Supplementary Information :

Machine Learning Accelerating Structure Prediction of PtSnO Nanoclusters under Working Conditions

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1. Computational details

All the DFT calculations were performed by CP2K program package (version 9.1)[1]. The Gaussian and plane-wave (GPW) method was used, and the Perdew-Burke-Ernzerhof (PBE) model was adopted for the exchange-correlation functional. Double-ζ valence plus polarization (DZVP) basis sets of the MOLOPT type were used to represent the valence electrons of O, Sn and Pt. The norm-conserving Goedecker-Teter-Hutter (GTH) pseudopotential was used for the core electrons. The cutoff energy of the plane wave was set to 500 Ry. The convergence threshold was set to 1.0×10^{-5} hartree for the self-consistent field calculation and 4.5×10^{-4} hartree/bohr for geometry optimization.

The AIMD simulations were carried out with the time step of 1 fs and the CSVR thermostat with time constant of 50 fs. The supercell for AIMD was a cubic box of 20 × 20 × 20 Å, and all structures were kept in the center of the box during the AIMD runs. All GA runs were performed in a cubic box of 20 × 20 × 20 Å. For local relaxation of the each putative GM structure, a suitable cubic box with at least 5 Å thickness vacuum around the cluster was chosen.

Behler-Parrinello neural networks potentials were based on the atom-centered symmetry functions[2]. For each of the pair and triple, there were 10 radial functions and 4 angular functions to map the atomic centered environment with cutoff radius of 12 bohr (6.35 Å), respectively.

For each element, the symmetry function types[3] are as follow:

Radial symmetry function form:

$$G_i^2 = \sum_{j \neq i} e^{-\eta(r_{ij}-r_s)^2} f_c(r_{ij})$$

Where the parameter of η was set to 0.307795 and r_s was chosen from a list of [0.264562, 1.539104, 2.813645, 4.088187, 5.362729, 6.637271, 7.911813, 9.186355, 10.460896, 11.735438]. There were totally 10 radial symmetry functions applied for each element.

Angular symmetry function form:

$$G_i^3 = 2^{1-\zeta} \sum_{\substack{j,k \neq i \\ j<k}} (1 + \lambda cos\theta_{ijk})^{\zeta} e^{-\eta((r_{ij}-r_s)^2+(r_{ik}-r_s)^2+(r_{jk}-r_s)^2)} f_c(r_{ij}) f_c(r_{ik}) f_c(r_{jk})$$

Where the parameter of η was set to 0.011906, λ = 1 or -1, ζ = 1 or 4, and r_s = 0. There are 4 type combinations of these angular parameters so that 4 angular symmetry functions for each element were applied.

There were 8 members in the committee of neural network potentials (C-NNPs)[4]. Every member shared the same data set but was distinct to each other by using different random number seeds. For each cluster AIMD trajectory, 15 or 25 iterations of QbC active learning were performed. For each iteration, 20 candidates were selected, filtered the repeats and added into the data set. The configuration of the neural network was set to N-20-20-1 (N is the number of symmetry functions, 20 is the node number of hidden layers). The data set was randomly divided into training set and test set with the ratio of 9:1 for every training process. Every C-NNPs model was trained 100 epochs before being used in GA search.

For the GA search, the population size was 20 and each generation/cycle would generate 100 candidates. The cut-and-splice operator was chosen for pairing. The mutation probability was 30% and the mutation operators were randomly chosen from rattle, permutation and mirror.

The thermochemical data for gases was obtained from NIST-JANAF Thermochemical Tables[5] with linear interpolation method.

2. Figures and tables

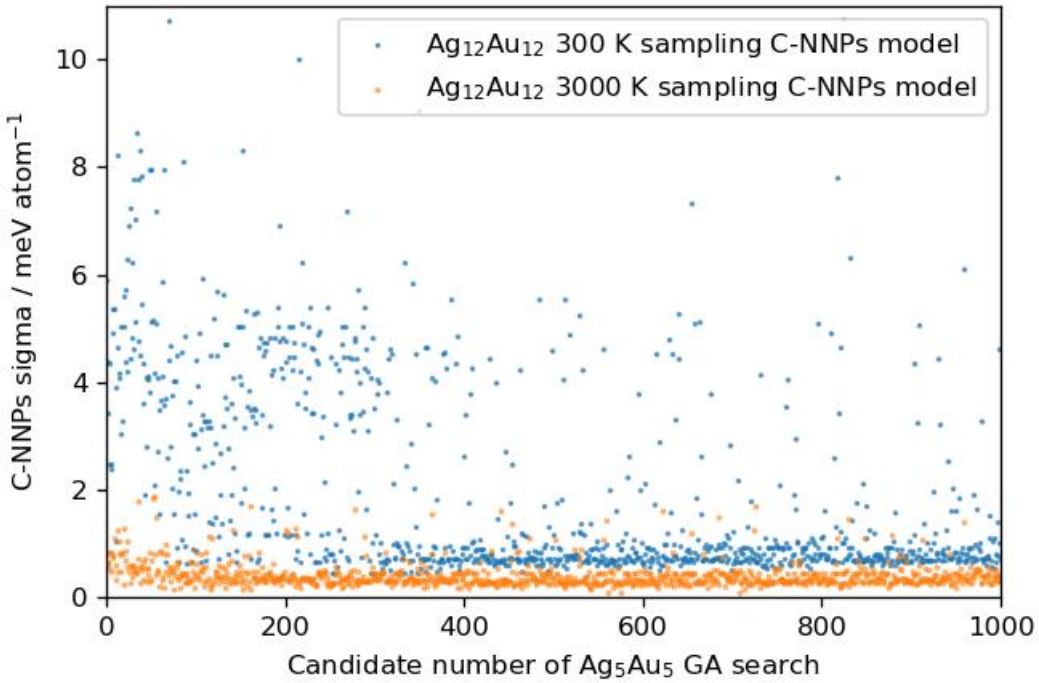


Figure S1. The C-NNPs sigma distribution of high temperature (3000 K) and low temperature (300 K) sampling C-NNPs model for Ag_5Au_5 GA run. Each model is trained with training set sampling by 15 iterations QbC of a reference $Ag_{12}Au_{12}$ AIMD trajectory for 20 ps (Δt = 1 fs) calculated by EMT potential[6] at corresponding temperature. The average sigma values of 300 K and 3000 K sampling model are 1.91 and 0.42 meV/atom, respectively. The max sigma values of 300 K and 3000 K sampling model are 10.75 and 1.87 meV/atom, respectively. High temperature simulating liquid sampling C-NNPs model performs more accurrate and stable while carrying out GA run.

