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Supporting Information

Unraveling Active Ensembles Consisting of Clusters and Single Atoms for Oxygen Reduction: A Synergy of Machine Learning and DFT Calculations

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Computational Details

CHE model

The ORR process is commonly be expressed as O_2 (g) + $2H_2O$ (l) + $4e^-$ →$4OH^-$; it is also summarized as the following electron steps (1)-(4) in alkaline conditions, where * refer to the active sites, and OH^*, O^*, and OOH^* represent the adsorbed intermediates. * + O_2 (g) + H_2O (l) + e^- → OOH^* + OH^- (1), OOH^* + e^-→ O^*+ OH^- (2), O^* + H_2O + e^- → OH^*+ OH^- (3), OH^* + e^-→ * + OH^- (4).

The Gibbs free energy value (ΔG) of each elementary step is calculated using the equation: $\Delta G = \Delta E + \Delta E_{ZPE} - T\Delta S + \Delta G_U + \Delta G_{pH}$. In this equation, ΔE represents the reaction energy, which is directly obtained from DFT calculations. ΔE_{ZPE} and ΔS are the changes in zero-point energy and entropy, respectively, and are derived from vibrational frequency calculations and standard thermodynamic data. $\Delta G_U = -eU$, where U is the applied potential. ΔG_{pH} accounts for the pH correction in the electrolyte and is computed as $\Delta G_{pH} = -kT\ln10\times pH$, with a pH value of 14 in this case. The Gibbs free energy of O_2 (G_{O2}) is calculated using the energies of H_2O and H_2, that is: $G_{O2} = G_{H2O} - 2G_{H2} + 4.92$ eV. The overpotential, used to assess the performance of ORR, is then determined by the following equations::

$$\eta^{ORR} = \Delta G^{max}/e + 1.23;$$

where ΔG represents the free energy changes of reaction (1-4), with 1.23 V corresponding to the equilibrium potential. A lower η value for a given catalyst indicates that less energy is required for ORR, thereby reflecting its higher catalytic activity for ORR.

Dissolution Potential

To evaluate the stability of the Pt_3M-M'NC ensemble, we computed the dissolution potentials (U_{diss}, V) of a metal single atom (M') in Pt_3M-M'NC, which is defined as: $U_{diss} = U^0_{M'} + \frac{\left[E_{M',bulk} - \left(E_{Pt_3M-M'NC} - E_{Pt_3M-NC}\right)\right]}{ne}$, where $U^0_{M'}$ is the standard dissolution potential of M' in the bulk form, $E_{Pt_3M-M'NC}$ and E_{Pt_3M-NC} are the total energies of Pt_3M-M'NC and Pt_3M-NC, n is the coefficient for the aqueous dissolution reaction: $M' + nH^+ \leftrightarrow M'^{n+} + H_2$.

Note 1 The calculation method for the distance between M'NC and the Pt_3M is based on the Cartesian coordinates of the M and M' atoms for candidates after structural relaxation.

Note 2 The 1521 catalysts consist of 39 single metals anchored on NC monolayers, forming 39 different substrate structures, categorized into four groups based on periodicity. These are: 4th period: ScNC, TiNC, VNC, CrNC, MnNC, FeNC, CoNC, NiNC, CuNC, ZnNC; 5th period: ZrNC, NbNC, MoNC, RuNC, RhNC, PdNC, AgNC; 6th period: HfNC, TaNC, WNC, ReNC, OsNC, IrNC, PtNC, AuNC, LaNC, CeNC, PrNC, NdNC, SmNC, EuNC, GdNC, TbNC, DyNC, HoNC, ErNC, TmNC, YbNC, LuNC. Moreover, in total, 39 distinct Pt_3M structures (where the selected metal is the same as the substrate single atom) are loaded onto 39 different substrates, forming 39 × 39 = 1521 catalyst configurations. For example, when M is Fe and M' is Co, the catalyst is defined as Pt_3Fe-CoNC.

Machine learning

```
import numpy as np

import pandas as pd

from sklearn.utils import shuffle

from sklearn.model_selection import cross_val_score, ShuffleSplit

from sklearn.metrics import mean_squared_error as mse

from sklearn.metrics import r2_score

from sklearn.model_selection import train_test_split

from sklearn.model_selection import train_test_split

from sklearn.preprocessing import MinMaxScaler

from sklearn.ensemble import GradientBoostingRegressor as GBR
```

GBR model

Machine learning (ML) is based on the gradient-boosted regression (GBR) algorithm. The training set D = $\{(x_1, y_1), (x_2, y_2), \ldots(x_n, y_n)\}$ is divided into J disjoint parts, where J is the number of leaf nodes in every regression tree. To minimize the loss function L, the decision tree parameter θ_m is defined as:

$$\theta_m = argmin_\theta \sum_{i=1}^{n} L(y_i, f_{m-1}(x_i) + t_m(x_i))$$

Where $t_m(x), f_{m-1}(x)$ is the m_{th} and the $(m\text{-}1)_{th}$ regression tree function after iterations. The GRB training process is summarized by four steps: (1) initializing a regression tree

function $argmin_{\theta}\sum_{i=1}^{n}L(y_i,c)$ where c is a constant number. (2) Calculate the negative gradient of the loss function as the estimated residual value r_{mi} = -$[\partial L(y_i,f(x_i)/\partial f(x_i)]_{f(x)=f_{m-1}(x)}$. (3) Use the new data set(x_i, r_{mi}) to obtain the updated regression tree function $f_m(x)$. (4) Repeat steps (2) and (3) to reach the final regression model, which is determined by:

$$f_M(x)=\sum_{m-1}^{M}t(x;\theta m)$$

Matlab Code:

```
clc;

clear;

close all;

data = readtable('pre1.csv');

X = table2array(data(:, 1:end-1));

y = table2array(data(:, end));

[X, mu, sigma] = zscore(X);

X_poly = [X, X.^2, X.^3, X.^4, X(:, 3).^2.*X(:, 4).^2, X(:, 4).^2.*X(:, 2).^2, X(:, 3).*X(:,

2),    X(:, 3).*X(:, 2).^2, X(:, 3).*X(:, 2).^3];

mdl_poly = fitlm(X_poly, y);

y_pred_poly = predict(mdl_poly, X_poly);

r_squared_poly = 1 - sum((y - y_pred_poly).^2) / sum((y - mean(y)).^2);
```

```
disp([num2str(r_squared_poly)]);

figure;

scatter(y, y_pred_poly, 'filled');

xlabel('actual value');

ylabel('estimated value');

title('xx');

grid on;

hold on;

plot([min(y), max(y)], [min(y), max(y)], 'r--', 'LineWidth', 2);

legend('estimated value vs. actual value', ' ideal angle ');

hold off;

figure;

plot(y, 'b-', 'LineWidth', 2);

hold on;

plot(y_pred_poly, 'r--', 'LineWidth', 2);

xlabel('index');

ylabel('value');

title('xx');

legend('actual value', 'estimated value');

grid on;

hold off;
```

% Coefficients of the extraction model

coefficients = mdl_poly.Coefficients.Estimate;

