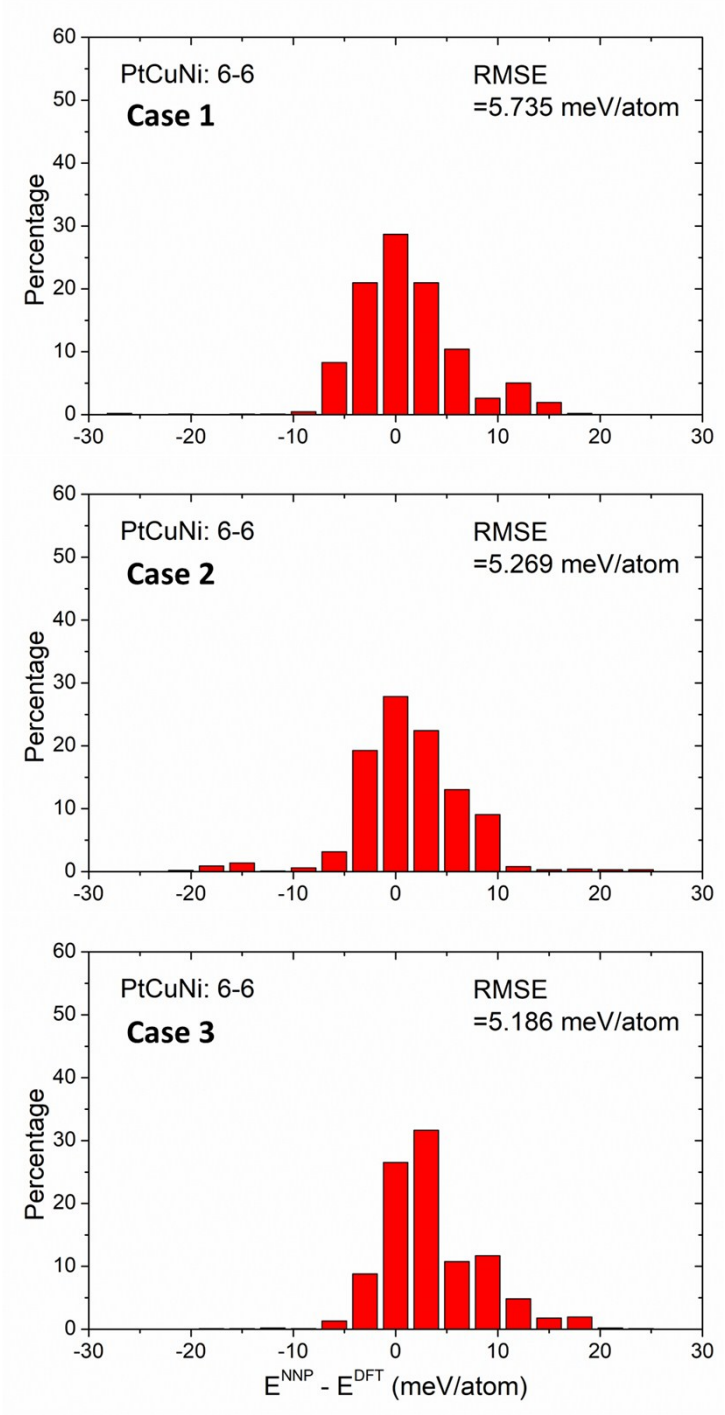

Figure S2. Evaluation of the accuracy of neural network with different training/test set using distribution of the energy difference between NNP and DFT energies for ternary nanoparticles.