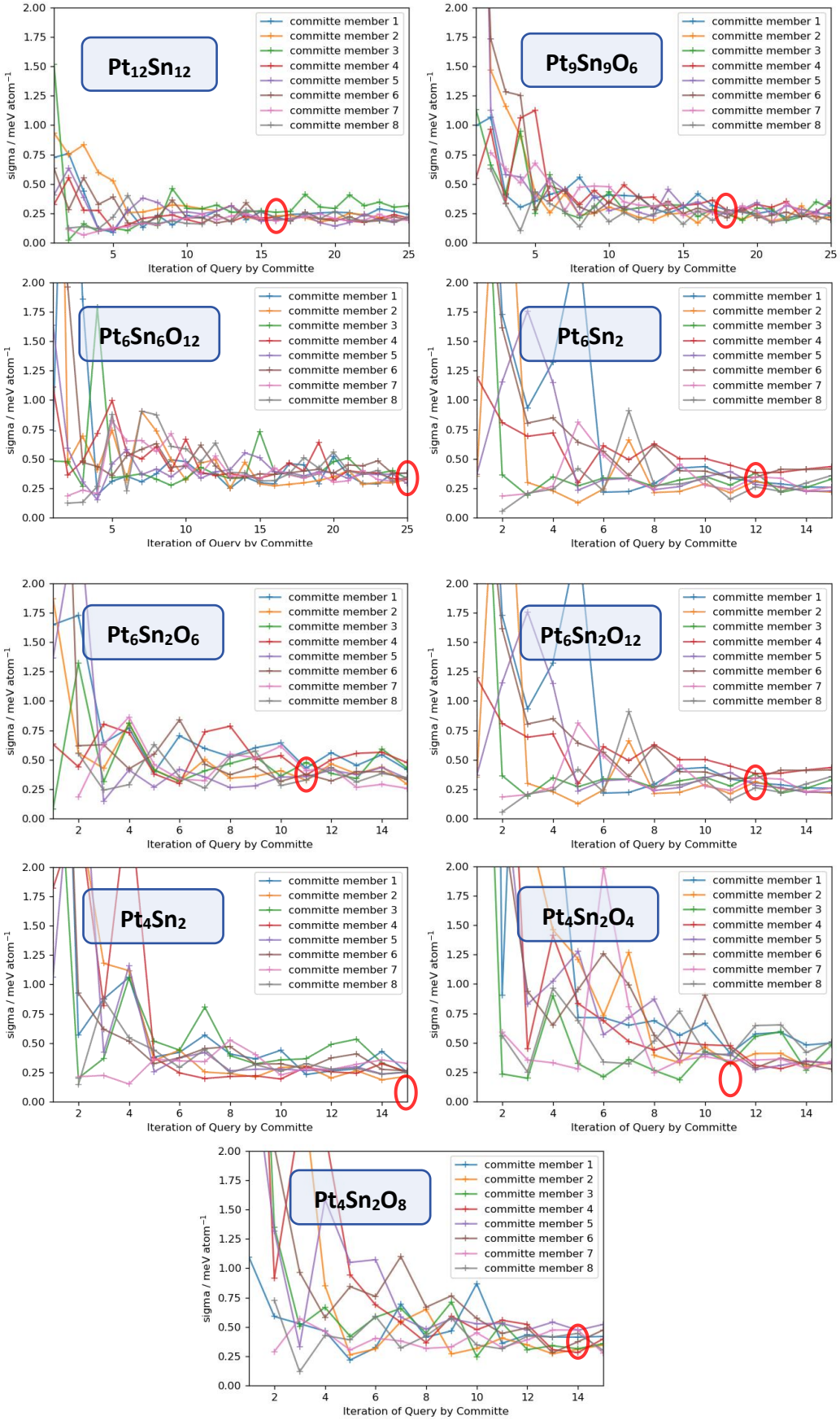


Figure S2. The C-NNPs model improving procedure with QbC active learning iterations to select training sets from reference AIMD trajectories. For each run, the

data set with lowest mean of test energy root mean square error (RMSE), highlighting by a red circle in each subplot, was chosen to construct final C-NNPs. Totally 931, 699 and 657 structures were chosen for constructing C-NNPs model of Pt:Sn atomic ratio 1:1, 2:1 and 3:1, respectively.

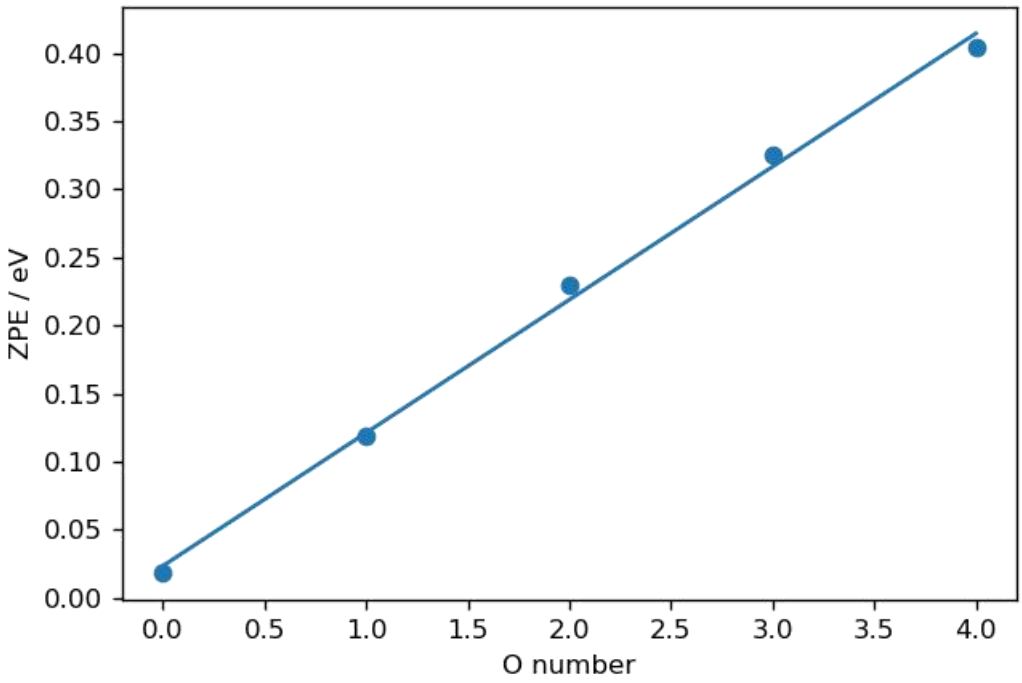


Figure S3. The linear fitting of ZPE increasing with O atoms for $Pt_1Sn_1O_y$. The the slope and coefficient of determination are 0.977 and 0.999, respectively.

