Supporting Information

Exploring electronic and energy descriptors to identify the dual metal center catalyst for CO_2ER towards C_2 product

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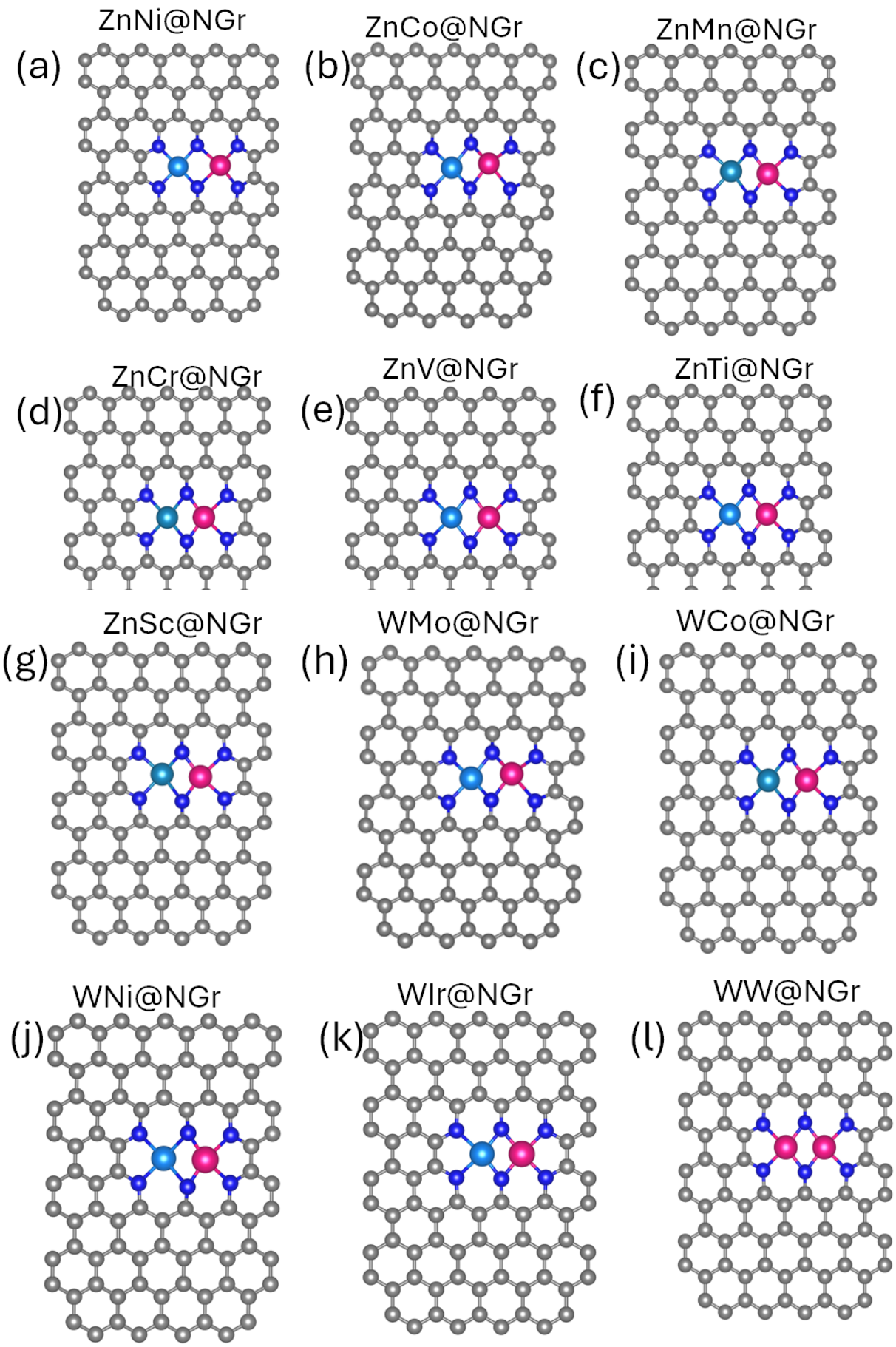
1.1 Computational details

In this study, we account for the subtle but significant effects of long-range weak van der Waals interactions by applying the Grimme DFT-D2 dispersion correction. This ensures our calculations accurately capture these interactions, which are often overlooked in standard DFT methods but are crucial for systems involving molecular adsorption or surface interactions. Also, we have performed Crystal Orbital Hamilton Population) (COHP) calculations with the help Lobster software. The entropy and zero-point energy (ZPE) values for free molecules are sourced from established chemical databases (e.g., https://janaf.nist.gov), while those for adsorbed molecules are provided in the supporting information (SI). The Gibbs free energy for the surface-anchored catalysts (SACs) considered in this study is calculated at U=0 V.