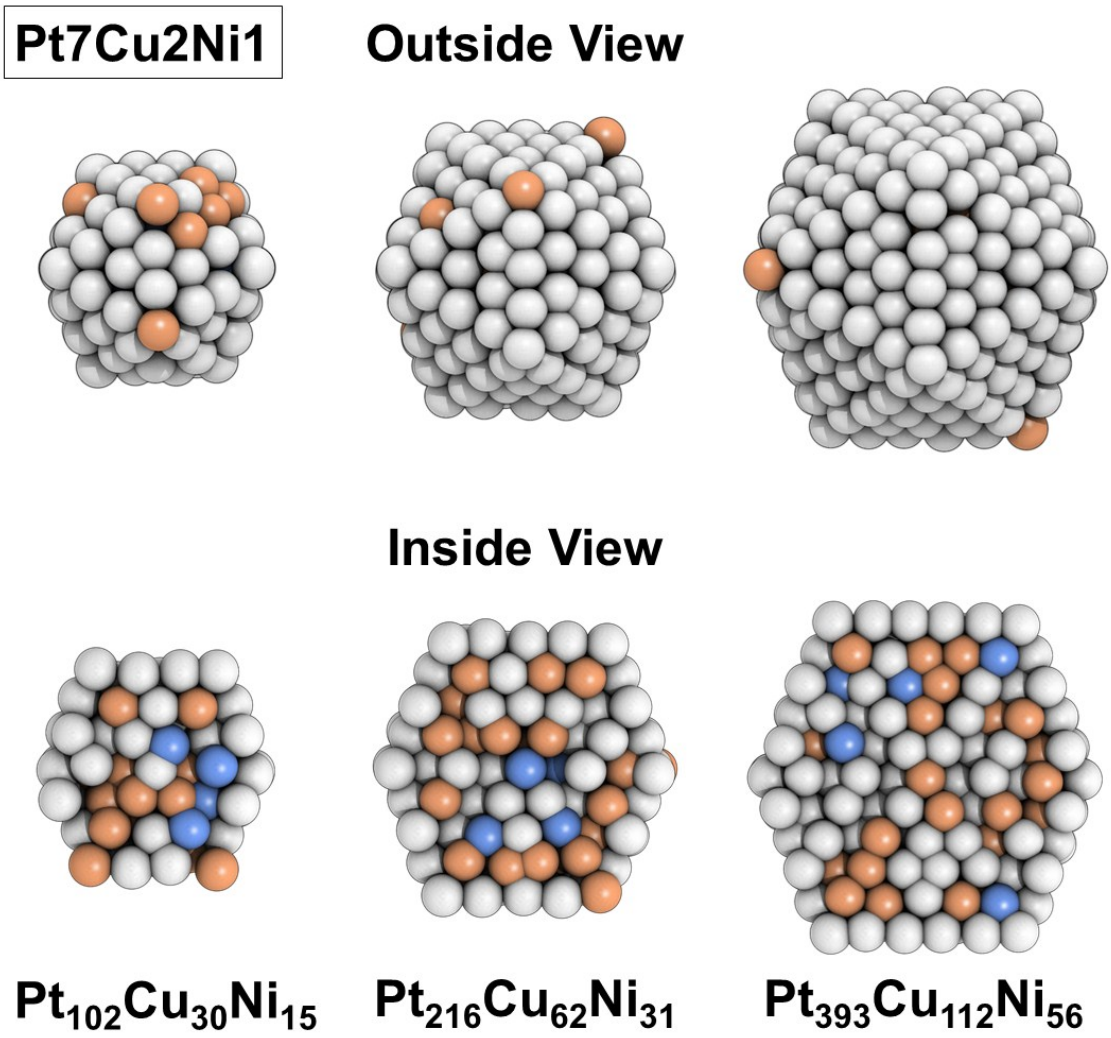

Figure S3. The outside and inside atomic arrangements of Pt7Cu1Ni1 nanoparticles from MC/MD simulations.