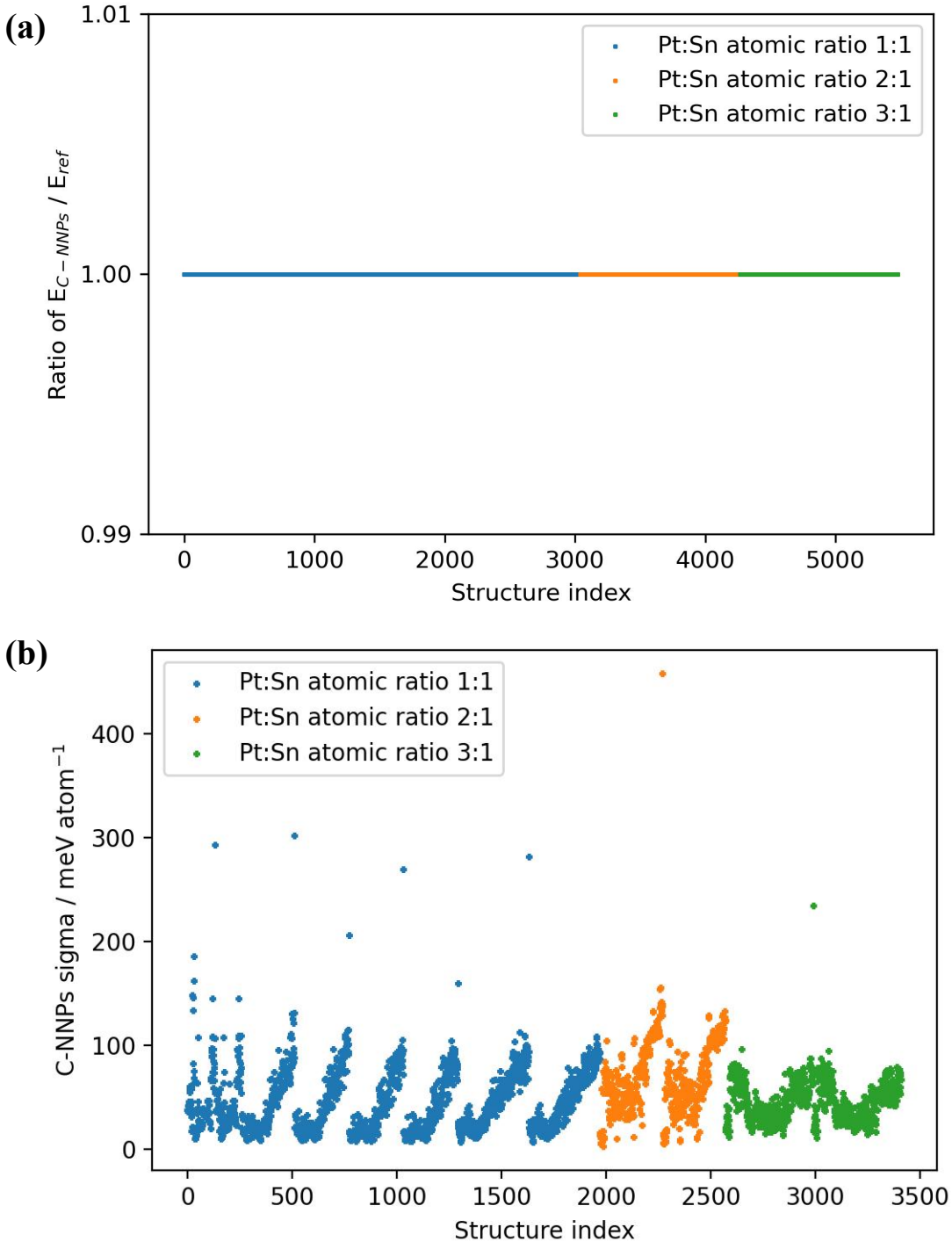


Figure S4. (a) Energy comparation of C-NNPs and DFT for reference structures with Pt:Sn atomic ratio of 1:1, 2:1 and 3:1. Training sets and test sets are included in reference structures. The ratio of ECNNPs/EDFT for each reference structure is 1.00, which indicates these C-NNPs can precisely predicet the DFT-level energy of reference AIMD trajectory. The mean values of C-NNPs sigma are 3.0, 3.5 and 3.4 meV/atom for reference structures of Pt:Sn atomic ratio 1:1, 2:1 and 3:1,respectively.

(b) The whole distributions of committee standard deviations (sigma) for each last population of GA run selected. The sigma of the most structures are lower than 100 meV/atom. For Pt:Sn atomic ratios 1:1, 2:1 and 3:1, the mean of committee sigma are 43.4, 45.1 and 68.5 meV/atom, respectively.

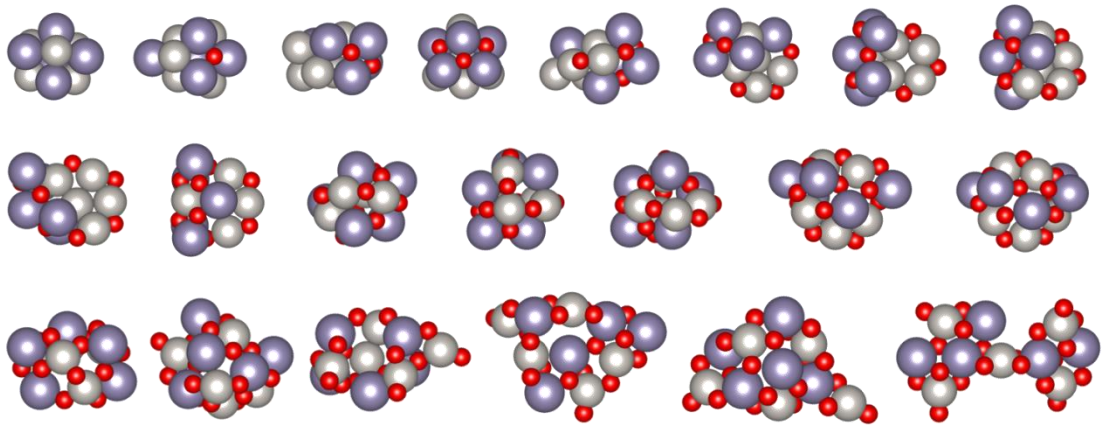


Figure S5. The most stable structures obtained for $Pt_5Sn_5O_y$ from GA runs without local relaxtion. Red, grey and dark purple refer elements of O, Pt and Sn, respectively.