(a)
ZnNi@NGr
(b)
ZnCo@NGr
(c)
ZnMn@NGr
(d)
ZnCr@NGr
(e)
ZnV@NGr
(f)
ZnTi@NGr
(g)
ZnSc@NGr
(h)
WMo@NGr
(i)
WCo@NGr
(j)
WNi@NGr
(k)
WIr@NGr
(l)
WW@NGr

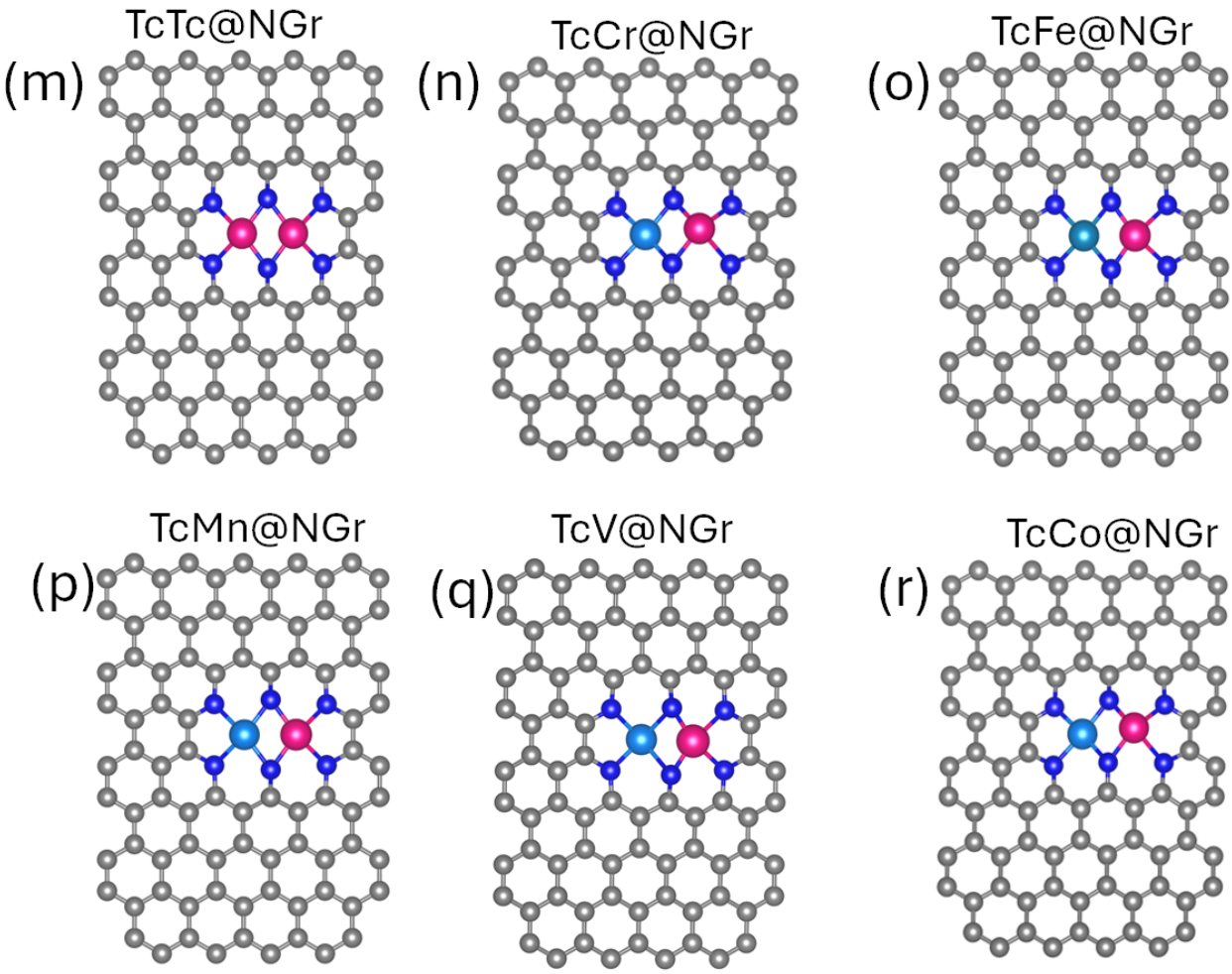


Fig. S1 Optimized structure of (a)ZnNi@NGr, (b) ZnCo@NGr, (c) ZnMn@NGr, (d) ZnCr@NGr, (e) ZnV@NGr, (f) ZnTi@NGr, (g) ZnSc@NGr, (h) WMo@NGr, (i) WCo@NGr, (j) WNi@NGr, (k) WIr@NGr, (l) WW@NGr, (m) TcTc@NGr, (n) TcCr@NGr, (o) TcFe@NGr, (p) TcMn@NGr, (q) TcV@NGr and (r) TcCo@NGr respectively.

Table S1 The obtained bond Lengths Between TM1 and TM2 in DACs.

DACs	Bond length (Å)
CuCu@NGr	2.3
CuPd@NGr	2.5
CuAu@NGr	2.65
CuAg@NGr	2.63
CuPt@NGr	2.63
CuZn@NGr	2.66
CuFe@NGr	2.45

CuNi@NGr	2.58
CuCo@NGr	2.51
CuOs@NGr	2.67
CuV@NGr	2.56
CuSc@NGr	2.46
CuTi@NGr	2.63
CuRh@NGr	2.47
CuRe@NGr	2.44
CuW@NGr	2.46
CuTa@NGr	2.57
CuTc@NGr	2.51
CuCd@NGr	2.45
CuMo@NGr	2.53
CuNb@NGr	2.55
CuIr@NGr	2.63
CuY@NGr	2.67
CuHf@NGr	2.68
CuLa@NGr	2.48
ZnNi@NGr	2.45
ZnCo@NGr	2.43
ZnMn@NGr	2.61
ZnCr@NGr	2.43
ZnV@NGr	2.44
Zn-Ti@NGr	2.46
ZnSc@NGr	2.56
ZnW@NGr	2.72
ZnTc@NGr	2.57
ZnRh@NGr	2.64
ZnRe@NGr	2.72
WMo@NGr	2.42
WFe@NGr	2.34
WV@NGr	2.61

WCo@NGr	2.36