The precise mathematical relationship is : $Y = \beta_0 + \beta_1 \times X_1 + \beta_2 \times X_2 + \beta_3 \times X_3 + \beta_4 \times X_4 + \beta_5 \times (X_1^2) + \beta_6 \times (X_2^2) + \beta_7 \times (X_3^2) + \beta_8 \times (X_4^2) + \beta_9 \times (X_1^3) + \beta_{10} \times (X_2^3) + \beta_{11} \times (X_3^3) + \beta_{12} \times (X_4^3) + \beta_{13} \times (X_1^4) + \beta_{14} \times (X_2^4) + \beta_{15} \times (X_3^4) + \beta_{16} \times (X_4^4) + \beta_{17} \times (X_3^2 \times X_4^2) + \beta_{18} \times (X_4^2 \times X_2^2) + \beta_{19} \times (X_3 \times X_2) + \beta_{20} \times (X_3 \times X_2^2) + \beta_{21} \times (X_3 \times X_2^3)$

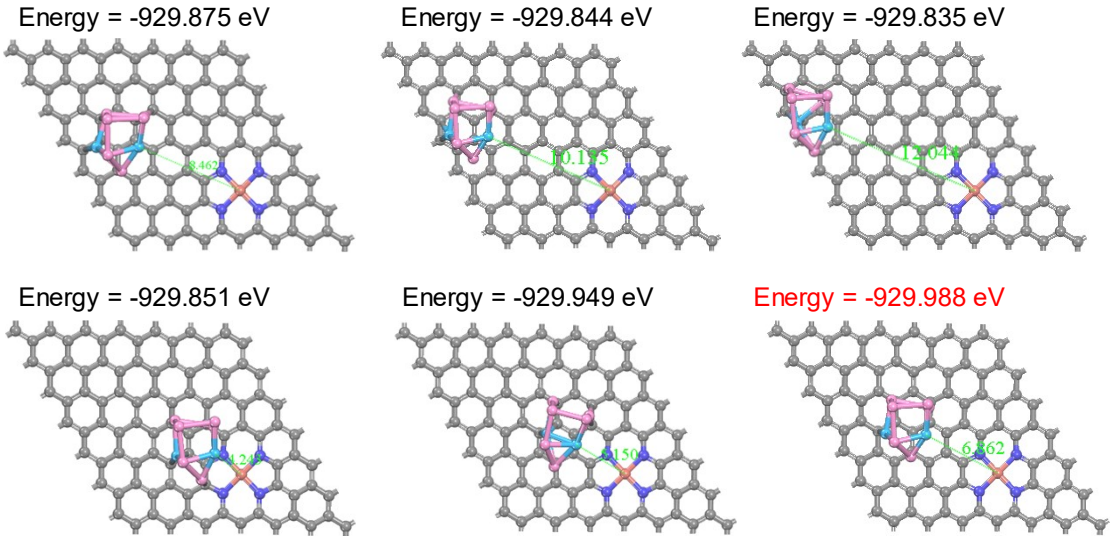

Figure S1. Configuration diagrams of Pt_3M-M'NC catalysts with different distances and their corresponding energies.

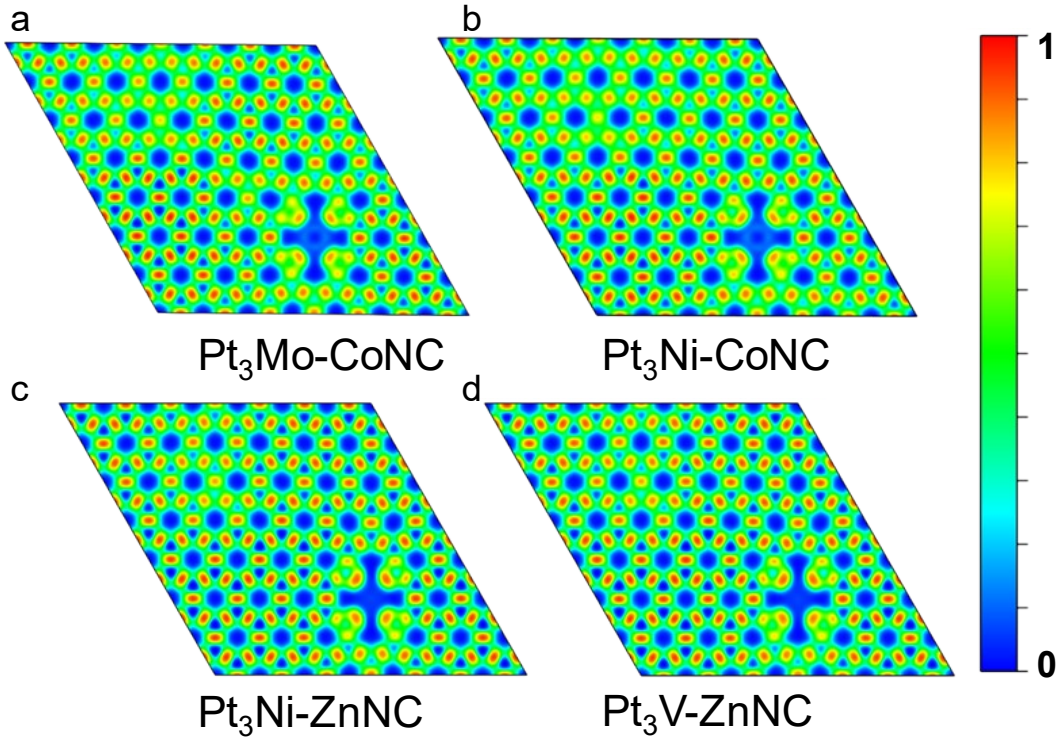

Figure S2. Electron localization function (ELF) maps of the (a) Pt_3Mo-CoNC (b) Pt_3Ni-CoNC, (c) Pt_3Ni-ZnNC, and (d) Pt_3V-ZnNC catalysts.

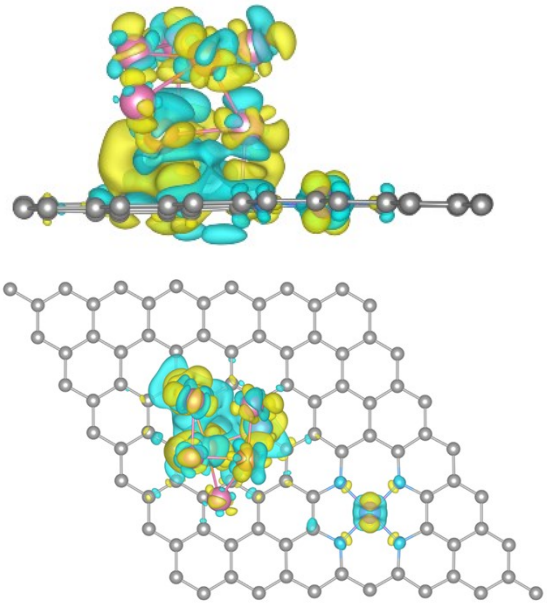

Figure S3. Charge density difference for the Pt_3Mo-CoNC catalyst.

