**A first-principles study on the electrochemical reaction activity of 3*d* transition metal single-atom catalysts in nitrogen-doped graphene: trends and hints**

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# Supporting information

# Reliability of data based on spin states

In the work of Lin et al. [1], a machine learning (ML) model was trained based on data from their previous work [2]. The spin states of single-atom catalysts (SACs) were not correctly treated in Ref. 2, resulting in the calculations yielding unreliable results in terms of physics. Consequently, the ML model in Ref. 1 was trained using the unreliable data from Ref. 2 and therefore is unconvincing.

According to Pauli’s Exclusion Principle, the magnetic moment should be determined by the unpaired electrons in the system. This is a basic principle in physics that one should obey, but the data in Ref. 2 does not. For example, as shown in Table S1, Fe supported on a single vacancy with three carbon atoms (FeC3-SV) has a magnetic moment of 1 in Ref. 2 (Table S1 and Table 34 in the supplementary materials of Ref. 2). Since the electron numbers of C and Fe in FeC3-SV are all even, the unpaired electrons (magnetic moment) should be even, rather than 1. This results in an incorrect ground state energy as well as free energy difference (). For example, FeC3-SV () and TcC3-SV () have outstanding HER performance in the study by Choi et al. [3], while the HER activity of Fe/TcC3-SV (Table S1 and Table 3 in the supplementary materials of Ref. 2) in the training data is relatively poor. The difference originates from the use of incorrect spin states, which can be proven by the following test calculation.

Based on Pauli’s Exclusion Principle, several spin states of each model were calculated, and the lowest energy one has been adopted. Following this protocol, the testing results match the ones in Ref. 3 well for FeC3-SV and TcC3-SV (Table S1). Keeping this fundamental principle in mind, it is easy to explain why our data (=0.71 V, =0.47 V, =0.49 V, =0.54 V) match the experimental observations [4,5] of ZnNx-G catalysts’ excellent ORR activity, but the data in Ref. 1 and 2 (=0.89 V, =1.44 V, =2.04 V, =1.33 V) do not. This also explains the large difference between the NiN4-G’s HER activity result in Ref. 2 ( = 0.22 eV) and an experimental result ( = 1.62 eV [6]), as well as the results in other theoretical studies ( = 1.20 eV [7], 1.35 eV [8], and 1.68 eV from our calculations).

**Table S1. The magnetic moment of a single metal atom supported on a single vacancy with three carbon atoms (MC3-SV) without adsorbates, and the adsorption free energy of H on the MC3-SV ().**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Metal | Magnetic moment |  | Reference | |
| FeC3-SV | 1 | -0.45 | Ref. 2 (UFe\_d= 3.29 eV) |
| 2 | 0.02 | Test (UFe\_d= 3.29 eV) | |
| 0 | 0.01 | Test (no U) | |
| - | 0.00 | Ref. 3 (no U) | |
| TcC3-SV | 1.99 | -0.37 | Ref. 2 | |
| 1 | -0.12 | Test | |
| - | -0.03 | Ref. 3 | |

# 2. Free energy calculation and machine learning method

## Free energy calculation

For the elementary reaction, the Gibbs free energy change () is estimated by the relation:

(S1)

where is the energy difference between products and reactants as obtained from calculation, *T* is room temperature (298.15 K), and and are the changes in the zero-point energy and entropy, respectively. The entropy for gas-phase molecules such as H2 can be obtained from the NIST database [9]. For adsorbed species, and are calculated using the following formulae:

(S2)

(S3)

where the characteristic vibrational temperature is equal to , and , , , , , and are the Planck constant, vibrational frequency, Boltzmann constant, vibrational entropy, gas constant, and temperature, respectively. In the frequency calculation, only the adsorbed atoms above the surface move, and the other atoms are fixed. We used the model proposed by Nørskov et al. [10], so the free energy of ) at , 298.15 K, and electrode potential was calculated using the free energy of 1/2 H2. Given that the free energy of gaseous water is equal to that of liquid water with a pressure of 0.035 bar at 298.15 K, gas-phase water at 0.035 bar was selected as the reference state. The free energy of O2 was obtained using , due to the poor description of the O2 high-spin ground state in DFT calculations [11].