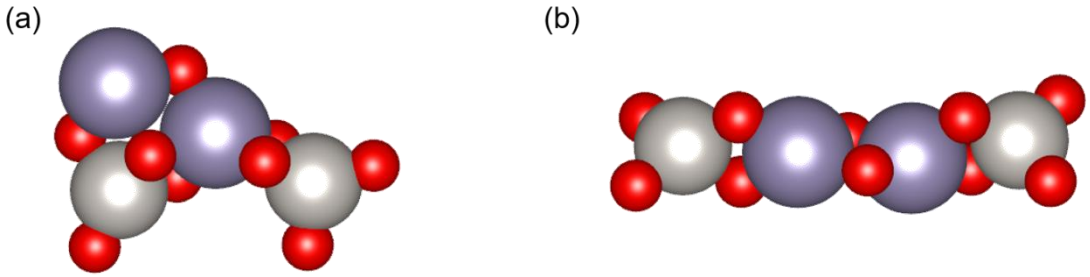


Figure S6. (a) The GM of $Pt_2Sn_2O_9$, found by GM runs and local relaxitons. (b) The predicted structure of $Pt_2Sn_2O_{10}$. Unfortunately, such a configuration of $Pt_2Sn_2O_{10}$ was not found after 5 independent GA runs. Red, grey and dark purple refer elements of O, Pt and Sn, respectively.

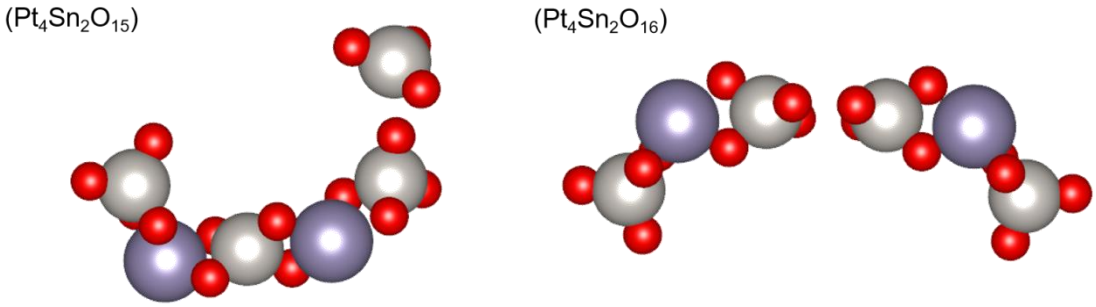


Figure S7. The GM of $Pt_2Sn_2O_{15}$ $Pt_2Sn_2O_{16}$, found after 5 independent GM runs but without local relaxitons. These structures are excluded to further analysis since they are separated to two parts of fragments. Red, grey and dark purple refer elements of O, Pt and Sn, respectively.

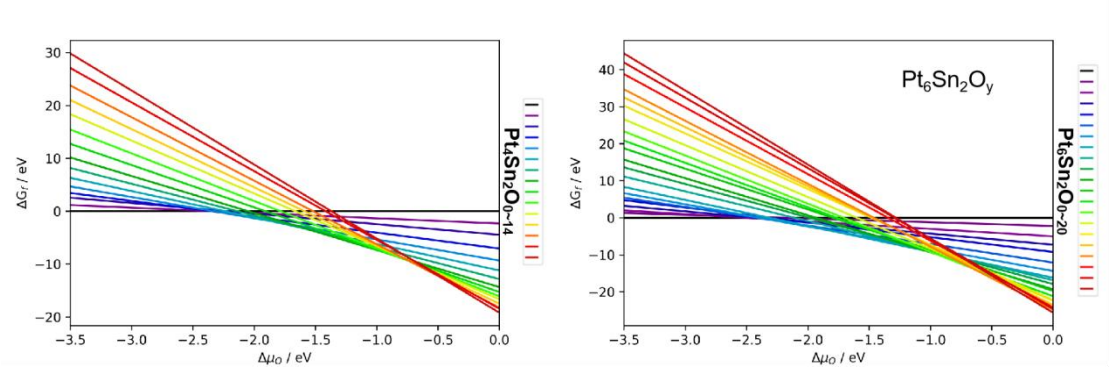


Figure S8. The phase diagrams as a function of $\Delta\mu_O$ for $Pt_4Sn_2O_y$ and $Pt_6Sn_2O_y$ most stable structure.

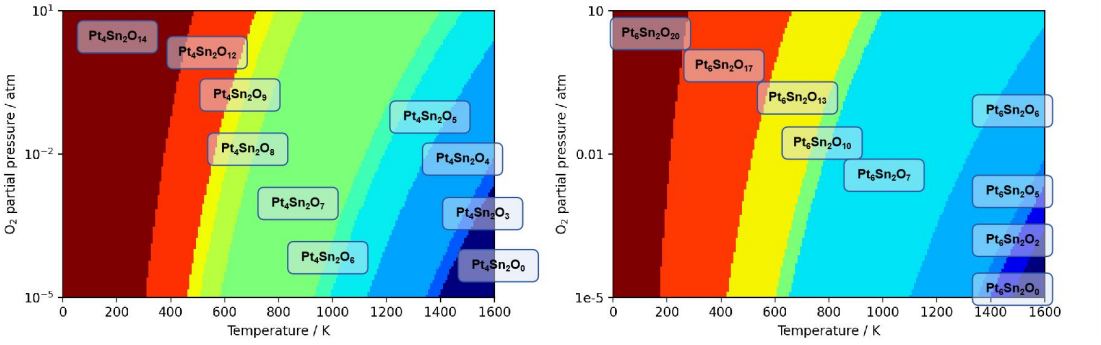
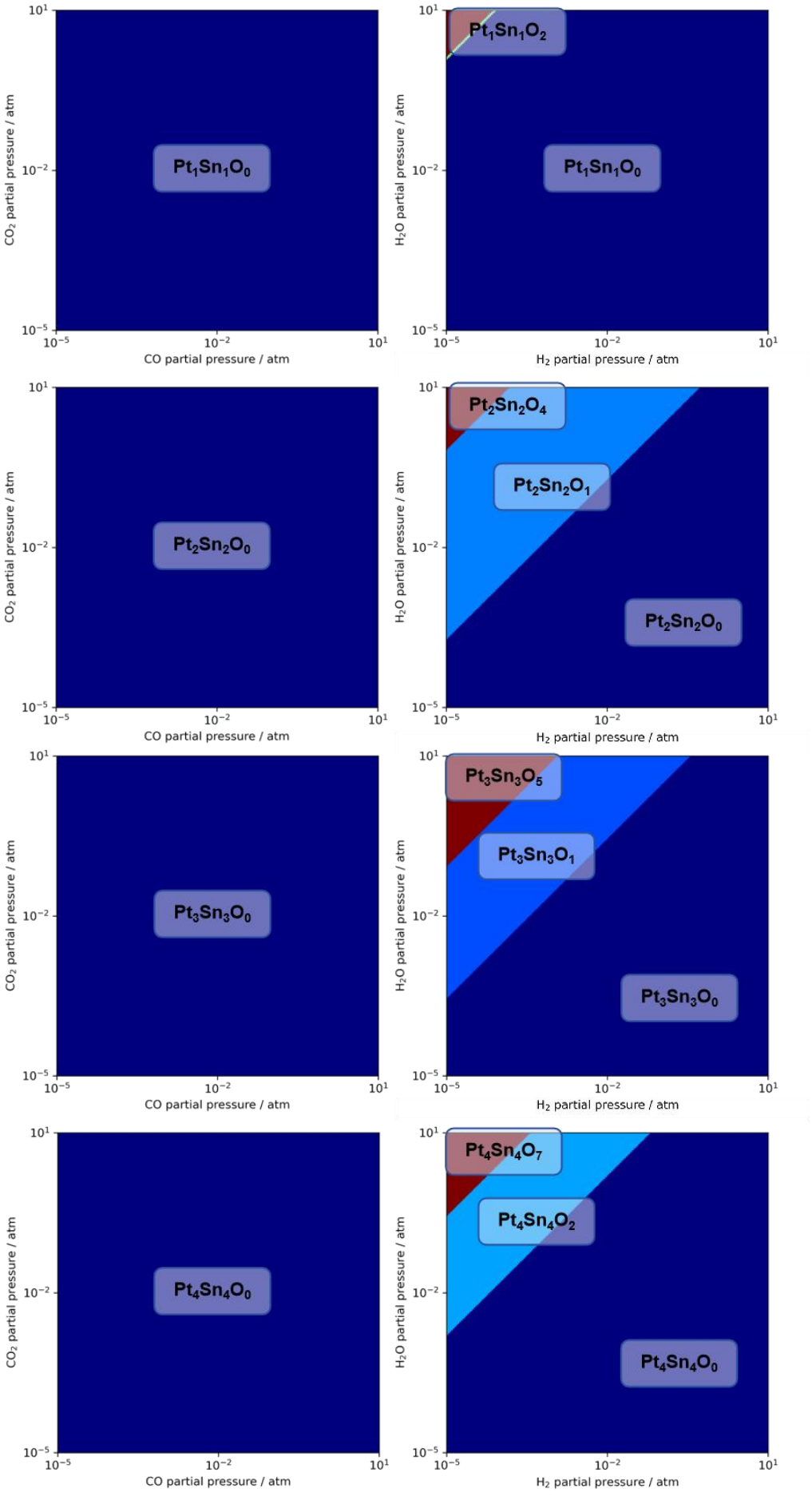