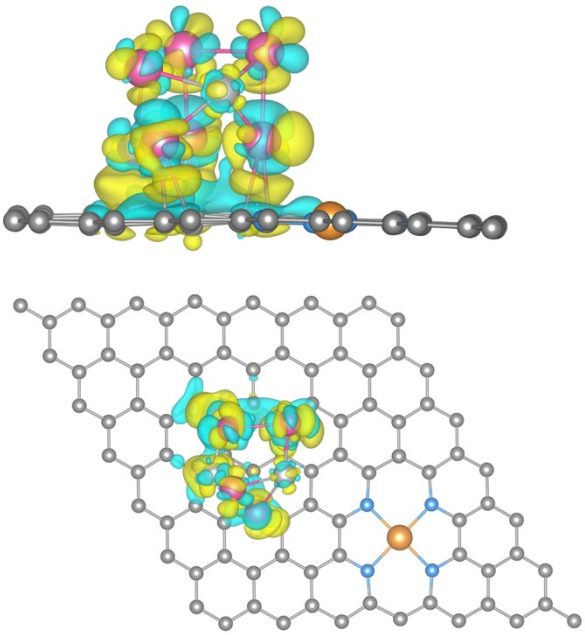

Figure S4. Charge density difference for the Pt_3Ni-ZnNC catalyst.

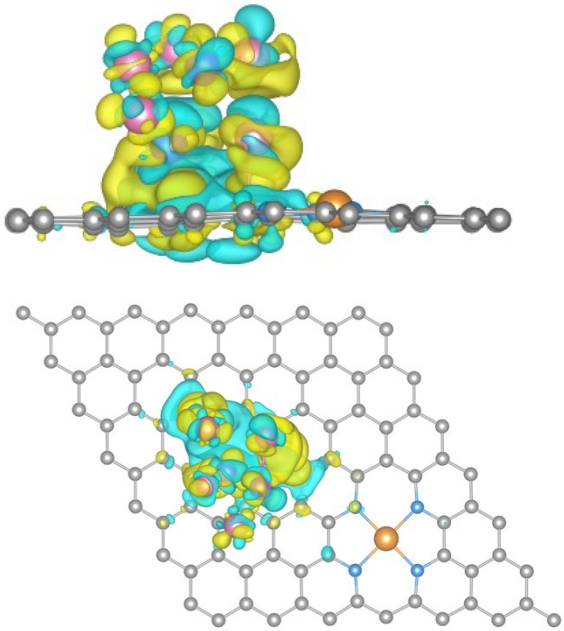

Figure S5 Charge density difference for the Pt_3V-ZnNC catalyst.

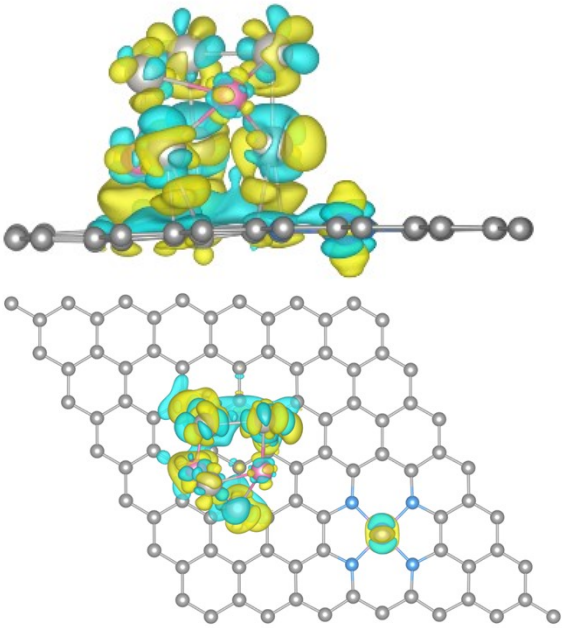

Figure S6. Charge density difference for the Pt_3Ni-CoNC catalyst.

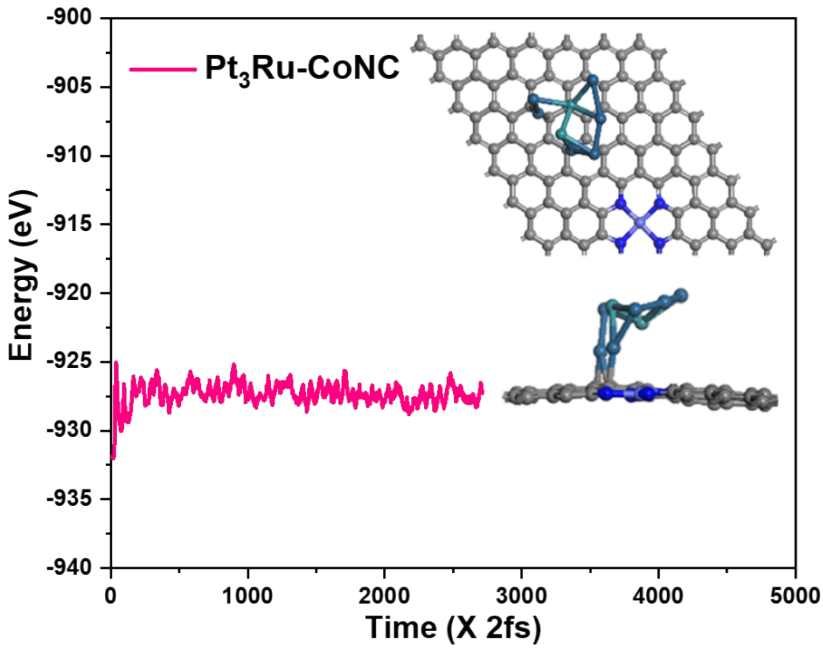

Figure S7. AIMD energy distributions of Pt_3Ru-CoNC catalyst.

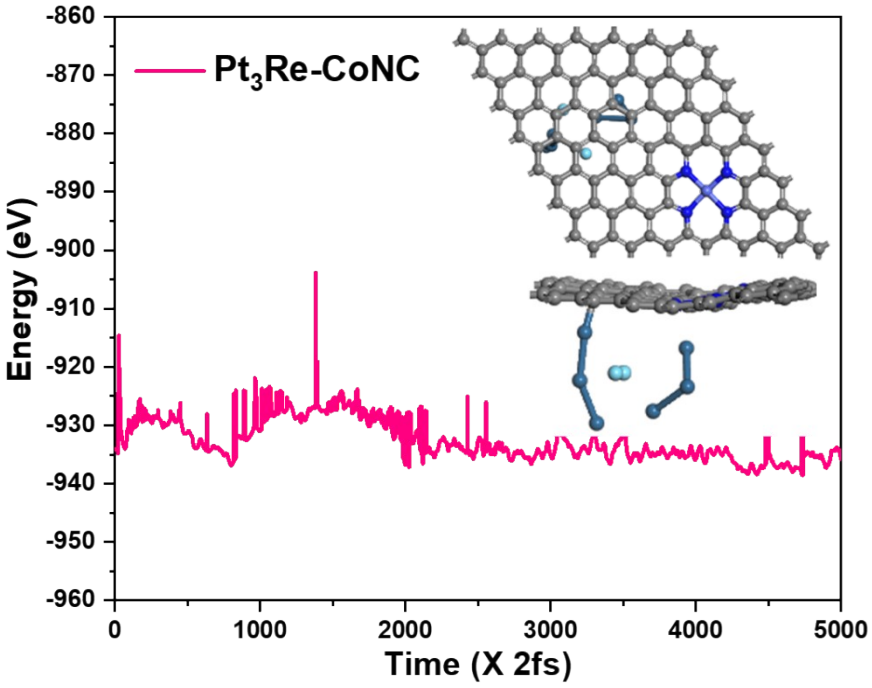

Figure S8. AIMD energy distributions of Pt_3Re-CoNC catalyst.

