Supplementary Material

Automated Search for Optimal Surface Phases in Grand Canonical Ensemble Powered by Machine Learning

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1. The architecture of global neural network potential

Scheme S1. Scheme of the HDNN architecture. The subscripts \((1, i, \ldots, N)\) 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 \(\{E_i, F_i, S_i\}\), i.e., energies, forces, and stresses. The overall properties, \(E_{\text{tot}}, F_{\text{tot}},\) and \(S_{\text{tot}}\), 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 \(E_{\text{tot}}\) of the structure can be composed as a linear combination of its atomic energy \(E_i\) from the output of NN

\[
E_{\text{tot}} = \sum_i E_i \tag{S1}
\]

Consistently, the atomic force can be analytically derived from the total energy, i.e., the force component \(F_{k,\alpha}\) (\(\alpha = x, y,\) or \(z\)) acting on atom \(k\) is the derivative of the total energy \(E_{\text{tot}}\) 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 \(i, G_{ji}\)

\[
F_{k,\alpha} = -\frac{\partial E_{\text{tot}}}{\partial R_{k,\alpha}} = -\sum_{i,j} \frac{\partial E_i}{\partial G_{ji}} \frac{\partial G_{ji}}{\partial R_{k,\alpha}} \tag{S2}
\]

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

\[
\sigma_{\alpha\beta} = -\frac{1}{V} \sum_{i,j,d} \frac{(r_d)_\alpha (r_d)_\beta}{r_d} \frac{\partial E_i}{\partial G_{ji}} \frac{\partial G_{ji}}{\partial r_d} \tag{S3}
\]

where \(r_d\) and \(r_d\) are the distance vector, constituted by \(G_{ji}\) and its module, respectively, and \(V\) is the volume of the structure.
2. SSW-NN simulation

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, \(R^n\) to a high energy configuration \(R'^{H}\) 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 \(N^n\) that defines the walking direction.

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

In the equation \(R\) is the current coordination vector of the structure and \(V_{\text{real}}\) represents the unmodified PES; \(R^n\) 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, \(\sim 4\) orders of magnitude faster than DFT.\(^1,3\) In our SSW-NN simulation for the surface oxides on Ag metal, the van der Waals correction was amended on G-NN PES by using D3 method with zero damping,\(^10,11\) since it is important for accurately describing the behaviors of Ag surface oxides.\(^12\)
2.3 Dataset generation and training of the initial Ag-C-H-O G-NN

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).

Before the ASOP simulation, an Ag-C-H-O G-NN potential is available from LASP G-NN library\(^1\). Now 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 Ag-C-H-O global dataset contains a variety of structural patterns 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 Ag-C-H-O potential. Listed data are the number of the structures in the global dataset, as distinguished by the chemical formula, the number of atoms (Natoms), the type of structures (cluster, bulk, layer) and its total number (Ntotal).

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3. DFT calculations

All DFT calculations are performed using the plane-wave VASP package.\textsuperscript{14} The kinetic energy cutoff was set as 450 eV, the electron-ion interaction was represented by the projector-augmented wave (PAW) pseudopotential, and the exchange functional was evaluated with the GGA-PBE.\textsuperscript{15} The Monkhorst−Pack k-mesh was 30 times the reciprocal lattice vectors (1/30 Å\textsuperscript{-1}) for optimization, and was 40 times the reciprocal lattice vectors (1/40 Å\textsuperscript{-1}) for single point calculations based on the optimized geometry, where the final energy is obtained. For all structures, the energy and force were converged to less than 10\textsuperscript{-6} eV and 0.05 eV/Å. The van der Waals interaction was considered by using DFT-D3 method with zero damping.\textsuperscript{10,11}
4. The Gibbs free energy computation

In this work, $\mu_{Ag}$ is set as the energy of a Ag atom in bulk silver.