WNi@NGr	2.45
WY@NGr	2.7
WHf@NGr	2.74
WIr@NGr	2.42
WW@NGr	2.39
WTc@NGr	2.54
TcTc@NGr	2.43
TcRh@NGr	2.72
TcCr@NGr	2.65
TcFe@NGr	2.53
TcMn@NGr	2.47
TcV@NGr	2.73
TcCo@NGr	2.55
TcNi@NGr	2.57

Table S2 The estimated zero-point energy (E_{ZPE}) and the product (TS) at T=300 K of different species of relevant free molecules for CO_2ER process

Intermediate	E_{ZPE} (eV)	TS (eV)
CO	0.13	0.60
O_2	0.24	0.64
CO_2	0.62	0.66
H_2O	0.56	0.67
H_2	0.27	0.40
CH_3OH	1.34	0.73
CH_4	1.57	0.59
CH_3CH_2OH	2.10	0.87
CH_3CHO	1.47	0.81
CH_2CH_2	1.34	0.68

Table S3 The estimated zero point energy (E_{ZPE}) and the product (TS) at T=300 K of different species along the reaction pathway of CO_2ER on TM_1TM_2@NGr

Intermediate	E_{ZPE} (eV)	TS (eV)
*COOH	0.60	0.21
*CO	0.20	0.13
*2CO	0.39	0.22
*COH	0.46	0.11
*CHO	0.47	0.11
*CO-CHO	0.68	0.30
*CHO-CO	0.69	0.28
*COH-CO	0.69	0.27
*C-CO	0.29	0.15
*CHOH-CO	1.01	0.16
*COH-CHO	0.92	0.25
*C-CHO	0.57	0.11
*CH-CHO	0.76	0.17
*C-CH_2O	0.79	0.18
*CH_2-CHO	1.08	0.20
*CH-CH_2O	1.07	0.19
*O	0.13	0.09
*CH_3-CHO	1.42	0.20
*CH_3-CH_2O	1.81	0.14
*C	0.11	0.08
*CH	0.17	0.11
*CH_2	0.29	0.12
*CH_3	0.41	0.13
*CH4	0.52	0.12