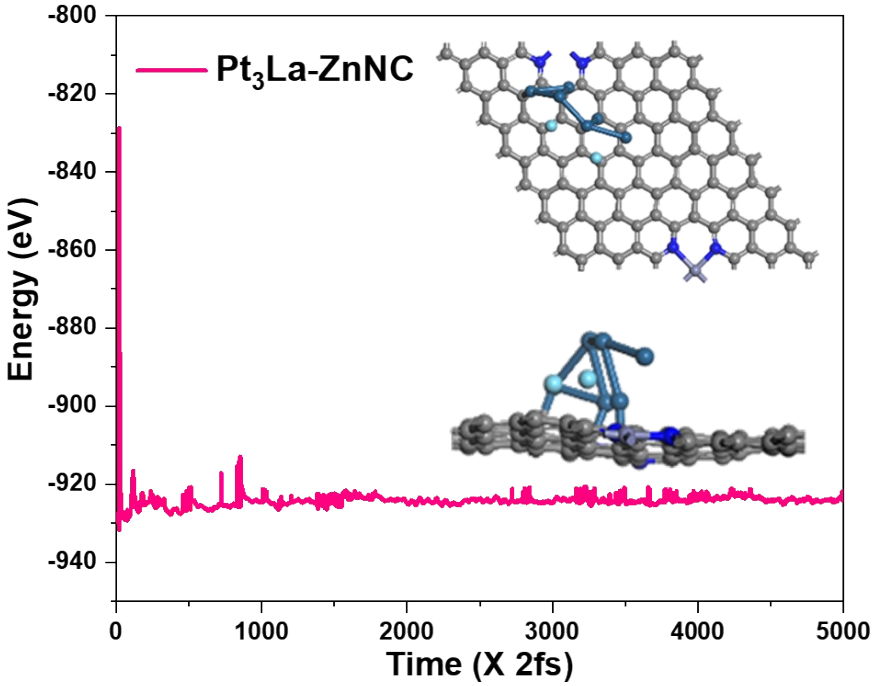

Figure S9. AIMD energy distributions of Pt_3La-ZnNC catalyst.

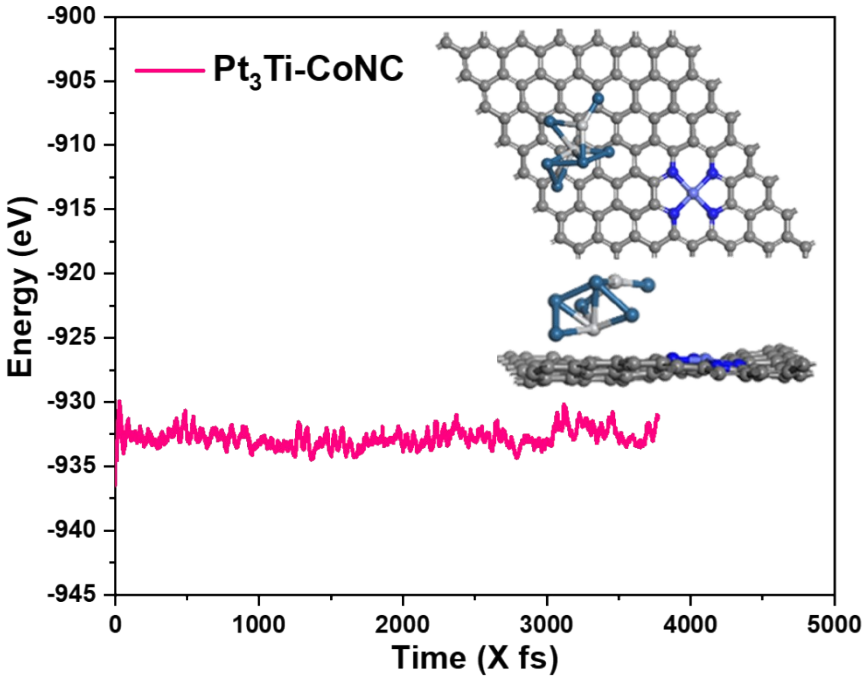

Figure S10. AIMD energy distributions of Pt_3Ti-CoNC catalyst.

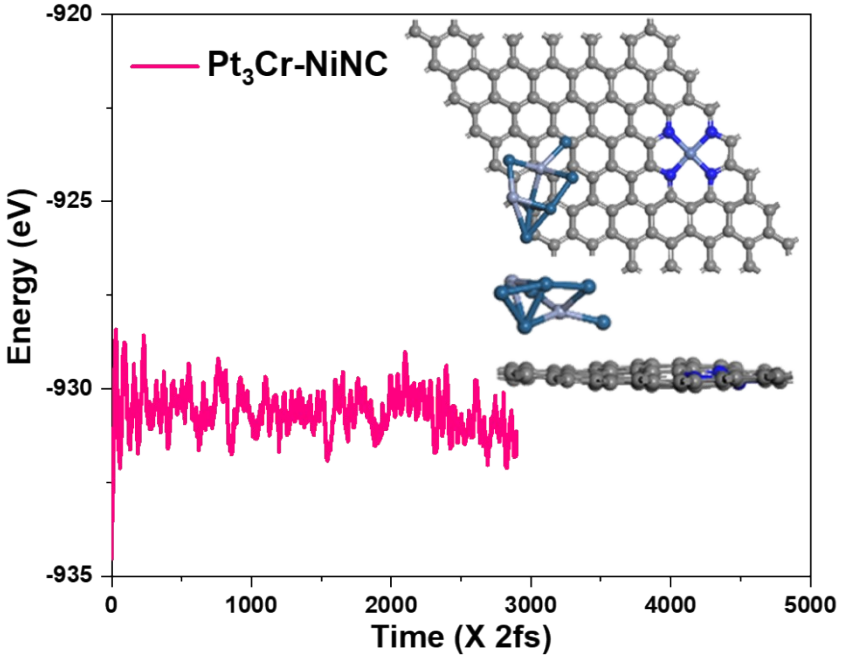

Figure S11. AIMD energy distributions of Pt_3Cr-NiNC catalyst.