For $\mu_O$, it can be calculated from the thermodynamics equation as

$$\mu_O(T,p) = (\mu_{O_2}(T,p^0=1\text{bar}) + k_B T \ln(P_{O_2}/p^0)) / 2$$

where $\mu_{O_2}(T,p^0)$ is the zero reference state of $\mu_{O_2}$. To avoid the use of DFT energy of spin-polarized O$_2$ molecule, the standard molar enthalpy of formation of Ag$_2$O (at 298.15 K, $\Delta_f H_m(\text{Ag}_2\text{O}) = -0.323$ eV$^{16}$) is then used to determine the $\mu_{O_2}$:

$$\mu_{O_2}(T,p^0) = (H(\text{Ag}_2\text{O}) - 2H(\text{Ag}) - \Delta_f H_m(\text{Ag}_2\text{O} \times 2 + \Delta \mu_{O_2}(T,p^0)$$

where $H(\text{Ag}_2\text{O})$ and $H(\text{Ag})$ is the enthalpy of bulk Ag$_2$O and Ag on 298.15 K, which can be approximated as the ZPE corrected total energies of a Ag$_2$O and Ag atom in bulk. $\Delta \mu_{O_2}(T,p^0)$ item is the chemical potential variation of 1 bar O$_2$ from 298.15 K (in enthalpy) to T (in free energy), as obtained to be -1.08 eV by thermodynamic equations under typical ethylene epoxidation condition, $T = 500$ K and 1 bar of O$_2$. 
5. **The benchmark of G-NN potential against DFT**

Table S2. Benchmark of G-NN potential against DFT for the calculated $\gamma$ values of 30 low energy surface oxides on Ag(111). Listed data are the stoichiometry of the structure, the $A$ value of its surface periodicity, the total number of atoms ($N_{\text{atoms}}$), the energies in NN ($E_{\text{NN}}$) and DFT ($E_{\text{DFT}}$) level, and the difference of NN and DFT energies ($E_{\text{NN-DFT}}$) in the unit of eV and meV/atom.

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<th>$E_{\text{DFT}}$ (eV)</th>
<th>$E_{\text{NN-DFT}}$ (eV)</th>
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**Table S3.** Benchmark of G-NN potential against DFT for the calculated $\gamma$ values of 30 low energy surface oxides on Ag(100). Listed data are the stoichiometry of the structure, the $A$ value of its surface periodicity, the total number of atoms ($N_{\text{atoms}}$), the energies in NN ($E_{\text{NN}}$) and DFT ($E_{\text{DFT}}$) level, and the difference of NN and DFT energies ($E_{\text{NN-DFT}}$) in the unit of eV and meV/atom.

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The benchmark of G-NN potential against DFT is conducted by comparing the $\gamma$ values of low energy 30 surface oxides on Ag(111) and Ag(100) with those calculated by DFT. The data can be found in Table S2 and S3, in which the maximum and root mean square (RMS) errors for the energy of surface oxides on Ag(111) are 5.327 and 2.627 meV/atom, while that on Ag(100) are 5.342 and 2.635 meV/atom, respectively.
6. The PES contour map construction

To construct the PES map, we utilized the Gaussian smearing method to map discrete grid points to a continuous contour plot. This is demonstrated in the following for Ag(111). Figure S1 left shows the data obtained from the phase database after the ASOP simulation, where each point corresponds to one composition with the specified Ag and O coverage and the color represents its $\gamma$ value (the lowest $\gamma$ value of the composition from the phase database). For each point, a Gaussian smearing with $\sigma=0.1$ (0.1 ML) is conducted for 2D-interpolation, see Eq. (9) in the main text. This will yield the smeared value for neighboring grid points. The final $\gamma$ value for each point is then obtained using Eq. (8) in the main text, i.e. the lowest value from all smeared values at this point.

By this method, the $\gamma$ value for local minima will not be affected and the value for other neighboring points may be reduced. To estimate the error of smearing, we have compared the $\gamma$ value of four compositions in the database (real) and in the PES map (smear), as shown in Figure S1. For the optimal phase (point 1) or the metastable phase locates in the high energy zone (point 2), both being local minima on PES, there are no errors after smearing. The smearing errors are present for the points adjacent to the local minima, such as point 3 and 4, where the smearing lowers their $\gamma$ values depending on the stability of the adjacent composition and the distance.