The recommended PAW potentials in the VASP manual were applied (Table S2). To reduce the influence of different spin configurations on energy, several spin states were studied for each model. For example, on a pure CoN3-G surface, the energy with magnetic moments of 0, 2, and 4 was considered, as the total number of electrons was even. Then the lowest energy (mag = 0) was adopted (Table S3). Similarly, the energies of the multiple spin states of \*OOH, \*O, \*OH, and \*H systems were also considered, and the lowest one was selected for subsequent reaction calculations.

## Machine learning method

For the ML method, the eXtreme Gradient Boosting (XGBoost) algorithm [12] was adopted, and the ML models were achieved using the scikit-learn package [13]. The impact of each feature was investigated using the Gini importance method [14]. XGBoost is an ensemble of decision trees (DT) and has been dominating Kaggle competitions. In the Gradient Boosting DT, the new regression models were sequentially created and the residuals made by prior models were reduced. The predicted value was obtained using the weighted sum of each sub-model:

(S4)

in which *K* stands for the number of sub-models, stands for the input features, andrepresents the sub-models. All the hyper-parameters were optimized until the best results were found. Generally, different ML models possess different indices to evaluate their prediction accuracy. We employed three indices to evaluate the prediction accuracy: coefficient of determination (*R*2), mean squared error (MSE), and Pearson correlation coefficient (*r*).

*R*2 is used to evaluate the fitness between actual and predicted values and is defined as:

(S5)

in which *y* stands for the values calculated by DFT, stands for the values predicted by ML models, and is the average value. The closer *R*2 is to 1, the better the fit between the predicted and actual values.

The MSE stands for the degree of variance between actual and predicted values, given by:

(S6)

The Pearson coefficient () represents the linear correlation between actual and predicted values, defined as:

(S7)

where the value of *r* is between –1 and 1, and the closer the absolute value of *r* is to 1, the stronger the linear correlation.

Variance () is used to measure the degree of deviation between a set of data and its expected value:

(S8)

where represents the values calculated by DFT, and the average value is taken as zero here. A small value means that the data is close to the expected value.

# 3. Figures and tables

Background pattern

Description automatically generated

**Figure S1. Three configurations of MN2-G.** (a) MN21-G. (b) MN22-G. (c) MN23-G. The yellow, blue, and grey balls represent transition metal, nitrogen, and carbon atoms, respectively.

Chart, scatter chart

Description automatically generated

**Figure S2. Linear relationship of *vs.* , and the relationship between OER overpotential and ()** (a, c)before and(b, d)after removing the points with different rate-determining steps.

**Table S2. Recommended PAW potentials of each atom in the VASP manual.**

|  |  |  |
| --- | --- | --- |
| Atoms | Pseudopotential | Valency |
| H | H | 1 |
| C | C | 4 |
| N | N | 5 |
| O | O | 6 |
| Sc | Sc\_sv | 11 |
| Ti | Ti\_sv | 12 |
| V | V\_sv | 13 |
| Cr | Cr\_pv | 12 |
| Mn | Mn\_pv | 13 |
| Fe | Fe | 8 |
| Co | Co | 9 |
| Ni | Ni | 10 |
| Cu | Cu | 11 |
| Zn | Zn | 12 |

**Table S3. Magnetic moment () and corresponding electron energies (eV) for CoN3-G structure.**

|  |  |  |  |
| --- | --- | --- | --- |
| Systems | Mag | Energy | ∆E |
| surface | **0** | **-647.40040** | 0.00 |
| 2 | -647.36164 | 0.04 |
| 4 | -646.14484 | 1.26 |
| \*OOH | **1** | **-662.13582** | 0.00 |
| 3 | -661.68175 | 0.45 |
| 5 | -660.45910 | 1.68 |
| \*O | 0 | -652.60038 | 0.38 |
| **2** | **-652.97767** | 0.00 |
| 4 | -652.36725 | 0.61 |
| \*OH | **1** | **-657.73523** | 0.00 |
| 3 | -657.25351 | 0.48 |
| 5 | -656.15972 | 1.58 |
| \*H | **1** | **-650.94144** | 0.00 |
| 3 | -650.29511 | 0.65 |
| 5 | -648.07846 | 2.86 |