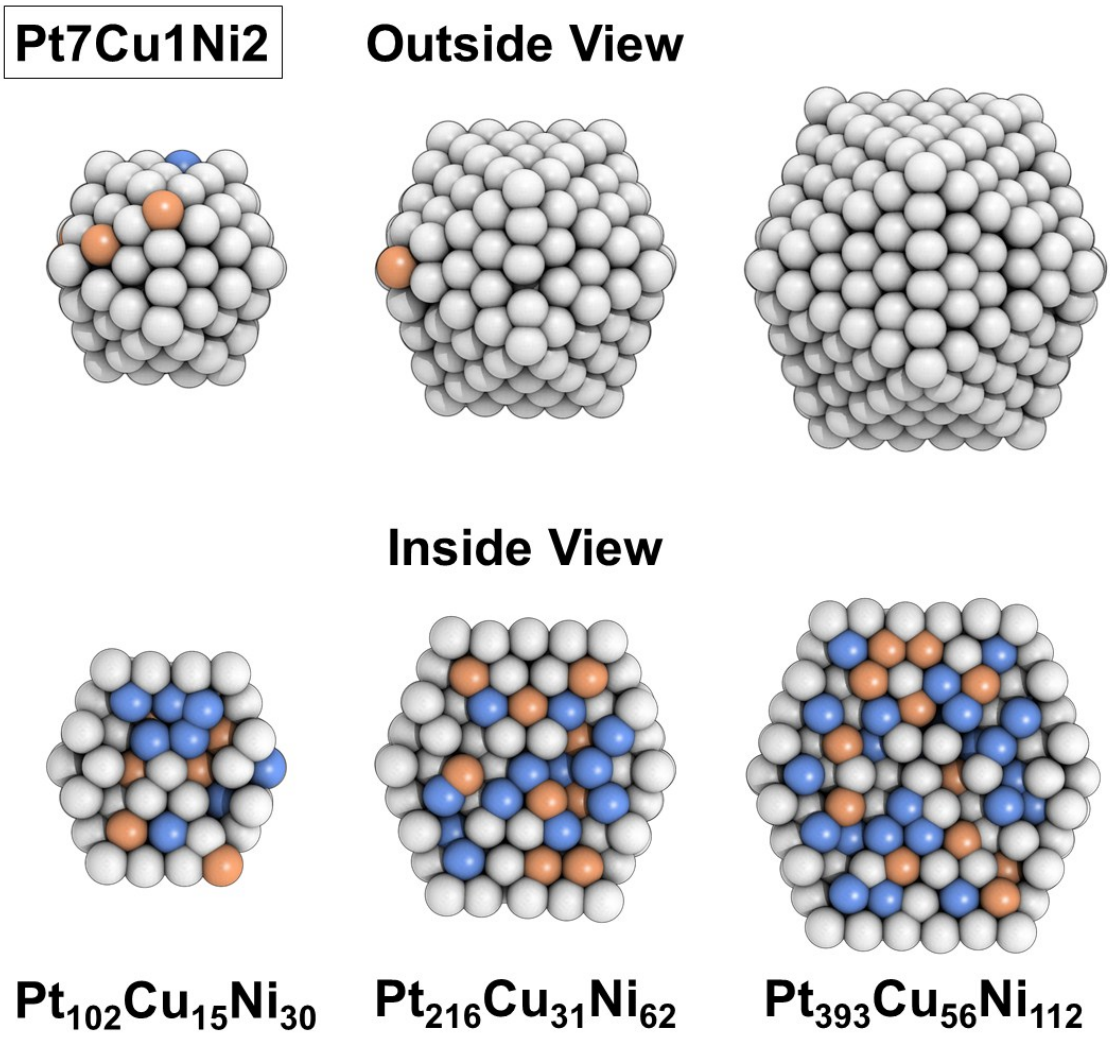

Figure S4. The outside and inside atomic arrangements of Pt7Cu1Ni2 nanoparticles from MC/MD simulations.