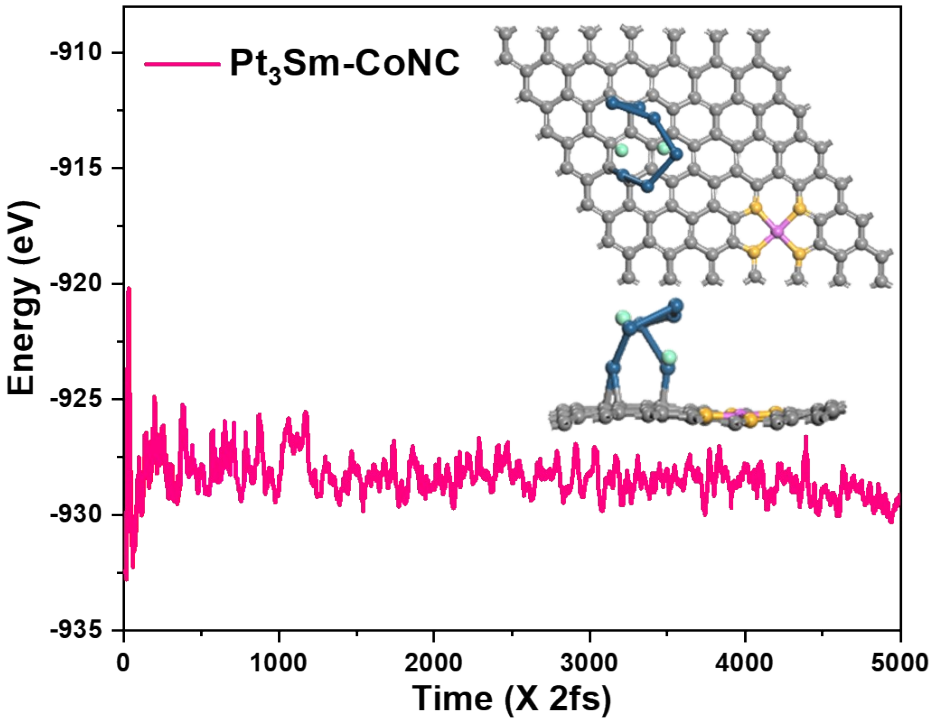

Figure S12. AIMD energy distributions of Pt_3Sm-CoNC catalyst.

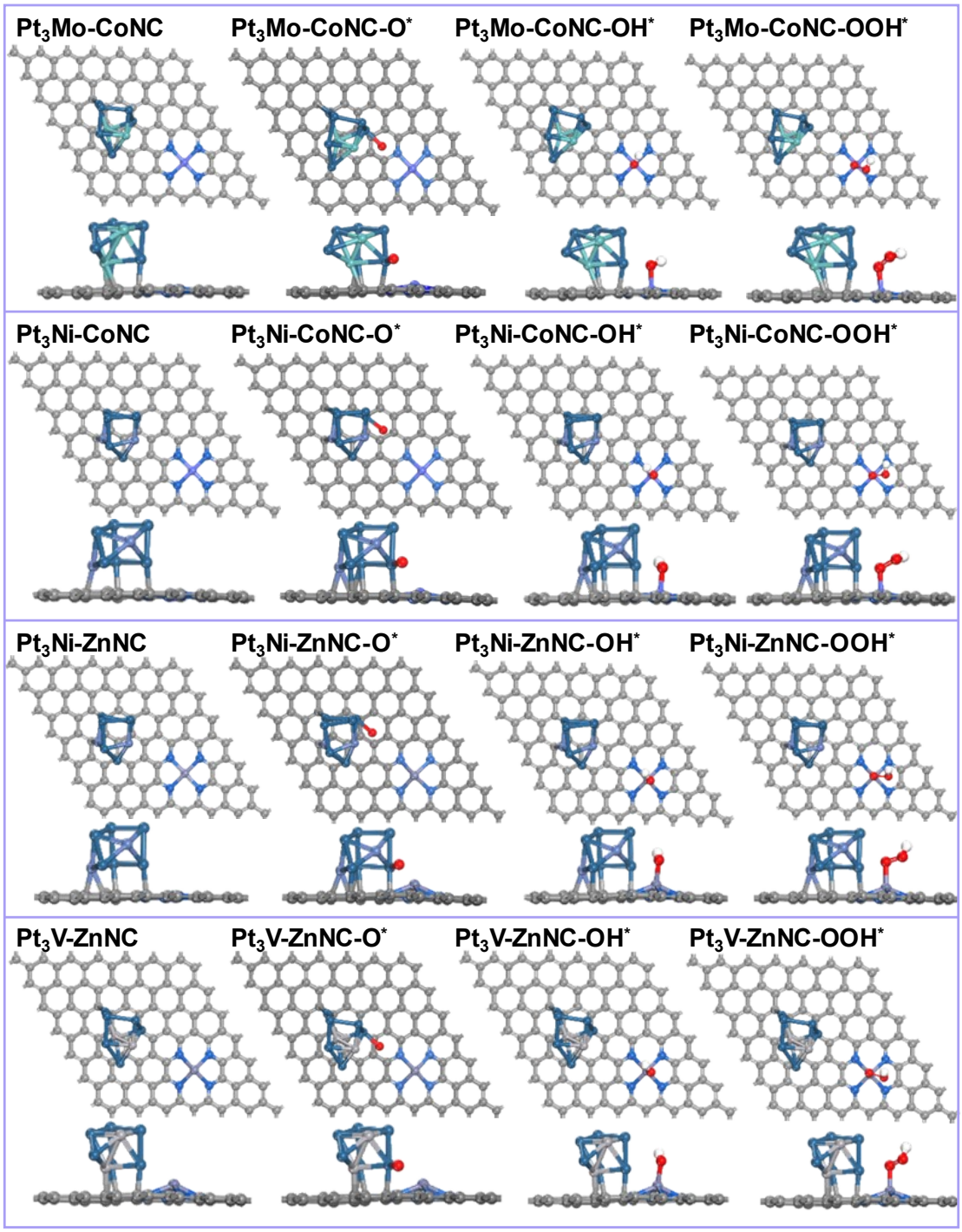

Figure S13 Catalyst and intermediate configurations.

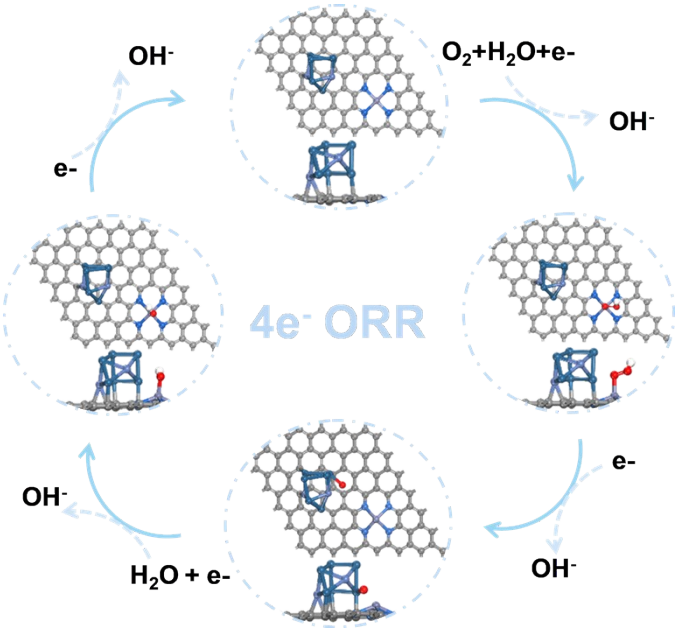

Figure S14 Reaction pathways for 4e- ORR process.

Note S3 We calculated the energies of the configurations of the intermediates at different sites, which are listed in Table S2. The results reveal that the energy of the structure in which the metal single atom (M') serves as the active site to adsorb *OH and *OOH is lower than that of the structure in which M (the metal of Pt_3M) and Pt serve as the active sites. Thus, the *OOH and *OH prefer to adsorb on the metal single-atom sites, while *O is more likely to adsorb on the Pt sites.

Table S1 Computed energies of catalysts and intermediates, and corresponding ΔE_{ZPE}-$T\Delta S$ values.

