Supporting Information

Resolving Activation Entropy of CO oxidation in the Solid-Gas and Solid-Liquid Conditions from Machine Learning Simulation

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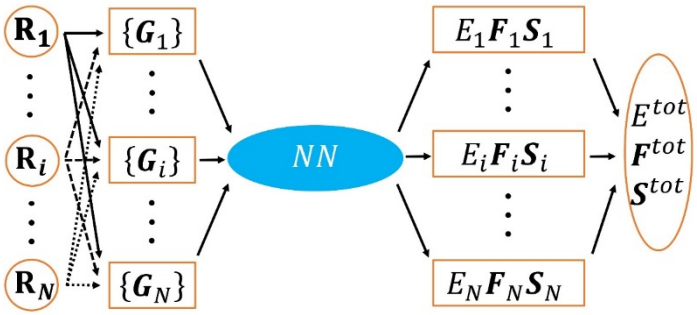
1. G-NN potential architecture



Scheme S1. Scheme of the HDNN architecture. The subscripts (1, *i*, …, *N*) are atom indices and represent the total atoms in a structure. The inputs of NN are a set of structural descriptors {***G***}, which are constructed from the Cartesian coordinates {**R**} of the structure, while the outputs of NN are the atomic properties {E_i, $\boldsymbol{F}_i$, $\boldsymbol{S}_i$}, *i.e.*, energies, forces, and stresses. The overall properties, E^{tot}, $\boldsymbol{F}^{tot}$, and $\boldsymbol{S}^{tot}$, can be calculated from the individual atomic contributions.

In this work, we utilized the high dimensional neural network (HDNN) scheme to construct the global NN (G-NN) potential, as shown in **Scheme S1**. The input nodes to NN are a set of structural descriptors of a structure, as discussed in our previous works. [1-3] The total energy E^{tot} of the structure can be composed as a linear combination of its atomic energy E^i from the output of NN

$$E^{tot} = \sum_i E_i \tag{S1}$$

Consistently, the atomic force can be analytically derived from the total energy, *i.e.*, the force component $F_{k,\alpha}$ (α = *x*, *y*, or *z*) acting on atom *k* is the derivative of the total energy E^{tot} with respect to coordinate $R_{k,\alpha}$. In combination with Eq. S1, the force component $F_{k,\alpha}$ then is related to the derivatives of the atomic energy E^i with respect to the j^{th} structural descriptors of atom *i*, $G_{j,i}$

$$F_{k,\alpha} = -\frac{\partial E^{tot}}{\partial \mathrm{R}_{k,\alpha}} = -\sum_{i,j} \frac{\partial E_i}{\partial G_{j,i}} \frac{\partial G_{j,i}}{\partial \mathrm{R}_{k,\alpha}} \tag{S2}$$

Similarly, the element $\sigma_{\alpha\beta}$ of static stress tensor matrix can be analytically derived as

$$\sigma_{\alpha\beta} = -\frac{1}{V}\sum_{i,j,d} \frac{(\boldsymbol{r}_d)_\alpha (\boldsymbol{r}_d)_\beta}{r_d} \frac{\partial E_i}{\partial G_{j,i}} \frac{\partial G_{j,i}}{\partial r_d} \tag{S3}$$

where $\boldsymbol{r}_d$ and r_d are the distance vector, constituted by $G_{j,i}$ and its module, respectively, and *V* is the volume of the structure.

2. SSW-NN method for generating G-NN potential

2.1 SSW method

The stochastic surface walking (SSW) algorithm[4] has an automated climbing mechanism to manipulate a structure configuration from a minimum to a high-energy configuration along one random mode direction. The method was initially developed for aperiodic systems, such as molecules and clusters[5], and has been extended to periodic crystals[6].

The SSW method inherits the idea of bias-potential driven constrained-Broyden-dimer (BP-CBD) method for TS location[7]. In one particular SSW step a modified PES V, as shown in Eq. S4, is utilized for moving from the current minimum, $\mathbf{R}^m$ to a high energy configuration $\mathbf{R}^H$ by adding a series of bias Gaussian potential v_n (n=1...H). The bias potentials are added one by one consecutively along the direction $\mathbf{N}^n$ that defines the walking direction.

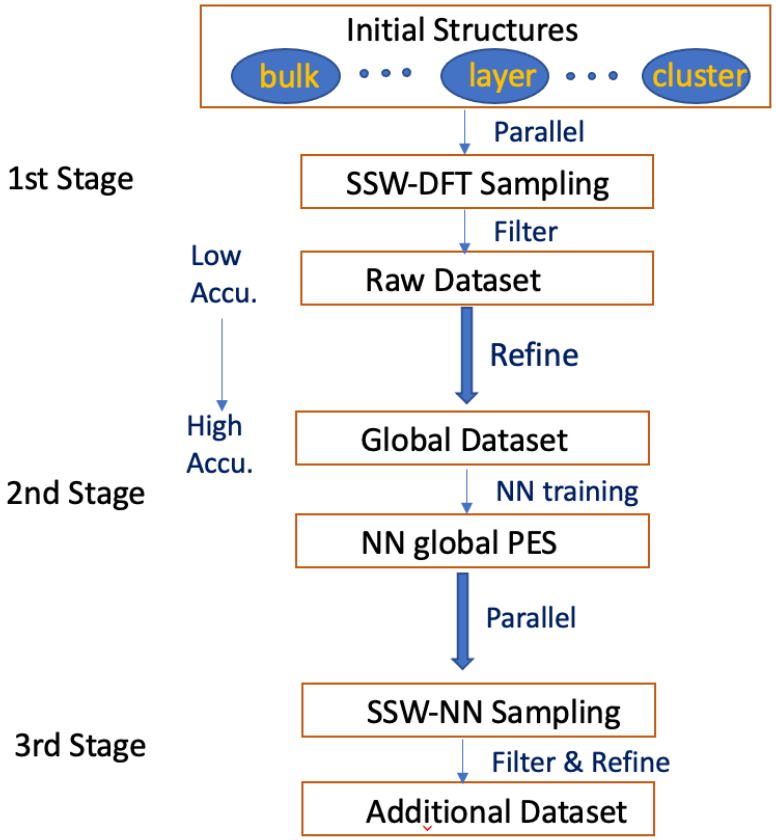
$$V = V_{real} + \sum_{n=1}^{H} v_n = V_{real} + \sum_{n=1}^{H} w_n \times \exp\left[-\left(\left(\boldsymbol{R} - \boldsymbol{R}^{n-1}\right)\cdot \boldsymbol{N}^n\right)^2 / (2 \times ds^2)\right] \quad \text{(S4)}$$