1.2 Aggregation energy calculation

We know that the positive aggregation energy favors the stable catalytic site else they will strongly bind with each other which leads to the formation of cluster growth. For this investigation, we have computed the aggregation energy of 19 DACs that shows either methanol or ethanol production from CO_2ER. The aggregation energy can be estimated by using the following formula

$$E_{aggregation} = E_{TM1TM2@NGr} - (E_{TM1} + E_{TM2} + E_{NGr})$$

In this context, $E_{aggregation}$ represents the aggregation energy of the dual-atom catalyst, while $E_{TM1\ TM2@NGr}$ is the total energy of the dual-atom catalyst supported on nitrogen-doped graphene. E_{NGr} represents the energy of pristine nitrogen-doped graphene without any transition metal atoms. On the other hand, E_{TM1} and E_{TM2} are the energies of TM_1 and ETM_2 in a vacuum. . The obtained $E_{aggregation}$ is presented in Fig. s2 which shows that there is small positive value of it's for all system which clearly indicates that the sites are stable which is crucial for this catalytic activity, and they are opposed to form nanoclusters.

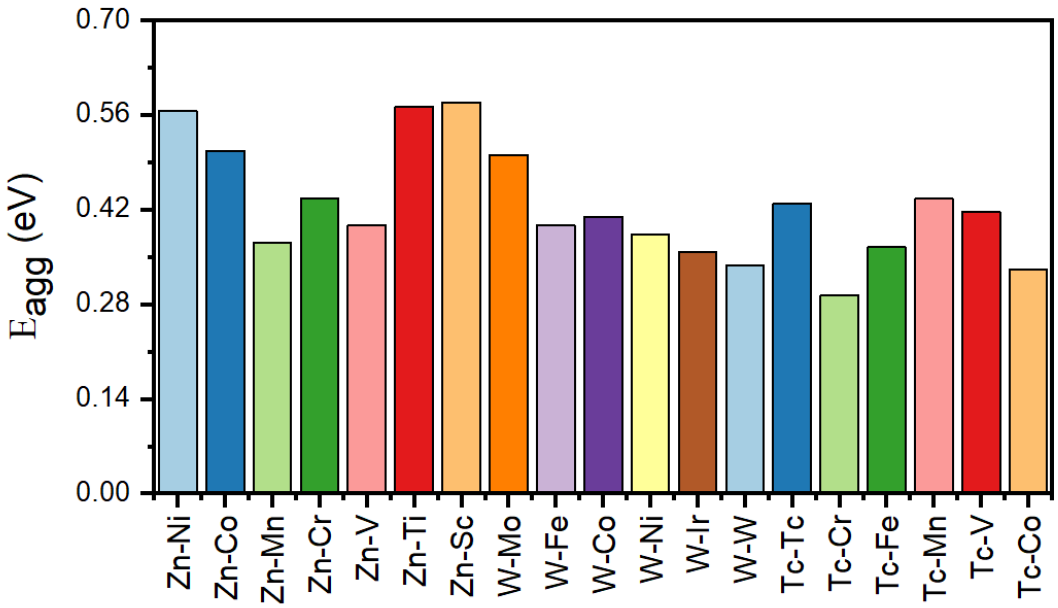


Fig. S2 The estimated aggregation energy of Zn-Ni, Zn-Co, Zn-Mn, Zn-Cr, Zn-V, Zn-Ti, Zn-Sc W-Mo, W-Fe, W-Co, W-Ni, W-W, W-Ir, Tc-Tc, Tc-Cr, Tc-Fe, Tc-Mn, Tc-V, and Tc-Co in DACs.