Figure S9. The 2-D phase diagrams as a function of p_{O2} and T for every stoichiometry of $Pt_4Sn_2O_y$ and $Pt_6Sn_2O_y$ most stable structure.


$Pt_1Sn_1O_0$
$Pt_1Sn_1O_2$
$Pt_2Sn_2O_0$
$Pt_2Sn_2O_4$
$Pt_2Sn_2O_1$
$Pt_3Sn_3O_0$
$Pt_3Sn_3O_5$
$Pt_3Sn_3O_1$
$Pt_4Sn_4O_0$
$Pt_4Sn_4O_7$
$Pt_4Sn_4O_2$
CO_2 partial pressure / atm
H_2O partial pressure / atm
CO partial pressure / atm
H_2 partial pressure / atm
10^{1}
10^{-2}
10^{-5}

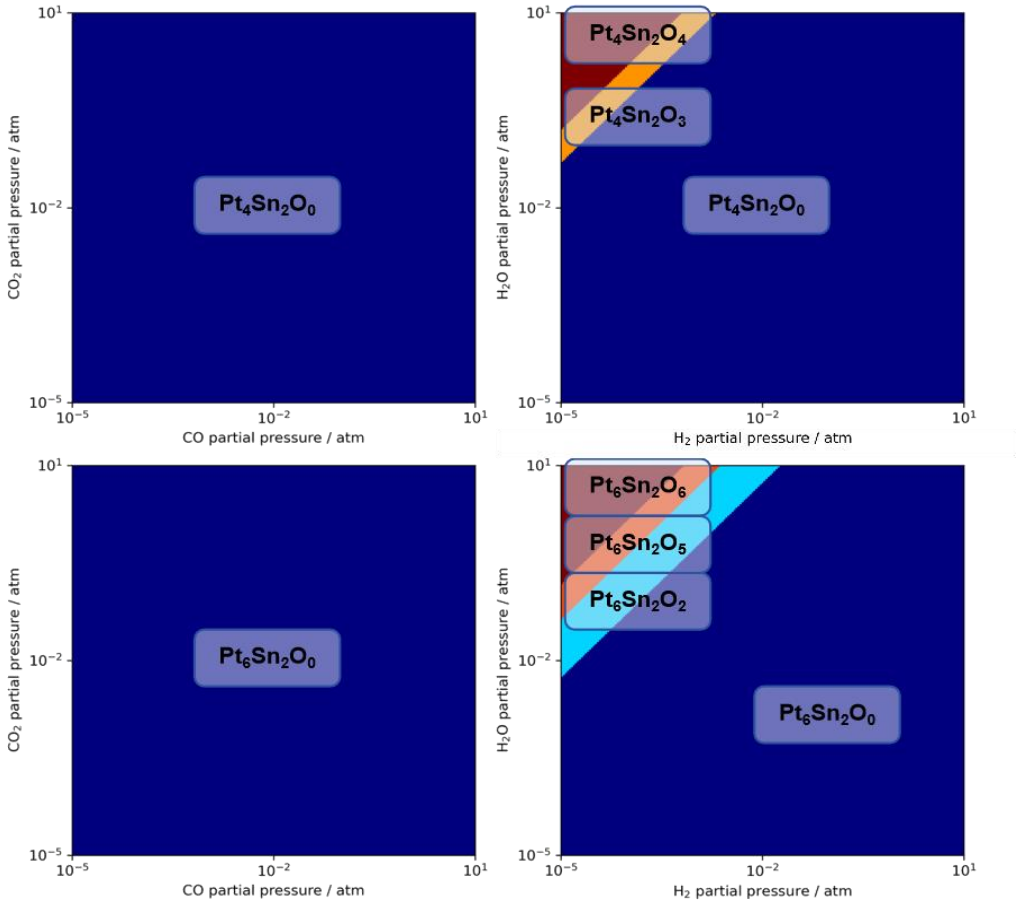


Figure S10. The 2-D phase diagrams under 823 K with CO_2/CO or H_2O/H_2 pairs. Partial oxidation states only appear in the H_2O/H_2 pairs, probably due to the different oxidizability between CO_2 and H_2O, which C-O bond of CO_2 is much more stable than H-O bond of H_2O. The partial pressures of H_2 and H_2O dominate the oxidation states of PtSn clusters of DHP reaction.