In the equation **R** is the current coordination vector of the structure and V_{real} represents the unmodified PES; $\mathbf{R}^n$ is the n^{th} local minima along the movement trajectory on the modified PES that is created after adding *n* Gaussian functions. The Gaussian function can be further controlled by its height *w* and its width *ds*. Once the maximum number of Gaussian functions (*e.g.* H=9) is reached, all bias potentials are removed and the local optimization is performed to quench the structure to a new minimum.

2.2 SSW-NN method

SSW-NN method is a machine-learning potential based global optimization method, which combines the global neural network (G-NN) potential with SSW method for fast and accurate global PES exploration as implemented in LASP code.[8] While traditional DFT calculations are frustrated for the global optimization of complex systems due to the high computational cost, SSW-NN method provides a general solution for PES scanning with both high efficiency and high accuracy.[9] The G-NN potential is trained based on DFT dataset and delivers a high speed of PES evaluation, ~4 orders of magnitude faster than DFT.[1–3]

2.3 Construction of the quaternary Pt-C-H-O G-NN potential



Scheme S2. Procedure for the generation of the global training dataset by SSW global optimization. In the first stage, the SSW sampling is typically performed by low accuracy DFT calculations. In the second stage, the global dataset is first refined with high accuracy DFT setups, and then a NN training is performed based on the accurate global dataset. In the third stage, an /additional dataset is generated by SSW sampling utilizing the previously obtained NN PES, and is fed into the global dataset. A new cycle of NN training then starts based on the new global dataset (back to stage 2).

The Pt–C–H–O G-NN potential is now available from LASP G-NN library [13]. Here we briefly introduce the procedure to generate this initial G-NN potential.

The quality of the potential energy surface (PES) of G-NN is largely determined by its training dataset. We utilized the stochastic surface walking (SSW) global optimization to generate a global dataset, which is fully automated and does not need a priori knowledge on the system, such as the structural motif, *e.g.* bonding patterns and symmetry. The final obtained Pt–C–H–O global dataset contains a variety of structural patternsi. on the global PES, as summarized in **Table S1**. In brief, the SSW-NN method involves three stages to generate the global dataset (see **Scheme S2**), as described below.

(i) **The first stage** generates a raw dataset, which contains the most common atomic environment and serves to build an initial NN PES. This is done by performing density functional theory (DFT) SSW global optimization in a massively parallel way. In this stage, the DFT calculations have low accuracy setups and small unit cells to speed up the SSW search. By collecting and screening the structures from SSW trajectories, a raw dataset is obtained.

(ii) **The second stage** trains a NN global PES. This is done by refining the dataset using DFT calculations with high accuracy setups, followed by NN training on the accurate global dataset. The NN architecture applied in this stage utilizes a small set of structural descriptors and a small network size.

(iii) **The third stage** iteratively expands the global dataset. It targets to increase the predictive power of NN PES by incorporating more structural patterns into the dataset. This is done by performing SSW PES search using the NN PES obtained in the second stage, starting from a variety of initial structures. These initial structures are randomly constructed, and also include large systems with many atoms per unit cell. The structures from all the SSW trajectories are collected and filtered to generate an additional dataset. The new dataset is then fed to the global dataset to start a new cycle of NN training (back to stage 2).

Table S1. Structure information of the final dataset for G-NN training of Pt–C–H–O potential. Listed data are the number of the structures in the global dataset, as distinguished by the species, the number of atoms (N_{atoms}), the type of structures, including cluster ($N_{cluster}$), bulk (N_{bulk}), layer (N_{layer}), and its total number (N_{total}).

Species	N_{atoms}	$N_{cluster}$	N_{layer}	N_{bulk}	N_{total}
Pt16	16	211	1	795	1007
Pt31	31	0	0	7	7
Pt32	32	0	3	12	15
O4	4	0	37	0	37
O11	11	0	198	98	296
C1-O1-Pt16	18	0	3335	0	3335
C1-O2-Pt44	47	4273	0	0	4273
H1-Pt15	16	0	0	365	365
H1-Pt23	24	0	7	32	39
H1-Pt26	27	0	17	0	17