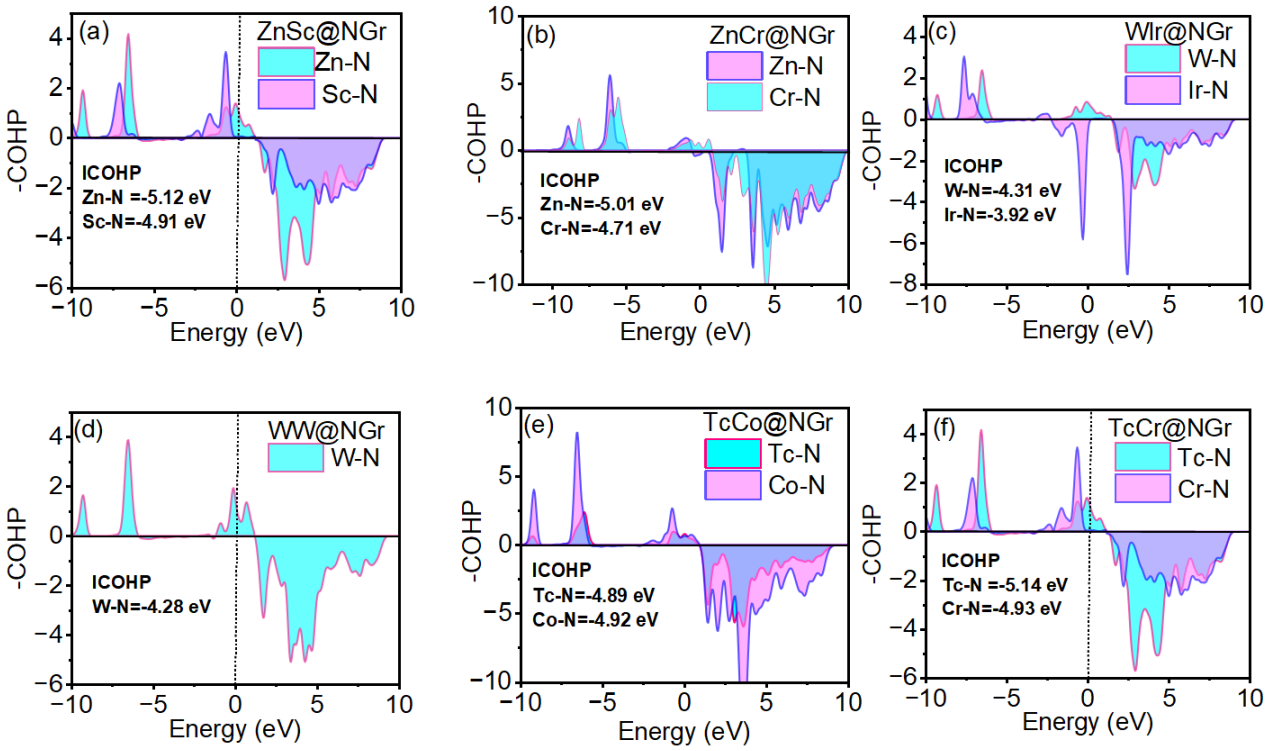
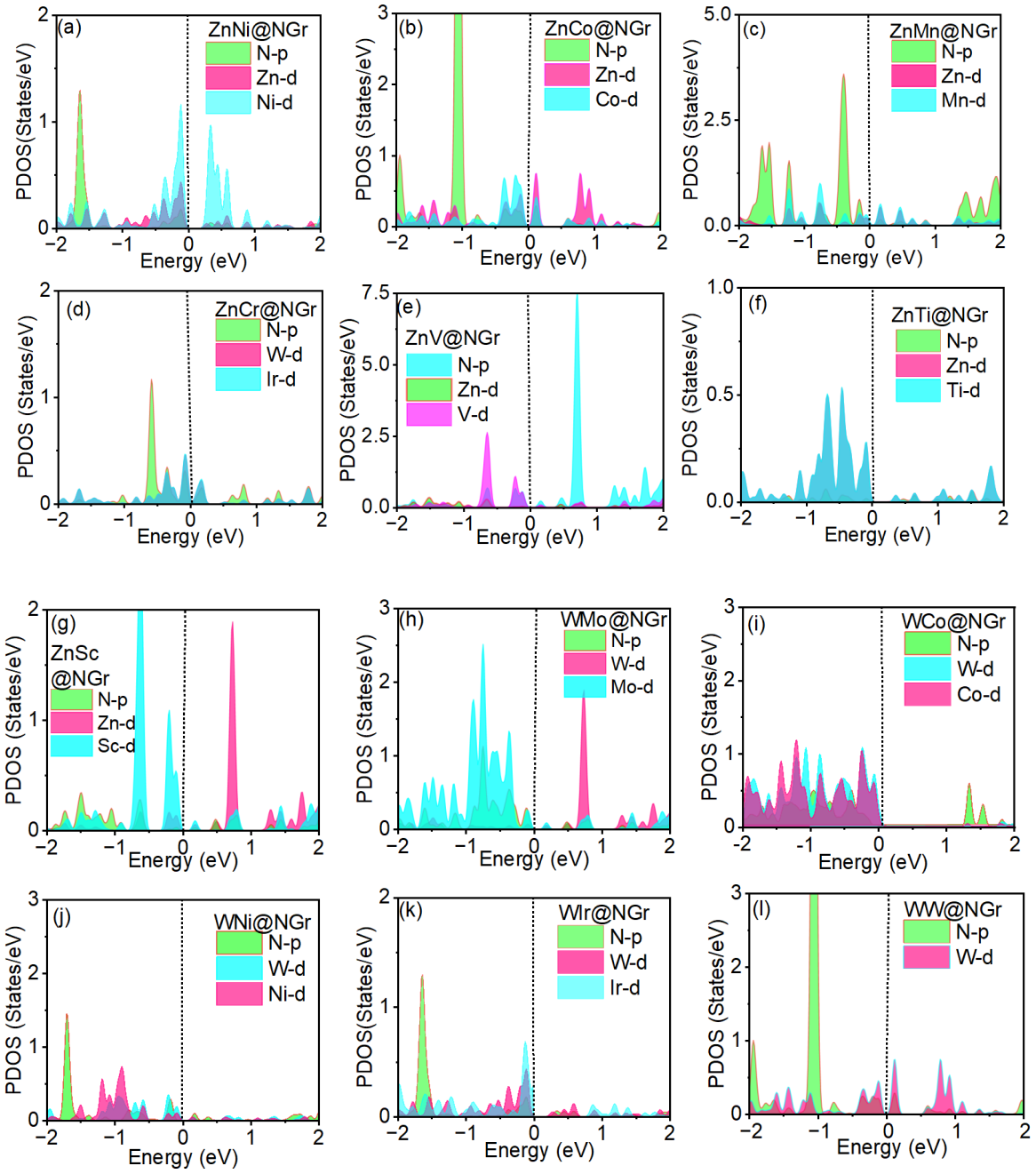