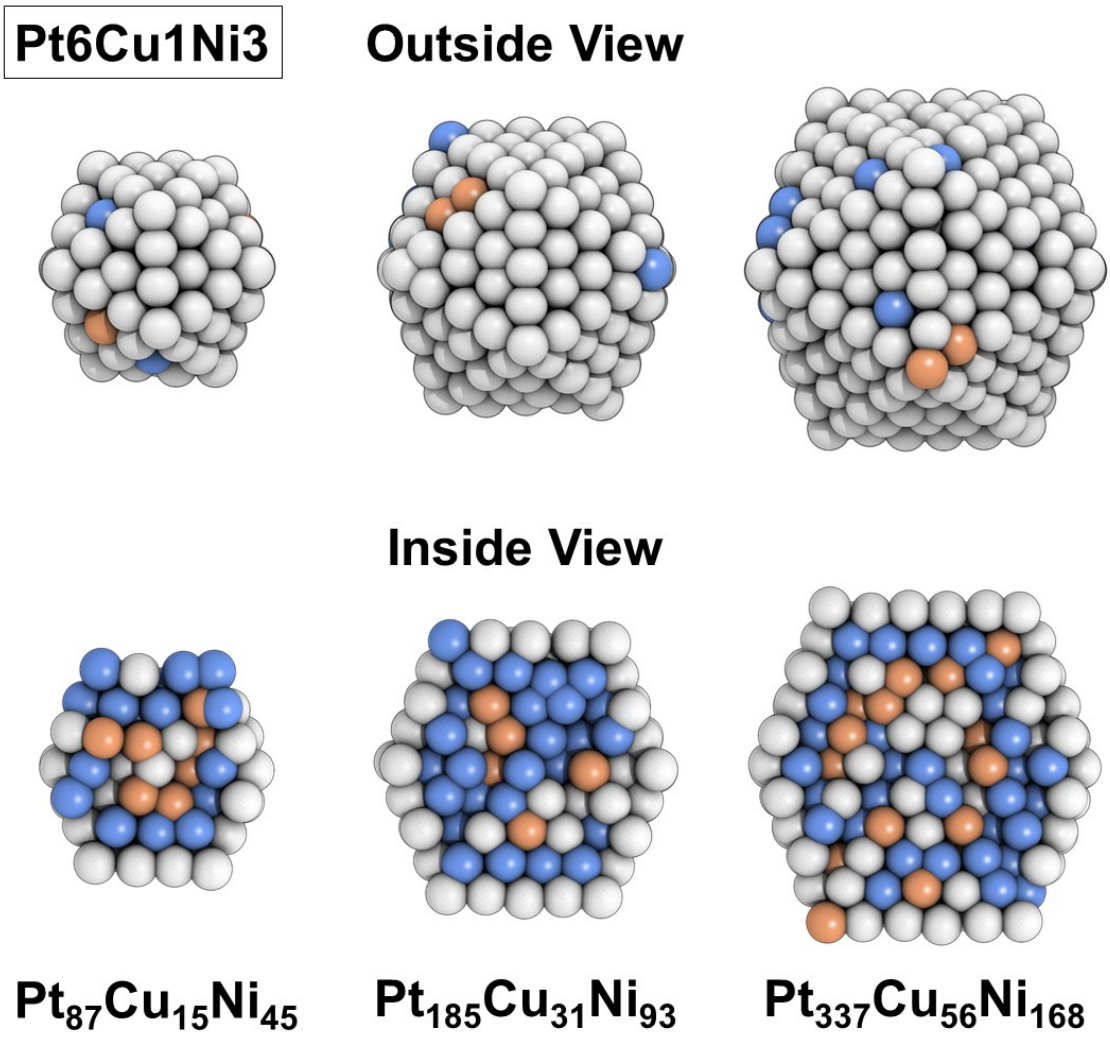

Figure S5. The outside and inside atomic arrangements of Pt6Cu1Ni3 nanoparticles from MC/MD simulations.