H1-Pt27	28	0	18	0	18
H1-C1-O3-Pt36	41	0	75	10	85
H2	2	1	0	0	1
H2-Pt14	16	0	69	626	695
H2-Pt27	29	0	24	22	46
H2-Pt28	30	0	29	0	29
H2-C1	3	4	0	0	4
H2-C1-O1	4	103	0	0	103
H2-C1-O2	5	40	0	0	40
H2-C1-O2-Pt12	17	0	994	38	1032
H2-C1-O2-Pt16	21	0	50	0	50
H2-C1-O2-Pt27	32	0	35	0	35
H2-C1-O2-Pt36	41	0	3528	0	3528
H2-C1-O3	6	11	0	0	11
H2-C1-O3-Pt36	42	0	235	0	235
H2-C2	4	86	0	0	86
H2-C2-O3-Pt26	33	0	55	0	55
H2-C2-O3-Pt27	34	0	226	4	230
H2-C2-O3-Pt36	43	0	124	0	124
H2-C3-O2-Pt25	32	0	22	0	22
H2-C3-O2-Pt26	33	0	331	3	334
H2-C3-O2-Pt27	34	0	267	0	267
H2-C3-O4-Pt33	42	0	321	3	324
H2-C3-O4-Pt35	44	0	348	3	351
H2-C3-O4-Pt36	45	0	715	21	736
H2-C4-O1-Pt26	33	0	87	0	87
H2-C4-O1-Pt27	34	0	302	1	303
H2-C4-O2-Pt25	33	0	126	1	127
H2-C4-O3	9	60	0	0	60
H2-C4-O4	10	2	0	0	2
H2-C4-O5	11	8	0	0	8
H2-C5-O3	10	6	0	0	6
H2-C5-O4	11	4	0	0	4
H2-C6-O2	10	2	0	0	2
H2-C7-O1	10	2	0	0	2
H3-Pt26	29	0	33	0	33
H3-C1	4	7	0	0	7
H3-C1-O2-Pt18	24	0	36	0	36
H3-C1-O2-Pt36	42	0	481	0	481
H3-C1-O3-Pt35	42	0	66	33	99
H3-C2-O2-Pt26	33	0	53	0	53
H3-C2-O2-Pt27	34	0	247	1	248
H3-C2-O2-Pt36	43	0	47	0	47
H3-C2-O3-Pt23	31	0	2	0	2

H3-C2-O3-Pt24	32	0	12	1	13
H3-C2-O3-Pt27	35	0	8	0	8
H3-C2-O3-Pt34	42	0	477	0	477
H3-C2-O3-Pt36	44	0	566	1	567
H3-C2-O4-Pt32	41	0	47	16	63
H3-C2-O4-Pt33	42	0	79	0	79
H3-C2-O4-Pt35	44	0	356	5	361
H3-C3-O1-Pt26	33	0	15	0	15
H3-C3-O1-Pt27	34	0	209	3	212
H3-C3-O2-Pt25	33	0	202	1	203
H3-C3-O3-Pt35	44	0	390	4	394
H4-Pt12	16	2122	0	256	2378
H4-Pt17	21	0	0	170	170
H4-Pt20	24	0	28	0	28
H4-Pt24	28	0	28	0	28
H4-C1	5	128	0	0	128
H4-C1-O1	6	36	0	0	36
H4-C1-O1-Pt12	18	0	66	1	67
H4-C1-O2	7	0	7	0	7
H4-C1-O2-Pt36	43	0	896	0	896
H4-C1-O3-Pt27	35	0	256	0	256
H4-C1-O3-Pt36	44	0	1331	42	1373
H4-C2	6	34	0	0	34
H4-C2-O1	7	157	0	0	157
H4-C2-O2	8	51	3	4	58
H4-C2-O2-Pt27	35	0	5	0	5
H4-C2-O2-Pt33	41	0	34	0	34
H4-C2-O2-Pt36	44	0	30	0	30
H4-C2-O3-Pt34	43	0	22	0	22
H4-C2-O3-Pt36	45	0	20	0	20
H4-C2-O4-Pt11	21	0	2	1	3
H4-C2-O4-Pt12	22	0	20	381	401
H4-C2-O4-Pt24	34	0	16	1	17
H4-C2-O4-Pt26	36	0	3	0	3
H4-C2-O4-Pt27	37	0	10	0	10
H4-C2-O4-Pt32	42	0	6	0	6
H4-C2-O4-Pt36	46	0	1666	0	1666
H4-C3	7	52	0	0	52
H4-C3-O1	8	12	0	0	12
H4-C3-O2	9	1	0	0	1
H4-C3-O5-Pt36	48	0	6	4	10
H4-C4-O2	10	6	0	0	6
H4-C4-O3	11	2	0	0	2
H4-C4-O4	12	4	0	0	4

H4-C4-O4-Pt36	48	0	0	57	57
H4-C4-O5	13	1	0	0	1
H4-C5-O2	11	3	0	0	3
H4-C5-O3	12	21	0	0	21
H4-C5-O4	13	26	0	0	26
H4-C6-O1	11	7	0	0	7
H4-C6-O2	12	22	0	0	22
H4-C6-O3	13	46	0	0	46
H4-C7	11	3	0	0	3
H4-C7-O1	12	6	0	0	6
H4-C7-O2	13	54	0	0	54
H4-C8-O1	13	24	0	0	24
H4-C9	13	1	0	0	1
H5-Pt16	21	0	182	38	220
H5-C1-O2-Pt23	31	0	3	0	3
H5-C1-O3-Pt36	45	0	43	16	59
H5-C2-O2-Pt44	53	0	202	0	202
H6-Pt10	16	0	0	360	360
H6-Pt15	21	0	286	5	291
H6-Pt25	31	0	133	0	133
H6-Pt26	32	95	72	106	273
H6-C1-O2-Pt36	45	0	533	203	736
H6-C1-O3-Pt12	22	0	10	162	172
H6-C1-O3-Pt36	46	0	380	20	400
H6-C2	8	292	0	0	292
H6-C2-Pt26	34	0	58	0	58
H6-C2-Pt28	36	0	78	0	78
H6-C2-O1	9	23	16	20	59
H6-C2-O1-Pt45	54	0	285	0	285
H6-C3	9	88	0	0	88
H6-C3-O1	10	2	0	0	2
H6-C3-O1-Pt48	58	0	5	0	5
H6-C3-O1-Pt64	74	0	270	0	270
H6-C3-O2	11	60	0	0	60
H6-C4-O1-Pt64	75	0	22	0	22
H6-C4-O2	12	1	0	0	1
H6-C4-O2-Pt64	76	0	75	0	75
H6-C4-O3	13	5	0	0	5
H6-C4-O4	14	3	0	0	3
H6-C5-O2	13	18	0	0	18
H6-C5-O3	14	40	0	0	40
H6-C5-O4	15	51	0	0	51
H6-C6	12	78	0	0	78
H6-C6-Pt36	48	0	0	51	51