Fig. S3 The COHP plots of (a)ZnSc@NGr, (b) ZnCr@NGr, (c) WIr@NGr, (d) WW@NGr, (e) TcCo@NGr, and (f) TcCr@NGr demonstrating the chemical interaction between TM_1, TM_2 with their neighbouring nitrogen.


(a)
ZnNi@NGr
N-p
Zn-d
Ni-d
PDOS(States/eV)
Energy (eV)
(b)
ZnCo@NGr
N-p
Zn-d
Co-d
PDOS (States/eV)
Energy (eV)
(c)
ZnMn@NGr
N-p
Zn-d
Mn-d
PDOS (States/eV)
Energy (eV)
(d)
ZnCr@NGr
N-p
W-d
Ir-d
PDOS (States/eV)
Energy (eV)
(e)
ZnV@NGr
N-p
Zn-d
V-d
PDOS (States/eV)
Energy (eV)
(f)
ZnTi@NGr
N-p
Zn-d
Ti-d
PDOS (States/eV)
Energy (eV)
(g)
ZnSc
@NGr
N-p
Zn-d
Sc-d
PDOS (States/eV)
Energy (eV)
(h)
WMo@NGr
N-p
W-d
Mo-d
PDOS (States/eV)
Energy (eV)
(i)
WCo@NGr
N-p
W-d
Co-d
PDOS (States/eV)
Energy (eV)
(j)
WNi@NGr
N-p
W-d
Ni-d
PDOS (States/eV)
Energy (eV)
(k)
WIr@NGr
N-p
W-d
Ir-d
PDOS(States/eV)
Energy (eV)
(l)
WW@NGr
N-p
W-d
PDOS (States/eV)
Energy (eV)