**Figure S1.** The process of PES smearing for surface oxides on Ag(111), which maps the discrete data from the phase database (left) to the contour pot (right, see also in Figure 4). The $\gamma$ values of four compositions (1 ~ 4) in the database (real) and in the smearing PES map (smear) are also listed for comparison.
7. The geometries of surface oxides with the increasing of O coverage

Table S4. The geometries of optimal surface oxides in A = 8 with the specified O coverage (from O1 to O8) on Ag(111) and Ag(100).

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$\text{Ag}_5\text{O}_6$ 0.750 ML  $\text{Ag}_7\text{O}_6$

$\text{Ag}_5\text{O}_7$ 0.875 ML  $\text{Ag}_2\text{O}_7$

$\text{Ag}_7\text{O}_8$ 1.000 ML  $\text{Ag}_7\text{O}_8$
References

8. XYZ coordinates for the stable silver surface oxides shown in Figure 4(b) and Figure 5(b)

Here, all of these structures are provided in VASP POSCAR format.

(1) Ag$_5$O$_4$ on (v7×v7)R19 of Ag(111)

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1.08948 7.54818 0.00000
-0.00000 -0.00000 25.09070
H C O Ag
0 0 4 37
D
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0.968018 0.034751 0.496270
0.985051 0.484182 0.485680
0.534633 0.468550 0.497653
0.125000 0.625000 0.119566
0.375001 0.875000 0.119566
0.000000 0.000000 0.119566
0.250000 0.250000 0.119566
0.500000 0.500000 0.119566
0.750000 0.750000 0.119566
0.625000 0.125000 0.119566
0.875000 0.375000 0.119566
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0.333332 0.666667 0.213368
0.583332 0.916667 0.213368
0.208332 0.041666 0.213368
0.458332 0.291666 0.213368
0.708332 0.541667 0.213368
0.958332 0.791667 0.213368
0.833332 0.166666 0.213368
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0.791032 0.959577 0.307717
0.541254 0.705558 0.306969
0.294556 0.458748 0.306541
0.418544 0.083401 0.306541
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0.916562 0.581461 0.306504
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0.880505 0.378681 0.403851
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0.252269 0.249863 0.398302
0.372582 0.871220 0.398076
0.954254 0.760545 0.493665
(2) \( \text{Ag}_{10}\text{O}_9 \) on \( (2\sqrt{7} \times \sqrt{7})R19 \) of Ag(111)

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2.17534 15.07122 0.00000
-0.00000 -0.00000 25.04880

H C O Ag
0 0 9 74

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0.029477 0.986056 0.498553
0.007606 0.261489 0.491618
0.483156 0.779003 0.493006
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(3) Ag$_{12}$O$_6$ on p(4×4) of Ag(111)

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-0.000000 -0.000000 25.090700

H  C  O  Ag
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D
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0.998752  0.428082  0.489085
0.676531  0.751898  0.488712
0.321744  0.073870  0.489662
0.620660  0.373400  0.523687
0.998995  0.130600  0.523422
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0.250001  0.000000  0.119566
0.500001  0.000000  0.119566
0.750002  0.000000  0.119566
0.000000  0.250001  0.119566
0.250001  0.250001  0.119566
0.500001  0.250001  0.119566
0.750002  0.250001  0.119566
0.000000  0.500001  0.119566
0.250001  0.500001  0.119566
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0.750002  0.500001  0.119566
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0.500001  0.750002  0.119566
0.750002  0.750002  0.119566
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0.083532  0.667595  0.215308
0.332534  0.666975  0.213914
0.584292  0.667249  0.213889
0.833794  0.666708  0.215319
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| 0.417150 | 0.584336 | 0.305891 |
| 0.666588 | 0.584627 | 0.308249 |
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| 0.166580 | 0.835334 | 0.309222 |
| 0.415701 | 0.834428 | 0.306755 |
| 0.668248 | 0.835170 | 0.307052 |
| 0.915313 | 0.832706 | 0.309283 |
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| 0.249983 | 0.000644 | 0.403070 |
| 0.500616 | 0.999169 | 0.400003 |
| 0.752511 | 0.004396 | 0.399863 |
| 0.000505 | 0.250950 | 0.397493 |
| 0.247848 | 0.251983 | 0.400232 |
| 0.499676 | 0.251719 | 0.397528 |
| 0.747055 | 0.251294 | 0.399839 |
| 0.999806 | 0.500883 | 0.402623 |
| 0.252967 | 0.502997 | 0.399987 |
| 0.498867 | 0.498113 | 0.400119 |
| 0.750679 | 0.502194 | 0.402192 |
| 0.000098 | 0.750926 | 0.404610 |
| 0.249250 | 0.750958 | 0.402239 |
| 0.499656 | 0.750699 | 0.397712 |
| 0.750348 | 0.751429 | 0.402600 |
| 0.666513 | 0.568203 | 0.503309 |
| 0.422078 | 0.584381 | 0.493241 |
| 0.183043 | 0.601257 | 0.503038 |
| 0.165409 | 0.339596 | 0.493148 |
| 0.815660 | 0.419308 | 0.503504 |
| 0.576803 | 0.163845 | 0.492758 |
| 0.410864 | 0.328033 | 0.493280 |
| 0.148217 | 0.083917 | 0.504043 |
| 0.833592 | 0.174989 | 0.492673 |
| 0.332743 | 0.900525 | 0.503329 |
| 0.850029 | 0.935421 | 0.503315 |
| 0.588888 | 0.918741 | 0.492775 |