H6-C6-O1	13	422	0	0	422
H6-C6-O2	14	75	0	0	75
H6-C6-O3	15	29	0	0	29
H6-C7-O1	14	8	0	0	8
H6-C7-O2	15	19	0	0	19
H6-C7-O4	17	0	3	0	3
H6-C8	14	3	0	0	3
H6-C8-O1	15	7	0	0	7
H6-C9	15	2	0	0	2
H7-Pt25	32	0	0	117	117
H7-C1-O4-Pt34	46	0	64	32	96
H7-C1-O4-Pt36	48	0	62	34	96
H7-C2-Pt26	35	0	19	0	19
H7-C2-O2-Pt36	47	0	407	0	407
H7-C2-O5-Pt34	48	0	8	154	162
H8-Pt8	16	2986	0	1462	4448
H8-Pt16	24	0	27	21	48
H8-Pt20	28	0	16	0	16
H8-C1-O5-Pt36	50	0	75	79	154
H8-C2	10	0	1	0	1
H8-C2-O2	12	0	7	0	7
H8-C2-O2-Pt23	35	0	3	0	3
H8-C2-O2-Pt24	36	0	4	3	7
H8-C2-O2-Pt36	48	0	350	0	350
H8-C2-O3	13	0	6	0	6
H8-C2-O4-Pt34	48	0	209	98	307
H8-C2-O4-Pt35	49	0	89	72	161
H8-C2-O4-Pt36	50	0	3376	15	3391
H8-C3	11	4	0	0	4
H8-C3-O1-Pt36	48	0	401	0	401
H8-C3-O3	14	2	0	0	2
H8-C3-O3-Pt64	78	0	27	0	27
H8-C4-O1	13	4	0	0	4
H8-C5-O1	14	166	0	0	166
H8-C5-O3	16	10	0	0	10
H8-C5-O4	17	13	0	0	13
H8-C6-O1	15	8	0	0	8
H8-C6-O2	16	10	0	0	10
H8-C6-O3	17	27	0	0	27
H8-C7	15	3	0	0	3
H8-C7-O1	16	11	0	0	11
H8-C7-O2	17	56	0	0	56
H8-C7-O3	18	0	3	4	7
H8-C8	16	6	0	0	6

H8-C8-O1	17	53	0	0	53
H8-C8-O2	18	2	0	0	2
H8-C8-O3	19	0	6	2	8
H8-C9	17	19	0	0	19
H8-C9-O3	20	73	0	0	73
H8-C12-O6	26	0	2	0	2
H9-Pt23	32	145	0	0	145
H9-C2-Pt25	36	0	31	17	48
H9-C2-Pt26	37	0	68	30	98
H9-C2-O1-Pt34	46	0	57	0	57
H9-C2-O1-Pt35	47	0	67	39	106
H9-C2-O1-Pt36	48	0	428	1	429
H9-C3-O1-Pt35	48	0	216	0	216
H9-C9-O1	19	210	0	0	210
H10-Pt21	31	0	135	0	135
H10-Pt22	32	0	54	206	260
H10-O5-Pt12	27	0	618	4	622
H10-C3-O3-Pt64	80	0	2426	103	2529
H10-C4-O3	17	0	7	0	7
H10-C5-O4	19	3	0	0	3
H10-C5-O5	20	3	0	0	3
H10-C6	16	26	0	0	26
H10-C6-O1	17	3	0	0	3
H10-C6-O2	18	7	0	0	7
H10-C6-O3	19	10	0	0	10
H10-C6-O4-Pt64	84	0	766	95	861
H10-C7	17	3	0	0	3
H10-C7-O1	18	52	0	0	52
H10-C7-O2	19	34	0	0	34
H10-C7-O3	20	0	1	0	1
H10-C8	18	12	0	0	12
H10-C8-O1	19	36	0	0	36
H10-C8-O2	20	0	12	1	13
H10-C8-O3	21	0	1	1	2
H10-C9	19	65	0	0	65
H10-C9-O2	21	0	5	3	8
H10-C10-O1	21	0	3	1	4
H10-C12-O6	28	0	2	1	3
H10-C13-O5	28	0	6	7	13
H11-Pt5	16	0	41	1334	1375
H11-Pt21	32	0	0	218	218
H11-O5-Pt12	28	0	249	8	257
H11-C4-O3-Pt41	59	0	33	17	50
H11-C4-O3-Pt42	60	0	69	17	86