Structures	Energy (eV)	ΔE_{ZPE}-$T\Delta S$	Gibbs free energy (eV)
Pt_3Ni-ZnNC	-923.474	0.000	-923.474
Pt_3Ni-ZnNC-OOH*	-937.996	0.402	-937.594
Pt_3Ni-ZnNC-O*	-927.659	0.039	-927.620
Pt_3Ni-ZnNC-OH*	-933.804	0.303	-933.501
Pt_3Ni-CoNC	-929.588	0.000	-929.588
Pt_3Ni-CoNC-OOH*	-944.498	0.472	-944.026
Pt_3Ni-CoNC-O*	-934.369	0.049	-934.320
Pt_3Ni-CoNC-OH*	-939.882	0.333	-939.549
Pt_3V-ZnNC	-933.346	0.000	-933.346
Pt_3V-ZnNC-OOH*	-948.005	0.498	-947.507
Pt_3V-ZnNC-O*	-937.597	0.020	-937.577
Pt_3V-ZnNC-OH*	-943.667	0.320	-943.347
Pt_3Mo-CoNC	-940.542	0.000	-940.542
Pt_3Mo-CoNC-OOH*	-955.883	0.473	-955.410
Pt_3Mo-CoNC-O*	-946.060	0.018	-946.042
Pt_3Mo-CoNC-OH*	-951.011	0.423	-950.588

Table S2 Calculated energies of intermediates at different active sites.

Structures	Active site	Energy (eV)
Pt_3Ni-ZnNC-OOH*	Zn	-937.996
	Ni	-937.752
	Pt	-937.486
Pt_3Ni-ZnNC-OH*	Zn	-933.804
	Ni	-933.389
	Pt	-933.025
Pt_3Ni-ZnNC-O*	Zn	-927.320
	Ni	-927.527
	Pt	-927.659
Pt_3Ni-CoNC-OOH*	Co	-944.498
	Ni	-944.024
	Pt	-944.536
Pt_3Ni-CoNC-OH*	Co	-939.882
	Ni	-939.406
	Pt	-939.804
Pt_3Ni-CoNC-O*	Co	-934.007
	Ni	-934.204
	Pt	-934.369
	Zn	-948.005

Pt_3V-ZnNC-OOH*	V	-947.548
	Pt	-947.904
Pt_3V-ZnNC-OH*	Zn	-943.667
	V	-943.558
	Pt	-943.429
Pt_3V-ZnNC-O*	Zn	-937.028
	V	-937.336
	Pt	-937.597
Pt_3Mo-CoNC-OOH*	Co	-955.883
	Mo	-955.701
	Pt	-955.732
Pt_3Mo-CoNC-OH*	Co	-951.011
	Mo	-950.967
	Pt	-950.852
Pt_3Mo-CoNC-O*	Co	-945.968
	Mo	-945.900
	Pt	-946.060

Atomic coordinates:

1. Pt_3Ni-CoNC

1.0

17.2199993134	0.0000000000	0.0000000000
-8.6099996567	14.9129568585	0.0000000000
0.0000000000	0.0000000000	15.0000000000

C	N	Co	Ni	Pt
92	4	1	2	6

Cartesian

0.016875616	1.361254679	1.989149898
1.242164707	0.647371449	1.985549927
2.462890396	1.363193440	1.967850029
3.693000995	0.660345730	2.034149989
4.909938304	1.383027609	2.060400099
6.163037773	0.728647051	2.116950005
7.373001005	1.506357805	2.133150101
8.628338618	0.806940122	2.163449898
9.882557529	1.508296456	2.148450091
11.093640041	0.730138372	2.154899910
12.346222851	1.389589332	2.130000070
13.565743684	0.664223087	2.131950036
14.794993044	1.368860282	2.085149959
16.013135978	0.649459265	2.056649923
-1.202214293	3.503799304	1.988999918
0.014206419	2.782012195	1.951799914
1.232607555	3.491421406	1.902449951
2.456777398	2.779178663	1.927050054
3.668807077	3.499623560	1.991250068
4.890566054	2.798714723	2.039399967
6.098204700	3.506483503	2.074500024
11.158387539	3.511404796	2.093549967
12.366714509	2.805723776	2.094899788
13.590884737	3.513492556	2.060400099
14.800933993	2.790810789	2.047649994
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-1.211254882	4.925153260	1.980900094
0.006801899	5.636948673	1.960049942
1.227097241	4.912626253	1.913850009
2.452988729	5.645747267	1.977450103
3.674317134	4.917249326	2.050049677
4.901328158	5.637992665	2.053650096
6.101992471	4.933951853	2.062650025
11.155201233	4.937829155	2.074949965
12.362323605	5.638439772	2.059350014

13.587612856	4.927837682	2.043450102
-3.663468492	7.779641964	2.076150030
-2.433616350	7.073364727	2.044349983
-1.225117075	7.794853393	2.063099965
0.008782066	7.069338538	2.017050013
1.248880357	7.776659766	1.985399947
2.465387030	7.075899817	1.904099956
3.693603295	7.771589586	2.080049962
4.921648153	7.049652924	2.063549906
6.168634560	7.716112714	2.063700110
7.374895789	6.941533823	2.067300081
8.626960784	7.647811949	2.071050033
9.879371416	6.943323586	2.073599920
11.091487440	7.720288680	2.071799934
12.340282607	7.055767095	2.067450061
-4.910713294	9.886544441	2.093849927
-3.673197725	9.198013278	2.102549896
-2.447478287	9.924871233	2.155949995
-1.232090381	9.212329604	2.170350105
0.003530275	9.939038226	2.312700078
1.245436812	9.217251341	2.180099934
2.475288376	9.953056776	2.108999938
3.703591115	9.210093178	2.139149979
4.959962594	9.896089250	2.135849968
6.179483010	9.150441230	2.088749930
7.409076950	9.843148357	2.086200044
8.627478085	9.095561686	2.071050033
9.847515289	9.842700361	2.069400027
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-6.138499180	12.004184606	2.071499974
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-3.671906139	12.047730022	2.144099995
-2.439213522	11.356515326	2.191200033
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1.237171278	12.093364309	2.192850038
2.471414773	11.367252126	2.136149928
3.711426078	12.053844638	2.143950015
4.942397949	11.321469395	2.139749900
6.180171206	12.008062796	2.126700059
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4.950663996	14.157615585	2.151449919
6.178105592	13.433740717	2.128650025
7.406580251	14.138825519	2.083499953
8.630835926	13.421064378	2.060700282
7.317639156	2.889534412	2.110949904
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7.323407863	5.555225353	2.074650005
9.933270849	5.559103099	2.082750052
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3.608795608	8.838313159	4.312650114
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3.524503170	9.062156630	6.806250215
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1.173715366	6.313847488	6.311249882
2.374723777	5.303495002	4.234350175

2. Pt_3V-ZnNC

1.0

17.2199993134	0.0000000000	0.0000000000
-8.6099996567	14.9129568585	0.0000000000
0.0000000000	0.0000000000	15.0000000000

C	N	Zn	Pt	V
92	4	1	6	2

Cartesian

0.029618400	1.377957206	1.941149980
1.250774596	0.662284436	1.971300021
2.466937138	1.383027609	1.976849958
3.694378638	0.674363891	2.041649893
4.908905433	1.397045825	2.081549987