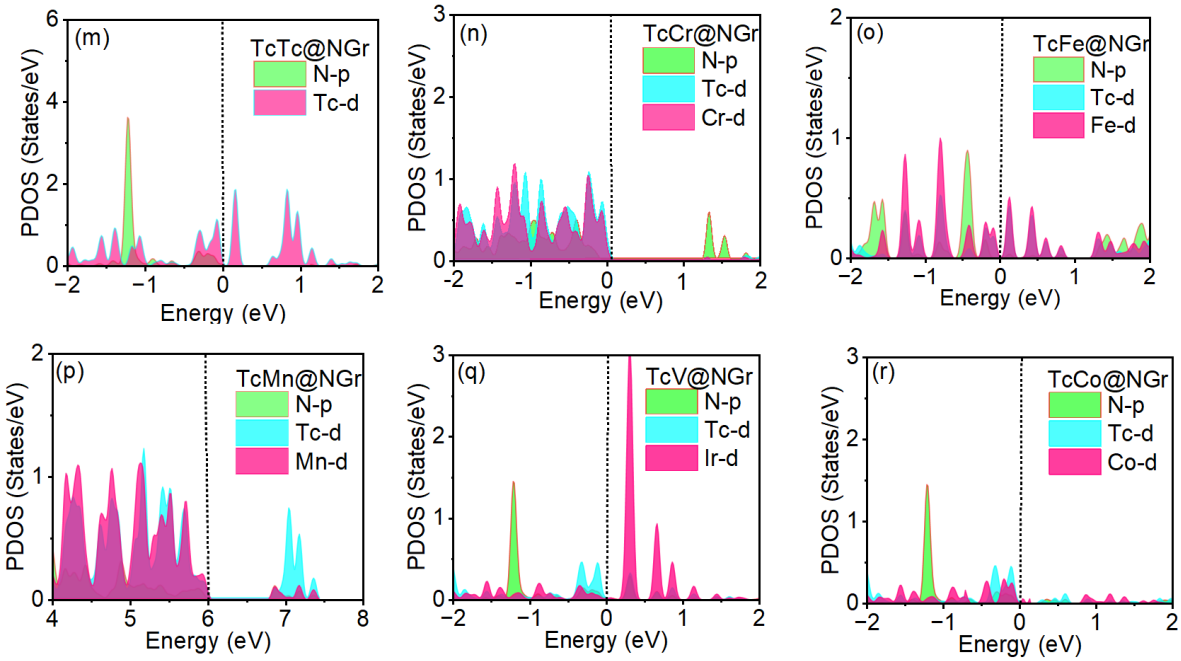
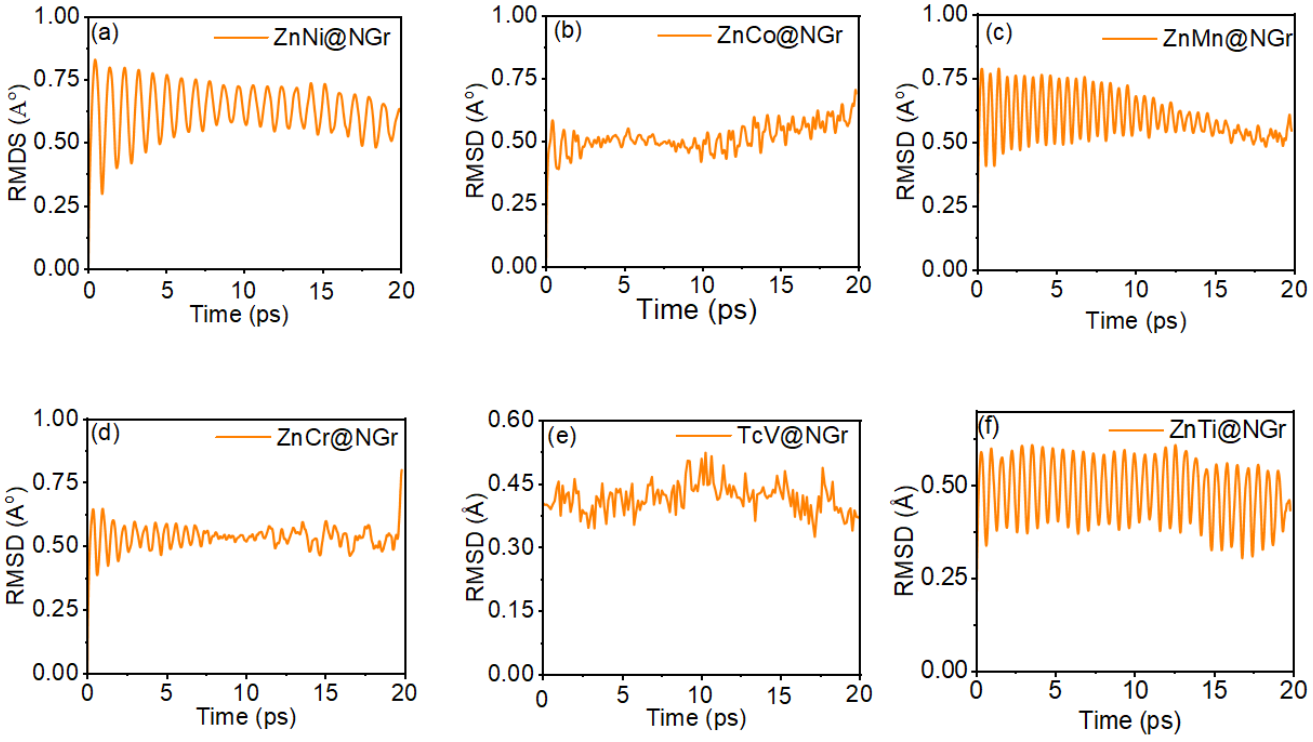
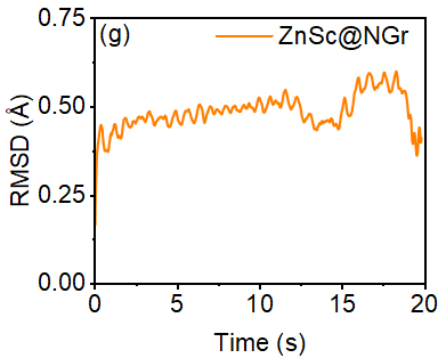
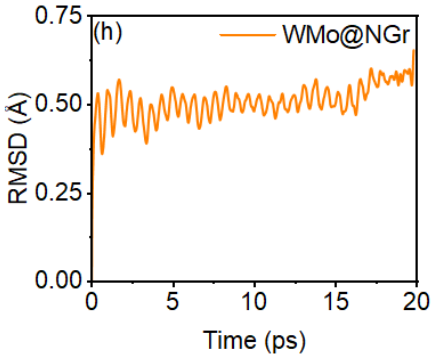
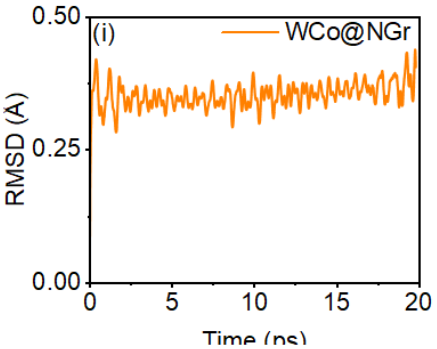