H11-C4-O3-Pt43	61	0	91	49	140
H11-C4-O3-Pt44	62	0	63	0	63
H11-C5-O2-Pt44	62	0	53	0	53
H12-Pt16	28	0	2	126	128
H12-O5-Pt12	29	0	267	32	299
H12-C2-O4-Pt12	30	0	4	428	432
H12-C3-O6	21	0	20	63	83
H12-C4-O1	17	1	0	0	1
H12-C4-O2	18	7	0	0	7
H12-C5-O2-Pt43	62	0	63	28	91
H12-C6-O3	21	0	0	1	1
H12-C6-O6	24	5231	70	56	5357
H12-C7	19	8	0	0	8
H12-C7-O1	20	27	0	0	27
H12-C7-O2	21	46	0	0	46
H12-C7-O3	22	0	1	1	2
H12-C8	20	10	0	0	10
H12-C8-O1	21	28	0	0	28
H12-C8-O3	23	0	3	1	4
H12-C9	21	45	0	0	45
H12-C9-O1	22	0	7	2	9
H12-C10	22	0	4	1	5
H12-C12-O4	28	0	0	2	2
H12-C12-O6	30	0	2	0	2
H12-C13-O5	30	0	5	6	11
H12-C14-O4	30	0	16	5	21
H12-C15-O3	30	0	7	1	8
H13-Pt19	32	0	0	53	53
H13-O5-Pt12	30	0	244	8	252
H14-Pt16	30	0	1	53	54
H14-Pt17	31	0	0	165	165
H14-Pt18	32	0	0	138	138
H14-O7	21	0	1	756	757
H14-C4-O4	22	0	8	0	8
H14-C4-O4-Pt64	86	0	510	86	596
H14-C7-O3	24	0	1	0	1
H14-C8	22	2	0	0	2
H14-C8-O1	23	1	0	0	1
H14-C8-O2	24	0	3	1	4
H14-C8-O3	25	0	1	0	1
H14-C9	23	54	0	0	54
H14-C10-O4	28	0	1	0	1
H14-C12-O6	32	0	4	0	4
H14-C13-O5	32	0	7	1	8

H14-C14-O4	32	0	2	2	4
H14-C15-O3	32	0	7	14	21
H14-C16-O2	32	0	5	6	11
H15-Pt6	21	0	650	0	650
H15-Pt16	31	0	1	254	255
H15-Pt17	32	0	0	257	257
H16-Pt5	21	0	950	58	1008
H16-Pt16	32	0	1	507	508
H16-O8	24	0	14	3911	3925
H16-C7-O1	24	1	0	0	1
H16-C8-O1	25	38	0	0	38
H16-C8-O2	26	0	5	0	5
H16-C9	25	18	0	0	18
H16-C10	26	2	0	0	2
H16-C10-O1	27	0	2	0	2
H16-C13-O5	34	0	13	1	14
H16-C14-O4	34	0	18	4	22
H16-C16-O2	34	0	2	3	5
H16-C17-O1	34	0	6	3	9
H16-C18	34	0	3	0	3
H17-Pt15	32	0	0	140	140
H18-Pt13	31	0	0	80	80
H18-C6-O4-Pt52	80	0	43	34	77
H18-C6-O6-Pt52	82	0	41	44	85
H18-C9	27	1	0	0	1
H18-C9-O5	32	0	1	0	1
H18-C10	28	0	3	0	3
H18-C13-O5	36	0	3	0	3
H18-C14-O4	36	0	10	2	12
H18-C15-O3	36	0	21	3	24
H18-C16-O2	36	0	4	1	5
H19-Pt13	32	0	0	64	64
H20-C2-Pt32	54	0	63	0	63
H20-C6-O4-Pt52	82	0	41	42	83
H20-C13-O5	38	0	1	0	1
H20-C14-O4	38	0	2	0	2
H20-C15-O3	38	0	4	1	5
H20-C16-O2	38	0	19	0	19
H22-C14-O4	40	0	1	2	3
H22-C17-O1	40	0	4	2	6
H22-C18	40	0	7	2	9
H23-Pt8	31	0	255	85	340
H23-Pt9	32	0	234	132	366
H23-O11-Pt16	50	0	145	1855	2000

H24-Pt8	32	0	62	113	175
H24-O11-Pt16	51	0	83	914	997
H24-C12-O12	48	1	0	0	1
H24-C16-O2	42	0	5	0	5
H25-O11-Pt16	52	0	52	746	798
H30-O15	45	124	4	94	222
H32-C1-O18-Pt32	83	0	166	647	813
H32-C1-O18-Pt36	87	0	2	17	19
H32-C1-O19-Pt35	87	0	16	131	147
H32-C2-O16-Pt35	85	0	17	174	191
H32-C2-O16-Pt36	86	0	8	192	200
H32-C2-O17-Pt35	86	0	27	92	119
H32-C2-O20-Pt36	90	0	6	140	146
H33-C1-O17-Pt36	87	0	1	18	19
H33-C1-O18-Pt35	87	0	27	162	189
H34-C1-O17-Pt35	87	0	23	111	134
H36-C2-O17-Pt35	90	0	0	32	32
H38-C2-O17-Pt35	92	0	0	38	38
H45-O22-Pt32	99	0	350	0	350
H48-O24-Pt24	96	0	14	104	118
H52-O22-Pt32	106	0	765	0	765
H67-O32-Pt48	147	0	0	2	2
H70-O32-Pt48	150	0	0	11	11
H78-O32-Pt48	158	0	1	70	71
H80-O32-Pt48	160	0	0	72	72
H81-C1-O42-Pt64	188	0	193	0	193
H84-O50-Pt62	196	0	0	51	51
H84-O50-Pt64	198	0	0	56	56
H84-C1-O45-Pt64	194	0	372	9	381
H84-C2-O50-Pt62	198	0	0	90	90
H84-C2-O50-Pt64	200	0	24	13	37
H84-C4-O47-Pt64	199	0	0	9	9
H88-C3-O52-Pt62	205	0	15	9	24
H88-C3-O52-Pt64	207	0	27	9	36
H91-C4-O54-Pt64	213	0	0	63	63
H92-C3-O53-Pt62	210	0	0	44	44
H92-C3-O53-Pt64	212	0	2	33	35
H94-C3-O54-Pt64	215	0	1	9	10
H94-C4-O54-Pt64	216	0	0	107	107
H98-O44-Pt64	206	0	127	0	127
total	--	18667	38903	22154	79724