**Table S4. Calculated electronic energies (eV) of MN2-G structures.**

|  |  |  |  |
| --- | --- | --- | --- |
| Metal | MN21-G | MN22-G | MN23-G |
| Sc | -647.484 | -647.490 | -647.416 |
| Ti | -648.757 | -648.794 | -648.697 |
| V | -648.904 | -648.897 | -648.840 |
| Cr | -649.189 | -649.263 | -648.976 |
| Mn | -649.408 | -649.093 | -649.190 |
| Fe | -648.222 | -647.773 | -647.890 |
| Co | -647.230 | -646.811 | -646.913 |
| Ni | -646.468 | -645.941 | -646.046 |
| Cu | -643.988 | -643.378 | -643.665 |
| Zn | -640.399 | -640.618 | -640.142 |

**Table S5. Binding energies (, eV) and cohesive energies (, eV) of single metal atom on MNx-G systems.**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Metal |  | MN1-G | | MN2-G | | MN3-G | | MN4-G | |
|  |  |  |  |  |  |  |  |
| Sc | -4.36 | -7.69 | -3.33 | -7.66 | -3.30 | -8.93 | -4.57 | -8.39 | -4.04 |
| Ti | -5.48 | -8.66 | -3.18 | -8.47 | -2.99 | -8.97 | -3.49 | -8.39 | -2.91 |
| V | -5.41 | -8.31 | -2.90 | -7.97 | -2.56 | -8.64 | -3.23 | -8.31 | -2.90 |
| Cr | -4.06 | -7.35 | -3.29 | -7.02 | -2.96 | -7.92 | -3.86 | -7.92 | -3.86 |
| Mn | -3.70 | -6.54 | -2.84 | -6.33 | -2.63 | -6.93 | -3.23 | -6.59 | -2.89 |
| Fe | -4.86 | -7.10 | -2.24 | -6.92 | -2.06 | -7.42 | -2.56 | -7.22 | -2.36 |
| Co | -5.15 | -7.43 | -2.28 | -7.41 | -2.26 | -7.98 | -2.83 | -7.68 | -2.53 |
| Ni | -5.18 | -8.09 | -2.90 | -8.25 | -3.07 | -8.59 | -3.40 | -8.08 | -2.89 |
| Cu | -3.49 | -6.31 | -2.82 | -5.82 | -2.33 | -5.80 | -2.32 | -5.17 | -1.68 |
| Zn | -1.10 | -3.02 | -1.92 | -2.46 | -1.36 | -3.33 | -2.23 | -3.39 | -2.29 |

**Table S6. Zero-point energy and entropy correction of the reaction intermediate species in free energy calculation.**

|  |  |  |  |
| --- | --- | --- | --- |
| Species | *E* (eV) | (eV) | *TS* (eV) |
| H2O | -14.22 | 0.57 | 0.67 |
| H2 | -6.77 | 0.27 | 0.40 |
| OOH | -18.29 | 0.73 | 0.73 |
| OH | -10.84 | 0.43 | 0.47 |
| O | -7.45 | 0.30 | 0.27 |
| H | -3.39 | 0.13 | 0.20 |

**Table S7.** **Reaction free energies (, eV) of ORR and OER on MN1-G structures.**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Metal |  |  |  |  |  |  |  |  |
| Sc | -1.85 | -1.36 | -2.21 | 0.50 | -0.50 | 2.21 | 1.36 | 1.85 |
| Ti | -3.01 | -2.02 | -1.44 | 1.55 | -1.55 | 1.44 | 2.02 | 3.01 |
| V | -2.88 | -3.49 | -0.06 | 1.39 | -1.39 | 0.06 | 3.49 | 2.88 |
| Cr | -2.63 | -3.43 | 0.08 | 1.06 | -1.06 | -0.08 | 3.43 | 2.63 |
| Mn | -1.89 | -2.81 | -0.29 | 0.06 | -0.06 | 0.29 | 2.81 | 1.89 |
| Fe | -1.78 | -2.53 | -0.47 | -0.15 | 0.15 | 0.47 | 2.53 | 1.78 |
| Co | -1.23 | -2.21 | -0.97 | -0.51 | 0.51 | 0.97 | 2.21 | 1.23 |
| Ni | -0.38 | -3.87 | 0.82 | -1.49 | 1.49 | -0.82 | 3.87 | 0.38 |
| Cu | 0.27 | -3.30 | 0.50 | -2.38 | 2.38 | -0.50 | 3.30 | -0.27 |
| Zn | -0.52 | -0.88 | -2.34 | -1.18 | 1.18 | 2.34 | 0.88 | 0.52 |