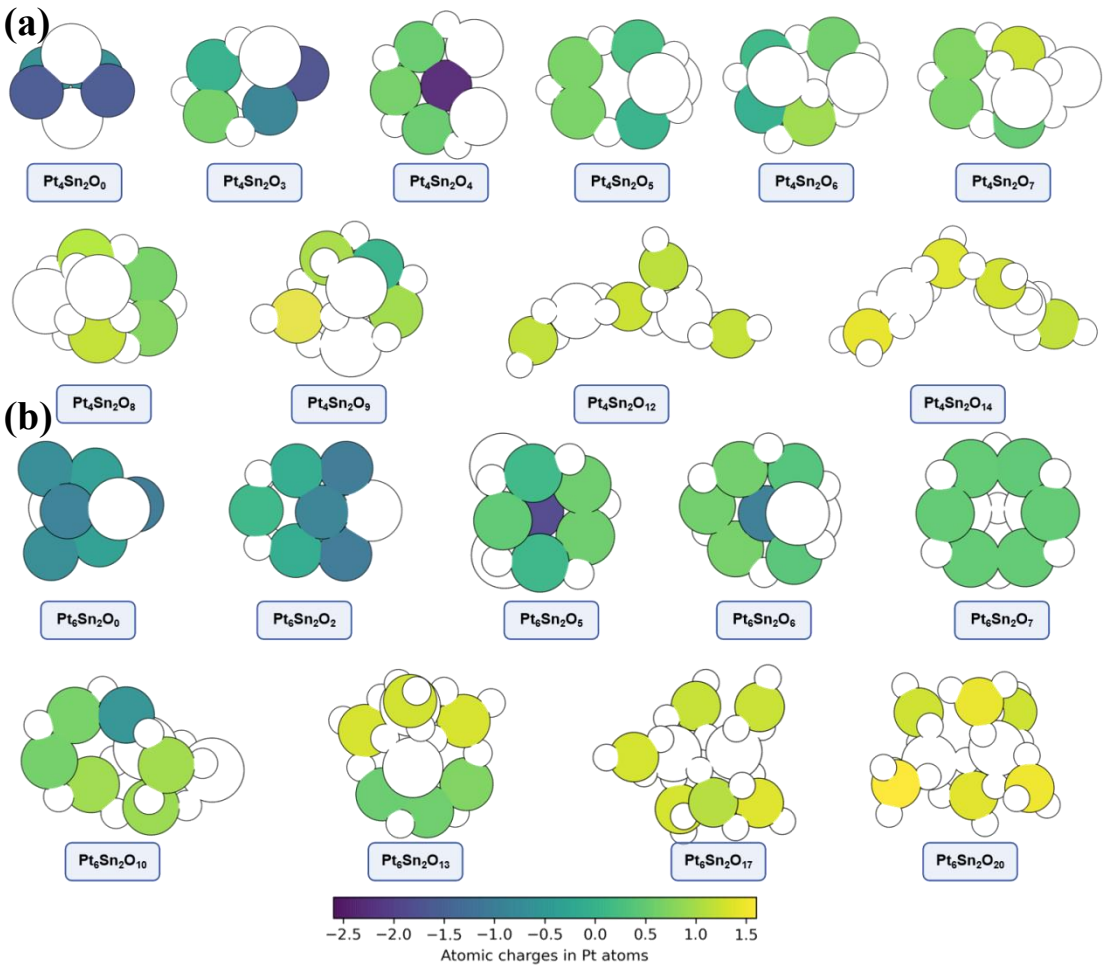


Figure S11. The atomic charges in Pt atoms for the GM structures of $Pt_4Sn_2O_y$ and $Pt_6Sn_2O_y$ comfirmed by phase diagrams. Pt atoms are colored according to their Bader charge in |e|. Sn and O atoms are presented as large and small white cycle, respectively.

Table 1. Bader charges distribution of each stoichiometry and coordination number of O atoms for Pt and Sn.

atom index	atomic symbol	bader charges/ |e|	coordination number of O
$Pt_1Sn_1O_0$			
1	Pt	-1.95	0
2	Sn	1.95	0
$Pt_1Sn_1O_2$			
1	Pt	-0.10	1
2	Sn	1.97	1
3	O	-0.58	
4	O	-1.28	
$Pt_1Sn_1O_3$			
1	Pt	1.10	3
2	Sn	2.04	2
3	O	-1.29	
4	O	-1.29	
5	O	-0.56	
$Pt_1Sn_1O_4$			
1	Pt	1.58	4
2	Sn	2.06	2
3	O	-0.55	
4	O	-0.55	
5	O	-1.26	
6	O	-1.27	
$Pt_2Sn_2O_0$			
1	Pt	-2.25	0
2	Pt	-2.26	0
3	Sn	2.26	0
4	Sn	2.25	0
$Pt_2Sn_2O_1$			
1	Pt	-1.24	0
2	Pt	-1.23	0
3	Sn	2.19	1

4	Sn	2.19	1
5	O	-1.91	
$Pt_2Sn_2O_4$			
1	Pt	0.50	2
2	Pt	0.49	2
3	Sn	2.12	2
4	Sn	2.12	2
5	O	-1.25	
6	O	-0.69	
7	O	-1.23	
8	O	-2.07	
$Pt_2Sn_2O_7$			
1	Pt	1.41	4
2	Pt	1.15	3
3	Sn	2.82	4
4	Sn	2.18	3
5	O	-1.45	
6	O	-1.61	
7	O	-1.15	
8	O	-0.50	
9	O	-1.17	
10	O	-1.13	
11	O	-0.54	
$Pt_2Sn_2O_8$			
1	Pt	1.44	4
2	Pt	1.44	4
3	Sn	2.90	4
4	Sn	2.96	4
5	O	-1.65	
6	O	-0.49	
7	O	-1.10	
8	O	-1.12	
9	O	-1.65	
10	O	-0.49	

11	O	-1.09	
12	O	-1.14	
$Pt_3Sn_3O_0$			
1	Pt	-2.41	0
2	Pt	-2.48	0
3	Pt	-1.89	0
4	Sn	2.21	0
5	Sn	2.30	0
6	Sn	2.27	0
$Pt_3Sn_3O_1$			
1	Pt	-1.24	0
2	Pt	-1.78	0
3	Pt	-1.77	0
4	Sn	2.17	1
5	Sn	2.19	1
6	Sn	2.46	1
7	O	-2.03	
$Pt_3Sn_3O_5$			
1	Pt	0.21	2
2	Pt	0.10	2
3	Pt	0.23	2
4	Sn	1.79	1
5	Sn	2.05	2
6	Sn	2.04	2
7	O	-0.66	
8	O	-0.66	
9	O	-2.16	
10	O	-1.46	
11	O	-1.47	
$Pt_3Sn_3O_7$			
1	Pt	1.11	4
2	Pt	0.54	2
3	Pt	0.57	2
4	Sn	2.27	3