3. Calculation setups for DFT calculation

All DFT calculations were carried out by Vienna ab initio simulation package (VASP)[10] with the projected augmented wave (PAW) potential to represent electron-ion interaction. A Perdew-Burke-Ernzerhof (PBE) exchange and correlation functional was employed within generalized gradient approximation (GGA).[11] For Pt initial cell optimization, the plane-wave basis set cutoff was 500 eV and the Monkhorst-Pack scheme in Brillouin zone *k*-point sampling was 40 times compared to the reciprocal lattice vectors. In other surface calculations, the cutoff was 450 eV and *k*-point was set to 25 times. The energy and force convergence were uniformly set to 5×10^{-6} eV and 0.01 eV/ in all calculations.

4. Structural information of the most stable IS and TS from SSW-NN global optimization for all reactions investigated

Table S2. Structural information of the most stable IS and TS from SSW-NN global optimization for all reactions investigated. The most stable TS structure is obtained by SSW-NN global optimization with constrained C–O_a distance. Listed data include the CO coverage (ML), O/OH coverage (ML), CO site and O/OH. The notation b: bridge, h: hollow, t: top site. Reaction 1-4 refer to CO+O (g), CO+OH (g), CO+O (aq), CO+OH (aq) in the main text, Reaction 5-6 are CO+O (g) at two high coverages; Reaction 7 is CO+OH (aq) at a high coverage.

Reaction	CO coverage	O/OH coverage	CO site		O/OH site	
			IS	TS	IS	TS
1	0.11	0.11	h	t	h	b
2	0.11	0.11	h	t	b	t
3	0.06	0.06	b	t	h	b
4	0.06	0.06	h	t	t	t
5	0.25	0.25	t	t	h	b
6	0.50	0.25	h t	t t	h	b
7	0.25	0.06	h h h b	t h h b	t	t

5. Benchmark of G-NN against DFT calculations

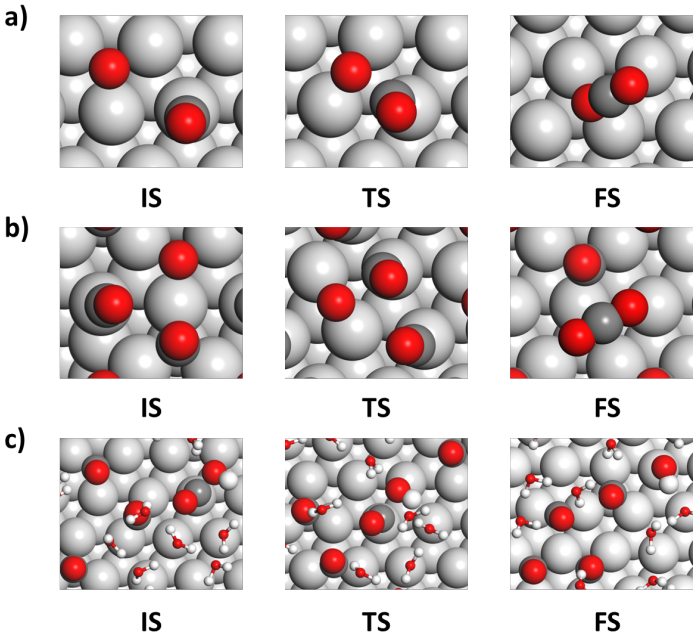
Table S3. Benchmark of G-NN against DFT calculations for four reactions investigated in this work. Listed data includes the structure, total atom number per cell (N_{atom}), NN energy (E_{NN}), DFT energy (E_{DFT}) and energy differences between DFT energy and NN energy (E_{diff}) in the unit of eV and meV/atom. For each reaction, five data are utilized for comparison: IS and TS from Table S2; MD_1 to MD_3 taken randomly from US MD simulation.

Structure	N_{atom}	E_{NN}(eV/cell)	E_{DFT}(eV/cell)	E_{NN-DFT} (eV)	E_{Diff}(meV/atom)
IS	39	-230.306	-230.386	0.0807	2.069
TS	39	-229.333	-229.397	0.0640	1.641
MD_1	39	-229.500	-229.554	0.0540	1.385
MD_2	39	-229.634	-229.682	0.0481	1.233
MD_3	39	-229.272	-229.289	0.0175	0.449
IS	40	-234.299	-234.369	0.0699	1.748
TS	40	-233.939	-233.982	0.0433	1.082
MD_1	40	-233.433	-233.405	-0.0284	-0.710
MD_2	40	-233.159	-233.180	0.0206	0.516
MD_3	40	-233.606	-233.587	-0.0182	-0.456
IS	187	-983.757	-983.758	0.0002	0.001
TS	187	-982.821	-982.737	-0.0836	-0.447
MD_1	187	-977.313	-977.354	0.0409	0.219
MD_2	187	-976.678	-976.564	-0.1139	-0.609
MD_3	187	-977.369	-977.397	0.0276	0.148
IS	188	-987.975	-987.842	-0.1326	-0.705
TS	188	-987.012	-986.813	-0.1993	-1.060
MD_1	188	-982.11	-981.993	-0.1162	-0.618
MD_2	188	-980.01	-980.041	0.0312	0.166
MD_3	188	-981.48	-981.477	-0.0032	-0.017

* Mean error between DFT energy and NN energy is 0.961 meV/atom.