**Table S8.** **Reaction free energies (, eV) of ORR and OER on MN2-G structures.**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Metal |  |  |  |  |  |  |  |  |
| Sc | -2.53 | -1.13 | -2.21 | 0.95 | -0.95 | 2.21 | 1.13 | 2.53 |
| Ti | -2.92 | -2.91 | -0.71 | 1.62 | -1.62 | 0.71 | 2.91 | 2.92 |
| V | -2.89 | -3.52 | -0.05 | 1.54 | -1.54 | 0.05 | 3.52 | 2.89 |
| Mn | -1.53 | -2.96 | -0.34 | -0.09 | 0.09 | 0.34 | 2.96 | 1.53 |
| Fe | -1.39 | -2.54 | -0.74 | -0.24 | 0.24 | 0.74 | 2.54 | 1.39 |
| Co | -1.06 | -2.09 | -1.11 | -0.67 | 0.67 | 1.11 | 2.09 | 1.06 |
| Ni | -0.18 | -1.28 | -1.71 | -1.74 | 1.74 | 1.71 | 1.28 | 0.18 |
| Cu | -0.12 | -0.78 | -2.30 | -1.72 | 1.72 | 2.30 | 0.78 | 0.12 |
| Zn | -0.76 | -0.93 | -2.40 | -0.84 | 0.84 | 2.40 | 0.93 | 0.76 |

**Table S9.** **Reaction free energies (, eV) of ORR and OER on MN3-G structures.**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Metal |  |  |  |  |  |  |  |  |
| Sc | -2.56 | -1.10 | -2.26 | 1.00 | -1.00 | 2.26 | 1.10 | 2.56 |
| Ti | -3.45 | -2.95 | -0.66 | 2.14 | -2.14 | 0.66 | 2.95 | 3.45 |
| V | -3.16 | -3.45 | -0.11 | 1.80 | -1.80 | 0.11 | 3.45 | 3.16 |
| Cr | -2.38 | -3.39 | 0.22 | 0.63 | -0.63 | -0.22 | 3.39 | 2.38 |
| Mn | -1.58 | -2.95 | -0.35 | -0.04 | 0.04 | 0.35 | 2.95 | 1.58 |
| Fe | -1.46 | -2.42 | -0.85 | -0.18 | 0.18 | 0.85 | 2.42 | 1.46 |
| Co | -1.02 | -2.02 | -1.05 | -0.84 | 0.84 | 1.05 | 2.02 | 1.02 |
| Ni | -0.25 | -1.02 | -2.05 | -1.61 | 1.61 | 2.05 | 1.02 | 0.25 |
| Cu | 0.03 | -0.70 | -2.29 | -1.96 | 1.96 | 2.29 | 0.70 | -0.03 |
| Zn | -0.74 | -0.93 | -2.39 | -0.85 | 0.85 | 2.39 | 0.93 | 0.74 |

**Table S10.** **Reaction free energies (, eV) of ORR and OER on MN4-G structures.**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Metal |  |  |  |  |  |  |  |  |
| Sc | -3.25 | -1.38 | -2.26 | 1.97 | -1.97 | 2.26 | 1.38 | 3.25 |
| Ti | -3.37 | -3.79 | 0.12 | 2.12 | -2.12 | -0.12 | 3.79 | 3.37 |
| Cr | -1.75 | -3.35 | -0.14 | 0.04 | -0.04 | 0.14 | 3.35 | 1.75 |
| Mn | -1.14 | -2.81 | -0.39 | -0.58 | 0.58 | 0.39 | 2.81 | 1.14 |
| Fe | -1.15 | -2.42 | -0.70 | -0.65 | 0.65 | 0.70 | 2.42 | 1.15 |
| Co | -0.81 | -1.48 | -1.56 | -1.07 | 1.07 | 1.56 | 1.48 | 0.81 |
| Ni | 0.12 | -0.95 | -1.96 | -2.14 | 2.14 | 1.96 | 0.95 | -0.12 |
| Cu | 0.05 | -0.82 | -2.20 | -1.96 | 1.96 | 2.20 | 0.82 | -0.05 |
| Zn | -0.69 | -0.86 | -2.49 | -0.89 | 0.89 | 2.49 | 0.86 | 0.69 |