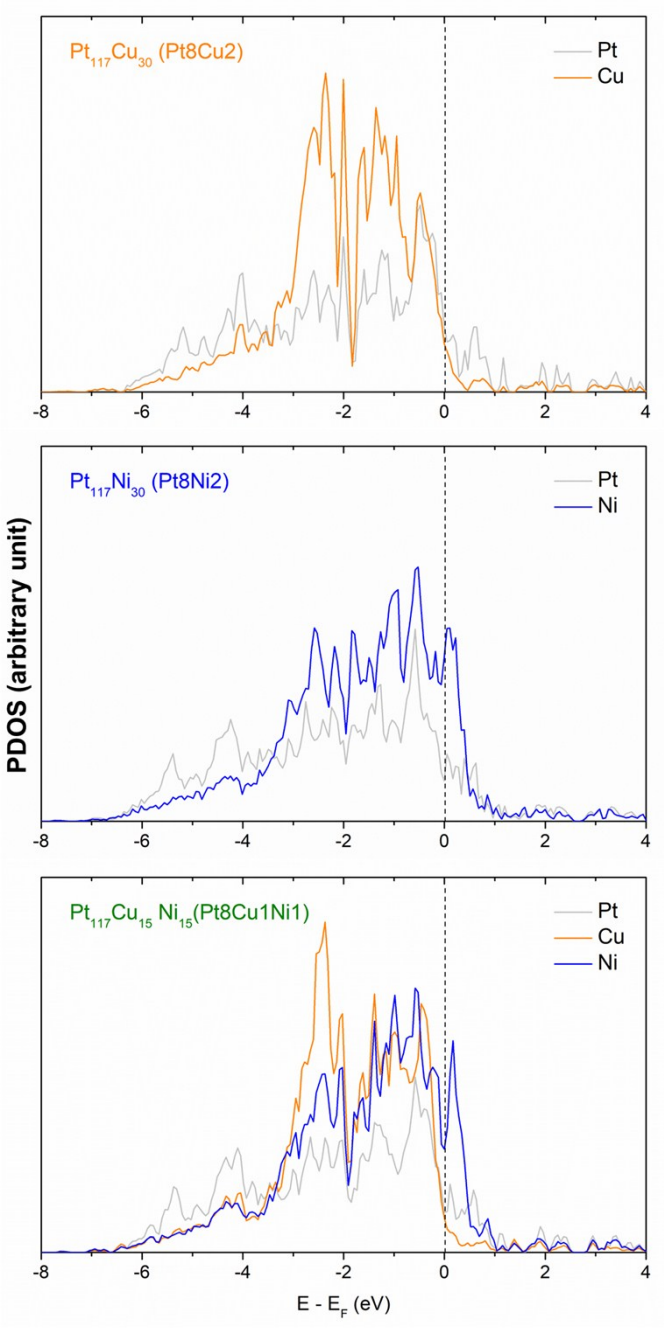

Figure S6. PDOS (*d* orbital) of Pt in the outermost shell and Cu or Ni in the core of M_{55}@Pt_{92} nanoparticles with respect to the Fermi level, E_F.

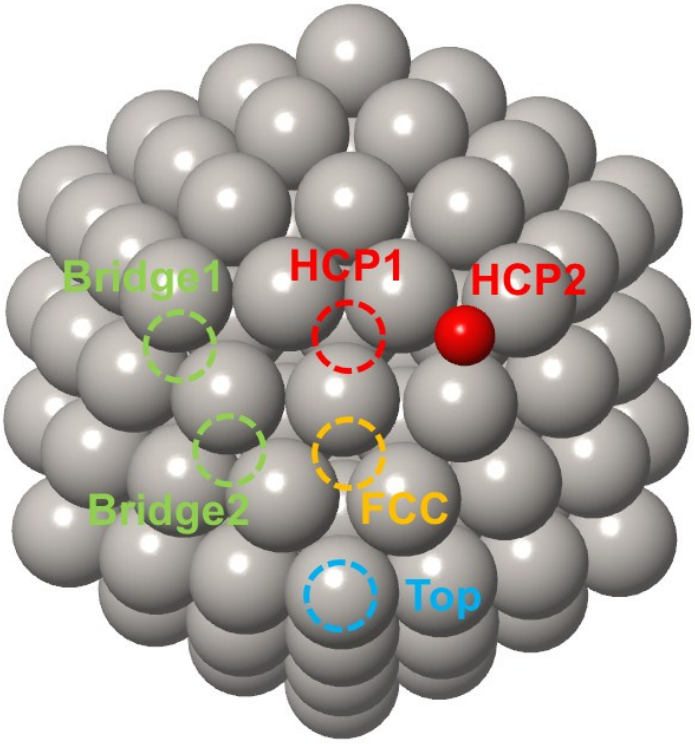

Figure S7. Oxygen adsorption sites on the outermost shell of nanoparticles. HCP2 is thermodynamically favorable oxygen adsorption site.