6. Reaction snapshots for reactions at high coverages

Figure S1. Reaction snapshots, including IS, TS and FS, from MD simulations. (a) CO+O(g) at 0.25 (1/4) ML CO and 0.25 ML O coverage. (b) CO+O(g) at 0.50 (1/2) ML CO and 0.25 O ML coverage. (c) CO+OH(aq) at 0.25 (1/4) ML CO and 0.06 (1/16) ML OH coverage. In (c) only the first layer water is shown for clarity. Atom representation scheme: big grey ball: Pt; small grey ball: C; red ball: O; white ball: H.



7. Free energy barriers from five US MD runs for different reactions

Table S4. The free energy barriers (eV) versus temperature (K) for 5 US MD runs. Reaction 1-7 is the same as Table S2.

Temperature	G_{a1}	G_{a2}	G_{a3}	G_{a4}	G_{a5}	Average
Reaction 1						
300	0.988	0.920	0.977	0.928	0.971	0.957
350	0.997	0.981	1.018	0.923	0.929	0.970
400	0.990	0.911	1.029	1.015	0.952	0.979
450	1.044	1.007	0.990	1.005	1.008	1.011
500	0.985	1.004	1.000	0.984	0.977	0.990
Reaction 2						
300	0.439	0.465	0.470	0.479	0.467	0.464
350	0.501	0.460	0.471	0.535	0.456	0.485
400	0.530	0.483	0.482	0.512	0.487	0.499
450	0.532	0.533	0.504	0.493	0.538	0.520
500	0.498	0.506	0.575	0.488	0.550	0.523
Reaction 3						
300	0.912	0.909	0.918	0.907	0.925	0.914
340	0.889	0.900	0.892	0.907	0.885	0.895
380	0.905	0.913	0.886	0.913	0.919	0.907
Reaction 4						
300	0.767	0.753	0.769	0.763	0.752	0.761
340	0.747	0.764	0.778	0.756	0.774	0.764
380	0.737	0.745	0.727	0.729	0.761	0.740
Reaction 5						
300	0.746	0.747	0.728	0.727	0.776	0.745
350	0.754	0.731	0.714	0.763	0.760	0.745
400	0.746	0.722	0.749	0.704	0.721	0.729
450	0.759	0.653	0.731	0.718	0.727	0.717
500	0.708	0.716	0.681	0.715	0.741	0.712
Reaction 6						
300	0.519	0.435	0.472	0.416	0.460	0.461
350	0.455	0.501	0.481	0.448	0.473	0.472
400	0.518	0.517	0.455	0.528	0.517	0.507
450	0.463	0.494	0.544	0.453	0.460	0.483

500	0.507	0.473	0.489	0.498	0.551	0.504
			Reaction 7			
300	0.660	0.646	0.658	0.648	0.645	0.651

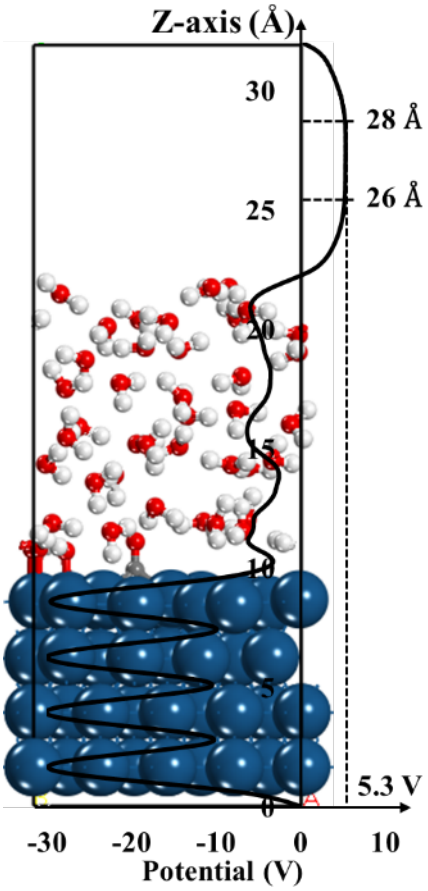
8. Vibrational frequencies for all reactions at the IS and TS

Table S5. Vibrational frequencies of reactions (zero K) calculated using the finite-difference method. Reaction 1-4 is the same as Table S2. Only the reacting atoms, *i.e.* CO+O (three atoms) and CO+OH (four atoms), are considered in the vibrational frequency calculations.

Mode	Frequency (cm^{-1})	Mode	Frequency(cm^{-1})	Mode	Frequency(cm^{-1})	Mode	Frequency(cm^{-1})
	Reaction 1				Reaction 3		
	IS		TS		IS		TS
1	1755.762	1	1978.382	1	1802.709	1	1945.782
2	410.2712	2	537.3907	2	423.8594	2	528.2637
3	375.7037	3	438.3887	3	414.3608	3	429.6135
4	374.8575	4	415.2197	4	386.4184	4	413.464
5	349.3218	5	317.2912	5	369.7458	5	320.0278
6	315.1153	6	308.5361	6	354.8447	6	293.5993
7	312.8553	7	157.6546	7	340.383	7	145.6499
8	182.7912	8	70.17999	8	210.617	8	82.46181
9	175.2133	9	-321.3488	9	80.06189	9	-322.9385
	Reaction 2				Reaction 4		
	IS		TS		IS		TS
1	3588.6	1	3633.998	1	3478.756	1	3286.028
2	1724.353	2	1950.822	2	1706.094	2	1839.966
3	758.5729	3	851.6303	3	1050.834	3	1022.805
4	699.7699	4	604.1073	4	703.981	4	891.1954
5	369.0914	5	534.6696	5	432.781	5	583.5844
6	362.2211	6	413.9605	6	361.9817	6	437.2186
7	351.2438	7	388.2487	7	355.5973	7	384.8151
8	305.192	8	313.2065	8	338.1487	8	331.1855
9	207.3558	9	149.2427	9	286.9582	9	214.0382
10	192.2998	10	127.9912	10	244.2128	10	160.0922
11	183.7685	11	74.18606	11	183.8395	11	70.14248
12	166.1139	12	-242.5571	12	178.7508	12	-253.3344