**Table S11.** **Adsorption free energies of H (, eV) on MNx-G structures.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Metal | MN1-G | MN2-G | MN3-G | MN4-G |
| Sc | 1.05 | 0.57 | 0.53 | -0.43 |
| Ti | -0.07 | -0.11 | -0.63 | -0.58 |
| V | -0.14 | -0.17 | -0.32 | -0.20 |
| Cr | 0.05 | 0.10 | 0.10 | 0.24 |
| Mn | 0.36 | 0.36 | 0.26 | 0.38 |
| Fe | 0.25 | 0.24 | -0.10 | 0.27 |
| Co | -0.51 | -0.05 | 0.04 | 0.12 |
| Ni | -0.25 | 0.27 | 0.02 | 1.68 |
| Cu | 0.16 | 1.39 | -0.02 | 1.75 |
| Zn | 1.01 | 0.81 | 0.89 | 0.87 |

**Table S12.** **Overpotential of ORR (, V) on MNx-G structures.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Metal | MN1-G | MN2-G | MN3-G | MN4-G |
| Sc | 1.73 | 2.18 | 2.23 | 3.20 |
| Ti | 2.78 | 2.85 | 3.37 | 3.35 |
| V | 2.62 | 2.77 | 3.03 | - |
| Cr | 2.29 | - | 1.86 | 1.37 |
| Mn | 1.29 | 1.14 | 1.19 | 0.84 |
| Fe | 1.08 | 0.99 | 1.05 | 0.58 |
| Co | 0.72 | 0.56 | 0.39 | 0.42 |
| Ni | 2.05 | 1.05 | 0.98 | 1.35 |
| Cu | 1.73 | 1.11 | 1.26 | 1.28 |
| Zn | 0.71 | 0.47 | 0.49 | 0.54 |

**Table S13. Overpotential of OER (, V) on MNx-G structures.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Metal | MN1-G | MN2-G | MN3-G | MN4-G |
| Sc | 0.98 | 1.30 | 1.33 | 2.02 |
| Ti | 1.78 | 1.69 | 2.22 | 2.56 |
| V | 2.26 | 2.29 | 2.22 | - |
| Cr | 2.20 | - | 2.16 | 2.12 |
| Mn | 1.58 | 1.73 | 1.72 | 1.58 |
| Fe | 1.30 | 1.31 | 1.19 | 1.19 |
| Co | 0.98 | 0.86 | 0.79 | 0.33 |
| Ni | 2.64 | 0.51 | 0.82 | 0.91 |
| Cu | 2.07 | 1.07 | 1.06 | 0.97 |
| Zn | 1.11 | 1.17 | 1.16 | 1.26 |

**Table S14. Overpotential of HER (, V) on MNx-G structures.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Metal | MN1-G | MN2-G | MN3-G | MN4-G |
| Sc | -1.05 | -0.57 | -0.53 | -0.43 |
| Ti | -0.07 | -0.11 | -0.63 | -0.58 |
| V | -0.14 | -0.17 | -0.32 | -0.20 |
| Cr | -0.05 | -0.10 | -0.10 | -0.24 |
| Mn | -0.36 | -0.36 | -0.26 | -0.38 |
| Fe | -0.25 | -0.24 | -0.10 | -0.27 |
| Co | -0.51 | -0.05 | -0.04 | -0.12 |
| Ni | -0.25 | -0.27 | -0.02 | -1.68 |
| Cu | -0.16 | -1.39 | -0.02 | -1.75 |
| Zn | -1.01 | -0.82 | -0.89 | -0.87 |

**Table S15.** **Bader charge analysis of transition metal single atom (*Q*, e). The negative values indicate electron donation.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Metal | MN1-G | MN2-G | MN3-G | MN4-G |
| Sc | -1.69 | -1.71 | -1.77 | -1.81 |
| Ti | -1.65 | -1.68 | -1.58 | -1.54 |
| V | -1.48 | -1.43 | -1.43 | -1.42 |
| Cr | -1.18 | -1.24 | -1.30 | -1.34 |
| Mn | -1.24 | -1.25 | -1.35 | -1.36 |
| Fe | -1.02 | -1.06 | -1.08 | -1.09 |
| Co | -0.78 | -0.80 | -0.81 | -0.90 |
| Ni | -1.04 | -0.64 | -0.74 | -0.84 |
| Cu | -0.71 | -0.76 | -0.88 | -0.93 |
| Zn | -0.95 | -1.03 | -1.05 | -1.15 |

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