5	Sn	1.78	2
6	Sn	2.22	3
7	O	-1.06	
8	O	-1.21	
9	O	-1.15	
10	O	-1.18	
11	O	-1.55	
12	O	-0.67	
13	O	-1.66	
$Pt_3Sn_3O_9$			
1	Pt	1.16	4
2	Pt	1.15	3
3	Pt	1.13	4
4	Sn	2.18	3
5	Sn	2.16	4
6	Sn	2.20	3
7	O	-1.64	
8	O	-1.42	
9	O	-1.04	
10	O	-0.70	
11	O	-0.49	
12	O	-1.65	
13	O	-1.49	
14	O	-1.04	
15	O	-0.51	
$Pt_3Sn_3O_{12}$			
1	Pt	1.17	4
2	Pt	1.50	4
3	Pt	1.49	4
4	Sn	2.81	4
5	Sn	2.40	4
6	Sn	4.00	6
7	O	-1.08	
8	O	-1.59	

9	O	-1.05	
10	O	-1.65	
11	O	-0.67	
12	O	-0.52	
13	O	-1.11	
14	O	-1.48	
15	O	-0.51	
16	O	-1.50	
17	O	-1.10	
18	O	-1.11	
$Pt_4Sn_4O_0$			
1	Pt	-2.45	0
2	Pt	-2.46	0
3	Pt	-2.46	0
4	Pt	-2.45	0
5	Sn	2.46	0
6	Sn	2.44	0
7	Sn	2.47	0
8	Sn	2.45	0
$Pt_4Sn_4O_2$			
1	Pt	-1.07	0
2	Pt	-0.93	0
3	Pt	-1.56	0
4	Pt	-1.89	0
5	Sn	2.77	1
6	Sn	2.10	2
7	Sn	2.37	1
8	Sn	2.33	2
9	O	-2.05	
10	O	-2.07	
$Pt_4Sn_4O_7$			
1	Pt	-0.21	2
2	Pt	0.59	2
3	Pt	0.60	2

4	Pt	-0.21	2
5	Sn	2.41	1
6	Sn	2.12	3
7	Sn	2.12	3
8	Sn	2.14	3
9	O	-2.14	
10	O	-1.62	
11	O	-0.68	
12	O	-0.71	
13	O	-0.68	
14	O	-2.10	
15	O	-1.63	
$Pt_4Sn_4O_9$			
1	Pt	1.08	4
2	Pt	0.30	2
3	Pt	0.30	2
4	Pt	1.10	4
5	Sn	1.88	2
6	Sn	2.19	4
7	Sn	2.20	4
8	Sn	1.88	2
9	O	-0.67	
10	O	-1.45	
11	O	-0.68	
12	O	-0.68	
13	O	-1.54	
14	O	-1.56	
15	O	-1.44	
16	O	-1.46	
17	O	-1.45	
$Pt_4Sn_4O_{12}$			
1	Pt	1.15	4
2	Pt	1.14	4
3	Pt	1.11	4

4	Pt	1.13	4
5	Sn	2.17	3
6	Sn	3.28	4
7	Sn	2.20	3
8	Sn	2.20	3
9	O	-1.11	
10	O	-1.12	
11	O	-1.36	
12	O	-1.30	
13	O	-1.58	
14	O	-1.10	
15	O	-1.23	
16	O	-1.57	
17	O	-1.12	
18	O	-0.62	
19	O	-1.11	
20	O	-1.15	
$Pt_4Sn_4O_{16}$			
1	Pt	1.21	4
2	Pt	1.47	4
3	Pt	1.13	4
4	Pt	1.49	4
5	Sn	4.00	6
6	Sn	2.34	3
7	Sn	3.00	4
8	Sn	4.00	6
9	O	-1.19	
10	O	-0.55	
11	O	-1.43	
12	O	-1.54	
13	O	-0.50	
14	O	-1.14	
15	O	-1.10	
16	O	-1.46	

17	O	-1.03	
18	O	-1.58	
19	O	-1.25	
20	O	-1.08	
21	O	-0.51	
22	O	-1.57	
23	O	-1.15	
24	O	-1.56	
$Pt_4Sn_2O_0$			
1	Pt	-1.60	0
2	Pt	-1.60	0
3	Pt	-0.66	0
4	Pt	-0.68	0
5	Sn	2.27	0
6	Sn	2.28	0
$Pt_4Sn_2O_3$			
1	Pt	0.63	2
2	Pt	-0.01	2
3	Pt	-0.89	1
4	Pt	-1.73	0
5	Sn	2.36	0
6	Sn	2.33	1
7	O	-0.73	
8	O	-0.68	
9	O	-1.28	
$Pt_4Sn_2O_4$			
1	Pt	0.54	2
2	Pt	-2.30	0
3	Pt	0.54	2
4	Pt	0.63	2
5	Sn	2.30	1
6	Sn	2.31	1
7	O	-1.34	
8	O	-0.68	

9	O	-1.33	
10	O	-0.68	
$Pt_4Sn_2O_5$			
1	Pt	0.67	2
2	Pt	0.67	2
3	Pt	0.00	2
4	Pt	0.24	2
5	Sn	2.08	2
6	Sn	2.02	2
7	O	-0.73	
8	O	-0.73	
9	O	-0.69	
10	O	-1.89	
11	O	-1.67	
$Pt_4Sn_2O_6$			
1	Pt	0.95	3
2	Pt	-0.07	2
3	Pt	0.11	2
4	Pt	0.61	2
5	Sn	2.24	1
6	Sn	2.17	3
7	O	-1.24	
8	O	-0.69	
9	O	-1.49	
10	O	-0.74	
11	O	-0.73	
12	O	-1.13	
$Pt_4Sn_2O_7$			
1	Pt	0.68	2
2	Pt	0.51	2
3	Pt	0.73	2
4	Pt	1.22	4
5	Sn	2.20	3
6	Sn	1.86	2

7	O	-0.73	
8	O	-1.15	
9	O	-1.10	
10	O	-1.17	
11	O	-0.69	
12	O	-0.69	
13	O	-1.67	
$Pt_4Sn_2O_8$			
1	Pt	0.66	2
2	Pt	0.75	2
3	Pt	1.09	3
4	Pt	1.20	4
5	Sn	2.19	3
6	Sn	2.62	4
7	O	-0.75	
8	O	-0.68	
9	O	-0.70	
10	O	-0.99	
11	O	-1.23	
12	O	1.53	
13	O	-1.44	
14	O	-1.18	
$Pt_4Sn_2O_9$			
1	Pt	0.96	3
2	Pt	1.43	4
3	Pt	0.01	2
4	Pt	1.01	3
5	Sn	3.29	4
6	Sn	2.24	2
7	O	-1.60	
8	O	-1.23	
9	O	-1.24	
10	O	-1.19	
11	O	-0.67	