9. Electrochemical potential for CO+OH(aq) reaction on Pt(111)

Figure S2. The electrostatic potential along *z* axis of the slab (black curve) with reference to the Fermi level averaged from 50 snapshots from the MD simulation of the IS of the CO+OH(aq) reaction. The electrochemical potential is thus calculated to be 0.7 V vs. RHE (5.3 - 4.6 = 0.7 V). The snapshot of a representative IS structure is shown as the background.



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10. XYZ coordinates for key reaction states

IS for CO+O (g)

Sample POSCAR

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0.000000000000	0.000000000000	21.881900000000

C O Pt

1 2 36

Cart

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TS for CO+O(g)

Sample POSCAR

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8.428600000000	0.000000000000	0.000000000000
-4.214300000000	7.299381718338	0.000000000000
0.000000000000	0.000000000000	21.881900000000

C	O	Pt
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Cart

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IS for CO+OH(g)
Sample POSCAR
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H C O Pt
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Cart
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-2.809530998000 6.488342174000 3.798738174000
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5.619072788000 1.622085591000 3.798738174000
2.809537932000 6.488342174000 3.798738174000

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1.385961716000	7.286567052000	8.391760933000
2.768557472000	4.878484830000	8.465874522000
4.206146511000	2.388334787000	8.465453146000
4.180211763000	7.288784637000	8.364015921000
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-0.029671602000	4.869850669000	8.386551294000
6.999548174000	2.406148289000	8.363677053000
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TS for CO+OH(g)

Sample POSCAR

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-4.214300000000	7.299381718338	0.000000000000
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H	C	O	Pt
1	1	2	36

Cart

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-1.404768824000	2.433131536000	1.504762825000
5.619069818000	0.000000089000	1.504762825000
2.809534962000	4.866256671000	1.504762825000
4.214300105000	2.433131536000	1.504762825000
2.809538748000	0.000000089000	1.504762825000
0.000003891000	4.866256671000	1.504762825000
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1.404765216000 4.055217038000 3.798738174000
0.000003859000 1.622085591000 3.798738174000
-2.809530998000 6.488342174000 3.798738174000
-1.404765854000 4.055217038000 3.798738174000
5.619072788000 1.622085591000 3.798738174000
2.809537932000 6.488342174000 3.798738174000
4.214303075000 4.055217038000 3.798738174000
2.814473282000 3.249907410000 6.090989504000
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1.396357964000 0.820875627000 6.093755196000
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4.215301530000 0.833375146000 6.105903392000
7.015548436000 0.809706876000 6.078474008000
4.205604400000 5.675530443000 6.080079866000
1.391568500000 7.301571323000 8.406938465000
2.795479712000 4.856936912000 8.514550811000
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-4.245967545000 7.273253628000 8.391152681000
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IS for CO+O(aq)
Sample POSCAR
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0.000000000000 9.732500000000 0.000000000000
0.000000000000 0.000000000000 32.022000000000
H C O Pt
80 1 42 64
Cart
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1.837616924000 6.476979048000 18.680242028000
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9.612565200000 6.994551143000 15.391098329000
1.744406749000 0.365643308000 17.887793721000
10.472799744000 5.449996465000 16.740670759000

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1.384960716000	2.798815805000	19.026875164000
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8.988340504000	0.532163480000	19.363035397000
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0.223629991000	3.377825501000	15.297266545000
2.584865230000	8.024497437000	17.222852417000
7.167155176000	4.692313359000	17.997874860000
5.439626634000	9.621525838000	20.540504565000
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TS for CO+O(aq)
Sample POSCAR
1.000000000000
11.238100000000 0.000000000000 0.000000000000
0.000000000000 9.732500000000 0.000000000000
0.000000000000 0.000000000000 32.022000000000
H C O Pt
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Cart
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5.521093864000	0.578360742000	10.879599089000
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0.000000889000	0.000000089000	1.624791635000
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8.427758840000	3.258283824000	6.203209221000
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8.461001704000	4.870865797000	8.576336354000
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IS for CO+OH(aq)

Sample POSCAR

1.000000000000

11.238100000000	0.000000000000	0.000000000000
0.000000000000	9.732500000000	0.000000000000
0.000000000000	0.000000000000	32.022000000000

H C O Pt

Cart

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1.387703491000	0.872269864000	20.632180839000
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5.276949269000	0.395677754000	15.012344110000
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6.888349533000	2.385190716000	20.834105766000
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7.977355562000	7.530771930000	12.428747877000
9.958015823000	0.070805549000	15.211733712000
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9.833371162000	2.433128119000	1.624791622000
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2.799796721000	3.287957556000	6.211557400000
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8.420700641000	3.284611968000	6.179228769000
8.419611164000	8.150851881000	6.164859310000
9.848555443000	0.831001363000	6.206204438000
9.844322003000	5.701823202000	6.204555531000
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8.399095623000	4.944405303000	8.500536969000
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TS for CO+OH(aq)

Sample POSCAR

1.000000000000

11.238100000000	0.000000000000	0.000000000000
0.000000000000	9.732500000000	0.000000000000
0.000000000000	0.000000000000	32.022000000000

H	C	O	Pt
81	1	42	64

Cart

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7.586192771000	5.568765596000	16.865067160000
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