6.153050402	0.719401017	2.142599970
7.359655408	1.487418296	2.182950005
8.632471995	0.805747076	2.200200185
9.909335004	1.487269186	2.194050103
11.118006201	0.716567596	2.138099894
12.363615319	1.396449275	2.090549916
13.579605556	0.676600873	2.048700079
14.808941518	1.381685397	1.999049932
16.027170573	0.664819637	1.980149969
-1.186199628	3.519308730	1.912349984
0.027207598	2.798863833	1.894199923
1.239840025	3.518562958	1.858949997
2.456777269	2.804530675	1.924649924
3.662693887	3.527809104	1.964100078
4.877220521	2.816461020	2.054250017
6.086667156	3.510659246	2.120549977
11.185767314	3.511106576	2.147400007
12.395385998	2.815118809	2.083949894
13.611635047	3.524975572	2.014650106
14.819617149	2.803486684	1.969650015
-2.407097654	5.660511144	1.959000081
-1.192743133	4.942601115	1.906650066
0.017994704	5.660212924	1.875000000
1.236051485	4.939171366	1.824150011
2.453849615	5.655291632	1.873950027
3.664071689	4.940066025	1.945199892
4.878942806	5.643957504	2.059799954
6.086150881	4.959601862	2.122950107
11.180773019	4.957663212	2.128650025
12.390994580	5.651414331	2.058599889
13.608362396	4.940811796	2.005799934
-3.647712477	7.791721863	2.033099905
-2.421820926	7.082461540	1.988399997
-1.212030064	7.802310220	2.015250027
0.012570479	7.082461540	1.963950098
1.241992754	7.796642711	1.993949935
2.454280699	7.078733127	1.963649914
3.693431374	7.801713780	2.149649933
4.918376528	7.068741654	2.167500034
6.168978915	7.756079493	2.110349983
7.366543524	6.984334356	2.143650055
8.637379688	7.670032209	2.122050002

9.911315556	6.987017889	2.130899951
11.116456990	7.753395071	2.086350024
12.358793329	7.069934533	2.056649923
-4.896851293	9.903993185	2.068500146
-3.661229867	9.209793625	2.064749971
-2.436887718	9.930984071	2.109299898
-1.223480749	9.216505569	2.119499892
0.010762233	9.945898614	2.276099995
1.257748897	9.234699195	2.212950066
2.492250016	9.958277177	2.080650106
3.706432168	9.240068040	2.053049952
4.948253515	9.914878427	2.032649964
6.177416370	9.176985898	2.057100087
7.412865875	9.864324181	2.054399997
8.633591789	9.116588178	2.077650055
9.856640940	9.861491316	2.067900002
11.097256276	9.175047247	2.069550008
-6.131353118	12.017457385	2.065500095
-4.896420593	11.325943136	2.083799914
-3.665449107	12.052950423	2.120699957
-2.433530133	11.360690403	2.151149958
-1.205400342	12.092319873	2.187600061
0.018770143	11.389919493	2.209350094
1.243800744	12.098881596	2.151299939
2.479249223	11.372770302	2.084849998
3.716248067	12.060705025	2.053650096
4.946358795	11.334592842	2.027399987
6.185596200	12.024019108	2.034599930
7.411918516	11.297906925	2.041049972
8.635484969	12.011789876	2.042849958
9.859569236	11.292240305	2.057550028
-7.355953212	14.151948966	2.018549815
-6.130577872	13.443583301	2.052450031
-4.905719319	14.166563066	2.072550058
-3.667257097	13.480269219	2.120100036
-2.441020229	14.209809818	2.151750103
-1.199545289	13.523666191	2.181750163
0.021353058	14.269909762	2.187450081
1.243025818	13.525902617	2.153700069
2.489409477	14.209512931	2.118749991
3.716334284	13.484444295	2.075249925
4.957121541	14.169993260	2.053650096

6.185509470	13.447460603	2.035949975
7.414587648	14.153588952	2.013150081
8.638154101	13.437021578	2.023799792
7.264428944	2.848971194	2.191499993
10.006282727	2.846138107	2.220749930
7.268389406	5.623675895	2.194950208
10.003957179	5.626658537	2.176050022
8.633849413	4.239306075	2.299949974
3.946823938	7.786949459	4.373250157
0.673559961	9.457648452	4.355700016
3.346104447	8.709017345	6.674250215
0.765946013	9.127922306	6.845400184
0.646094226	6.650880685	6.407250613
1.918824340	4.829113614	4.977749884
3.028653479	6.458503174	6.358349919
1.562456439	7.178948293	4.155749828

3. Pt_3Mo-CoNC

1.0

17.2199993134	0.0000000000	0.0000000000
-8.6099996567	14.9129568585	0.0000000000
0.0000000000	0.0000000000	15.0000000000

C	N	Co	Pt	Mo
92	4	1	6	2

Cartesian

0.031684783	1.391378872	1.960049942
1.256371094	0.679732569	1.997399926
2.477957829	1.398835366	2.004750073
3.708240703	0.691215529	2.052150071
4.927158338	1.413450022	2.074200064
6.177158328	0.748928716	2.122950107
7.389532458	1.521867232	2.153099924
8.641426431	0.820361733	2.180399895
9.893577963	1.524104213	2.149799913
11.108191039	0.750867366	2.106000111
12.358190324	1.418073095	2.049000040
13.576591396	0.694049005	2.024249956
14.806443922	1.398238815	1.975800097
16.028375589	0.677943028	1.982399896
-1.187577238	3.534818157	1.898100078
0.028327006	2.813627488	1.914599910
1.246555708	3.528703763	1.911900043

2.470036714	2.817952341	1.977900043
3.685510195	3.537800798	2.021099925
4.907785960	2.828838695	2.056050003
6.120848831	3.533774165	2.094600052
11.164586305	3.536756807	2.062949985
12.379543895	2.831224897	2.019299939
13.599064183	3.539888559	1.964849979
14.814020490	2.820934983	1.942200065
-2.411316574	5.675275021	1.908000112
-1.192657173	4.956768553	1.859249957
0.021955550	5.672143047	1.829850040
1.240701040	4.950206829	1.890599951
2.463923395	5.665283104	2.020799965
3.690934933	4.947820627	2.055450082
4.908130571	5.648878796	2.120100036
6.120848574	4.955277454	2.119499892
11.161572818	4.957216104	2.057100087
12.375927147	5.662896902	2.012249976
13.597600163	4.955873893	1.957949996
-3.649951102	7.802160888	2.036099955
-2.423198216	7.096777865	1.952999979
-1.207810567	7.818862971	1.956000030
0.015239868	7.102295597	1.871849969
1.244661373	7.811407033	1.944749951
2.465215109	7.098269408	1.995299980
3.707551962	7.815731441	2.169300020
4.935423872	7.075303377	2.230649963
6.195239666	7.747579119	2.126700059
7.395386677	6.971956681	2.150700018
8.646850207	7.674803725	2.137050033
9.897625540	6.973149560	2.126700059
11.107330313	7.745640469	2.093549967
12.355004660	7.076198036	2.047050074
-4.893923895	9.911747787	2.107049972
-3.658216765	9.221874413	2.094150111
-2.433788784	9.945302174	2.136750072
-1.215731747	9.230821894	2.107649893
0.017650349	9.951565233	2.269649953
1.264550796	9.239918708	2.175149918
2.505337540	9.966627330	2.080650106
3.722188824	9.250954171	2.045100108
4.967108335	9.923678354	2.022299990