12	O	-0.53	
13	O	-0.64	
14	O	-1.15	
15	O	-0.68	
$Pt_4Sn_2O_{12}$			
1	Pt	1.14	3
2	Pt	1.19	3
3	Pt	1.19	3
4	Pt	1.26	4
5	Sn	4.00	5
6	Sn	4.00	4
7	O	-1.02	
8	O	-1.26	
9	O	-0.53	
10	O	-1.22	
11	O	-1.21	
12	O	-0.51	
13	O	-1.23	
14	O	-0.53	
15	O	-1.33	
16	O	-1.30	
17	O	-1.28	
18	O	-1.35	
$Pt_4Sn_2O_{14}$			
1	Pt	1.52	4
2	Pt	1.45	4
3	Pt	1.28	3
4	Pt	1.18	3
5	Sn	4.00	4
6	Sn	4.00	4
7	O	-0.49	
8	O	-1.33	
9	O	-0.39	
10	O	-1.32	

11	O	-0.39	
12	O	-1.37	
13	O	-1.23	
14	O	-0.61	
15	O	-1.33	
16	O	-1.44	
17	O	-0.53	
18	O	-1.27	
19	O	-1.31	
20	O	-0.40	
$Pt_6Sn_2O_0$			
1	Pt	-1.06	0
2	Pt	-0.39	0
3	Pt	-0.72	0
4	Pt	-0.96	0
5	Pt	-0.36	0
6	Pt	-0.74	0
7	Sn	1.98	0
8	Sn	2.24	0
$Pt_6Sn_2O_2$			
1	Pt	-0.15	1
2	Pt	-0.14	1
3	Pt	0.09	2
4	Pt	-1.06	0
5	Pt	-1.07	0
6	Pt	-0.92	0
7	Sn	2.17	0
8	Sn	2.48	0
9	O	-0.71	
10	O	-0.70	
$Pt_6Sn_2O_5$			
1	Pt	0.57	2
2	Pt	0.07	2
3	Pt	0.45	2

4	Pt	0.11	2
5	Pt	0.57	2
6	Pt	-1.88	0
7	Sn	2.18	1
8	Sn	2.21	1
9	O	-0.67	
10	O	-0.70	
11	O	-1.11	
12	O	-1.10	
13	O	-0.69	
$Pt_6Sn_2O_6$			
1	Pt	0.36	2
2	Pt	0.60	2
3	Pt	-0.98	0
4	Pt	0.61	2
5	Pt	0.63	2
6	Pt	0.39	2
7	Sn	1.98	1
8	Sn	1.88	1
9	O	-0.70	
10	O	-1.35	
11	O	-0.69	
12	O	-0.68	
13	O	-0.72	
14	O	-1.34	
$Pt_6Sn_2O_7$			
1	Pt	0.50	2
2	Pt	0.47	2
3	Pt	0.45	2
4	Pt	0.48	2
5	Pt	0.48	2
6	Pt	0.50	2
7	Sn	1.63	1
8	Sn	1.63	1

9	O	-0.68	
10	O	-0.68	
11	O	-0.69	
12	O	-0.69	
13	O	-0.68	
14	O	-2.04	
15	O	-0.68	
$Pt_6Sn_2O_{10}$			
1	Pt	0.96	3
2	Pt	0.92	3
3	Pt	0.97	3
4	Pt	0.62	2
5	Pt	-0.58	2
6	Pt	0.65	2
7	Sn	2.33	3
8	Sn	3.85	2
9	O	-0.69	
10	O	-0.64	
11	O	-0.62	
12	O	-1.16	
13	O	-1.11	
14	O	-2.04	
15	O	-0.68	
16	O	-1.41	
17	O	-0.66	
18	O	-0.69	
$Pt_6Sn_2O_{13}$			
1	Pt	0.59	2
2	Pt	1.34	4
3	Pt	0.72	2
4	Pt	0.54	2
5	Pt	1.32	4
6	Pt	1.28	3
7	Sn	1.95	3

8	Sn	4.00	6
9	O	-1.57	
10	O	-1.24	
11	O	-0.38	
12	O	-0.70	
13	O	-0.65	
14	O	-0.71	
15	O	-0.68	
16	O	-1.18	
17	O	-1.18	
18	O	-0.40	
19	O	-1.59	
20	O	-0.95	
21	O	-0.52	
$Pt_6Sn_2O_{17}$			
1	Pt	1.23	3
2	Pt	1.38	4
3	Pt	1.22	3
4	Pt	1.10	4
5	Pt	1.31	3
6	Pt	1.31	3
7	Sn	4.00	6
8	Sn	4.00	6
9	O	-0.47	
10	O	-1.10	
11	O	-1.04	
12	O	-1.19	
13	O	-1.12	
14	O	-0.53	
15	O	-1.50	
16	O	-0.50	
17	O	-1.16	
18	O	-1.55	
19	O	-0.56	

20	O	-0.64	
21	O	-0.93	
22	O	-0.47	
23	O	-1.15	
24	O	-0.52	
25	O	-1.10	
$Pt_6Sn_2O_{20}$			
1	Pt	1.39	4
2	Pt	1.50	4
3	Pt	1.76	4
4	Pt	1.27	3
5	Pt	1.27	3
6	Pt	1.46	3
7	Sn	4.00	6
8	Sn	4.00	6
9	O	-0.43	
10	O	-1.63	
11	O	-0.50	
12	O	-1.08	
13	O	-0.50	
14	O	-1.01	
15	O	-1.08	
16	O	-0.47	
17	O	-0.96	
18	O	-0.46	
19	O	-1.14	
20	O	-1.06	
21	O	-0.51	
22	O	-1.07	
23	O	-0.53	
24	O	-1.12	
25	O	-1.02	
26	O	-0.48	
27	O	-0.48	

28	O	-1.10

3. Reference

[1] Kuehne,Thomas D.; Iannuzzi,Marcella; Del Ben,Mauro; et al. CP2K: An electronic structure and molecular dynamics software package-Quickstep: Efficient and accurate electronic structure calculations. The Journal of Chemical Physics, **152** (19), (2020).

[2] Jörg Behler. Atom-centered symmetry functions for constructing high-dimensional neural network potentials. The Journal of Chemical Physics, **134**, 074106, (2011).

[3] Jörg Behler and Michele Parrinello. Generalized neural-network representation of high-dimensional potential-energy surfaces. Phys. Rev. Lett., **98**, 146401, (2007).

[4] Christoph Schran, Krystof Brezina, Ondrej Marsalek. Committee neural network potentials control generalization errors and enable active learning. J. Chem. Phys., **153** (10): 104105, (2020).

[5] NIST-JANAF Thermochemical Tables. NIST Standard Reference Database 13, Last Update to Data Content: 1998. https://janaf.nist.gov.

[6] K. W. Jacobsen, P. Stoltze, and J. K. Nørskov. A semi-empirical effective medium theory for metals and alloys. Surf. Sci., **366**, 394, (1996).