(4) $\text{Ag}_7\text{O}_5$ on $(2\sqrt{2} \times 2\sqrt{2})R45^\circ$ of Ag(100)
Structure
1.00000000
8.15300  0.00000  0.00000
-0.00000  8.15300  0.00000
-0.00000  -0.00000  24.14480
H    C    O    Ag
0    0    5    39
D
0.175264  0.253603  0.469880
0.502124  0.077399  0.469471
0.325450  0.750069  0.469893
0.750343  0.501762  0.514748
0.998494  0.926381  0.469855
0.000000  0.749996  0.124250
0.000000  0.249999  0.124250
0.249999  0.499998  0.124250
0.499998  0.749996  0.124250
0.249999  0.000000  0.124250
0.499998  0.249999  0.124250
0.749996  0.499998  0.124250
0.749996  0.000000  0.124250
0.000000  0.499998  0.208668
0.249999  0.749996  0.208668
0.000000  0.000000  0.208668
0.249999  0.249999  0.208668
0.499998  0.499998  0.208668
0.749996  0.749996  0.208668
0.499998  0.000000  0.208668
0.749996  0.249999  0.208668
0.499953  0.250521  0.294408
0.000186  0.250191  0.294421
0.499551  0.750689  0.294228
0.750060  0.500222  0.294454
0.249978  0.500279  0.294432
0.000411  0.750787  0.294299
0.250033  0.000301  0.294398
0.750016  0.000200  0.294391
0.250436  0.750140  0.378642
0.997378  0.506657  0.379674
0.756128  0.253905  0.379399
0.250388  0.002026  0.480583
0.250127  0.251834  0.378519
0.750421  0.002326  0.470205
0.936456  0.337421  0.483694
0.913198  0.688388  0.483813
0.500686  0.000632  0.378379
0.999659  0.000670  0.378478
0.744692  0.748191  0.379410
0.586695  0.315641  0.483402
0.564132  0.665821  0.483807
0.250460  0.501791  0.470471
(5) Ag$_3$O$_2$ on (2V2xV2)R45º of Ag(100)

Structure
1.00000000
4.07650 0.00000 0.00000
-0.00000 8.15300 0.00000
-0.00000 -0.00000 24.14480

H    C    O    Ag
0    0    2    19

D
0.999182 0.992528 0.479239
0.001144 0.506733 0.479283
0.000000 0.749996 0.124250
0.000000 0.249999 0.124250
0.499998 0.499998 0.124250
0.499998 0.000000 0.124250
0.000000 0.499998 0.208668
0.499998 0.749996 0.208668
0.000000 0.000000 0.208668
0.499998 0.249999 0.208668
0.500198 0.001471 0.294164
0.000230 0.749643 0.293334
0.000213 0.249756 0.295403
0.500278 0.498090 0.294173
0.499413 0.965271 0.469300
0.000999 0.996064 0.378565
0.000285 0.502525 0.378596
0.500121 0.249270 0.381447
0.000175 0.249388 0.473810
0.500548 0.535162 0.469789
0.500355 0.749204 0.376246