6.196013565	9.176091683	2.050200105
7.424919822	9.872078783	2.056349963
8.646075794	9.126282319	2.103599980
9.865165125	9.871781008	2.097900063
11.098203636	9.175495243	2.101500034
-6.125756267	12.033413696	2.081549987
-4.890393876	11.338172368	2.115449980
-3.660369494	12.068012520	2.146199942
-2.427675594	11.373217409	2.187450081
-1.197651083	12.104250441	2.217449918
0.026777026	11.397525652	2.238000110
1.253788050	12.108724181	2.182650045
2.490958815	11.383507102	2.104500085
3.724858469	12.075915565	2.063850090
4.956776673	11.346374077	2.025600001
6.192914375	12.041169187	2.032350004
7.418547468	11.309091721	2.038049921
8.643406662	12.023720444	2.050350085
9.868695400	11.304767312	2.072400078
-7.350012327	14.169396820	2.032949924
-6.121795677	13.460285385	2.063099965
-4.894612732	14.183415371	2.077500075
-3.655461287	13.497717073	2.127899900
-2.426297663	14.232627406	2.148600072
-1.190848670	13.537534520	2.194500044
0.029273725	14.282735433	2.194800004
1.252496336	13.540218942	2.172750011
2.490184403	14.236504707	2.121750042
3.717798432	13.502190814	2.079600021
4.958068388	14.186248236	2.045100108
6.187318486	13.464908457	2.032200024
7.417600621	14.167458170	2.016450092
8.643664286	13.450741464	2.032200024
7.330037329	2.900570098	2.133600041
9.957119964	2.901464980	2.131049931
7.333136776	5.589077960	2.168549895
9.954106862	5.591911270	2.116350085
8.647367508	4.247806449	2.472000048
4.108691592	7.785756580	4.337549955
0.838269695	9.266612708	4.332899898
3.445635726	8.601047577	6.683849841
0.918859424	9.150291897	6.842249930

0.460893090	6.688013709	6.577650011
0.993421924	4.560083852	5.141850114
2.841988452	6.341287704	6.022350043
1.633488920	6.799413672	4.192800075

4. Pt_3Ni-ZnNC

1.0

17.2199993134	0.0000000000	0.0000000000
-8.6099996567	14.9129568585	0.0000000000
0.0000000000	0.0000000000	15.0000000000

C	N	Zn	Pt	Ni
92	4	1	6	2

Cartesian

0.005079870	1.344701372	1.921950057
1.230455018	0.631563747	1.953149959
2.453161162	1.349026114	1.948800087
3.679311236	0.641704552	2.019750103
4.900725730	1.363789880	2.057849988
6.139618300	0.688382108	2.138850018
7.344329901	1.463259275	2.221049890
8.616457105	0.776815928	2.245050073
9.890048137	1.466391026	2.224199921
11.093640426	0.691364694	2.138400078
12.332791101	1.370799044	2.060249895
13.554894721	0.647222339	2.028900012
14.780786882	1.352008644	1.967700049
16.001339559	0.632309352	1.964250058
-1.213493378	3.487245886	1.882499903
0.004218984	2.765011226	1.874100007
1.223308829	3.479192841	1.857599951
2.449803065	2.767099208	1.908150092
3.664329827	3.477254191	1.970700100
4.881697642	2.778582224	2.028600052
6.105867101	3.472332899	2.116200104
11.129199646	3.476955971	2.104950026
12.353197569	2.786784156	2.013899982
13.572890034	3.495149598	1.939799935
14.785952776	2.775002920	1.920899972
-2.435166202	5.631281609	1.940850019
-1.217195766	4.909494724	1.900200024
0.000688709	5.618009275	1.916249916
1.215043294	4.896818384	1.868700050

2.446187086	5.626509649	1.969799995
3.671217687	4.902634781	2.029950097
4.894526259	5.623527007	2.003100067
6.112583296	4.937083383	2.084550038
11.130232453	4.940811796	2.081849948
12.354057557	5.627404308	1.996949986
13.574439116	4.916056447	1.941900104
-3.667429274	7.768606500	2.042400017
-2.442054190	7.058451517	2.012549937
-1.232177112	7.777852645	2.089800015
0.001377675	7.047564941	2.068800107
1.240959178	7.759956794	2.086350024
2.467195276	7.063820362	1.899600103
3.685423978	7.749965766	1.940700039
4.908301978	7.036678810	1.979550049
6.147970725	7.719393576	2.058750093
7.349409963	6.947499107	2.137499973
8.620848106	7.643188876	2.152500004
9.892631374	6.952569731	2.140799984
11.096137509	7.727148178	2.072099894
12.333566412	7.044731632	2.030400038
-4.914674012	9.879684942	2.078099996
-3.677761192	9.186232043	2.092349902
-2.452644631	9.909063365	2.165550068
-1.238462479	9.194434641	2.200499922
-0.005423968	9.930388521	2.329650074
1.236051485	9.207855863	2.253450081
2.476063816	9.932029396	2.157300040
3.694723602	9.177731669	2.113799974
4.939986954	9.881772925	2.143199891
6.166481190	9.143432399	2.099099904
7.397022489	9.829428471	2.107199952
8.621192974	9.080499589	2.112900093
9.842263242	9.833603548	2.079300061
11.079434007	9.150142565	2.069550008
-6.151844969	11.989421173	2.063549906
-4.914415682	11.301337118	2.095649913
-3.682238570	12.027747077	2.135999948
-2.448511863	11.338023036	2.190149948
-1.222447686	12.072336928	2.221350074
0.002239074	11.366357022	2.248350084
1.229163368	12.073232032	2.171849906

2.462201879	11.354278011	2.114249915
3.701008713	12.037589662	2.082600072
4.931032198	11.308048174	2.097600102
6.167084195	11.991061160	2.080950066
7.393493241	11.261817447	2.086949944
8.615424138	11.979429257	2.061000019
9.841832157	11.261817447	2.061599940
-7.378597728	14.122570543	2.005499974
-6.150983570	13.414502654	2.041349933
-4.924058634	14.136588204	2.056649923
-3.684218737	13.450592132	2.113500014
-2.458327250	14.179538069	2.151299939
-1.218745490	13.499655724	2.197950035
0.004735259	14.249479710	2.211600021
1.227183458	13.500848603	2.171849906
2.467883472	14.181476720	2.130150050
3.697736575	13.455215205	2.085750103
4.936973467	14.141061945	2.059350014
6.163210079	13.415994198	2.050350085
7.391426601	14.121824772	2.012849897
8.615681762	13.402572976	2.026650086
7.270025603	2.823768293	2.249099985
9.965299538	2.827049154	2.248350084
7.282251599	5.586841090	2.167650014
9.964094169	5.595192132	2.180700079
8.621450855	4.221410669	3.016650081
3.582104286	9.372196719	4.317900091
0.880889081	9.440647705	4.395149946
3.564195799	9.289877403	6.821700186
1.064885232	8.909894786	6.845700145
1.444585845	6.423308800	6.266099811
2.618817486	5.412508762	4.198500216
3.575474563	7.243968641	5.466299951
0.788934114	7.034889047	4.023000151