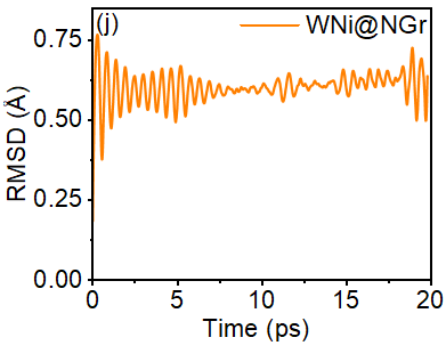
Fig. S4 The PDOS of (a)ZnNi@NGr, (b) ZnCo@NGr, (c) ZnMn@NGr, (d) ZnCr@NGr, (e) ZnV@NGr, (f) ZnTi@NGr, (g) ZnSc@NGr, (h) WMo@NGr, (i) WCo@NGr, (j) WNi@NGr, (k) WIr@NGr, (l) WW@NGr, (m) TcTc@NGr, (n) TcCr@NGr, (o) TcFe@NGr, (p) TcMn@NGr, (q) TcV@NGr and (r) TcCo@NGr showing the hybridization between TM_1-d, TM_2-d with N-p near the Fermi level.

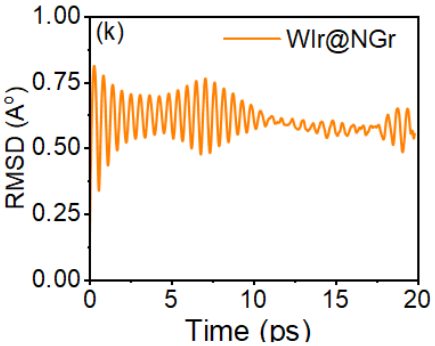


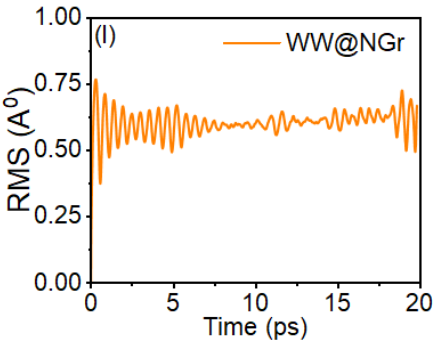

(g)
ZnSc@NGr
RMSD (Å)
Time (s)

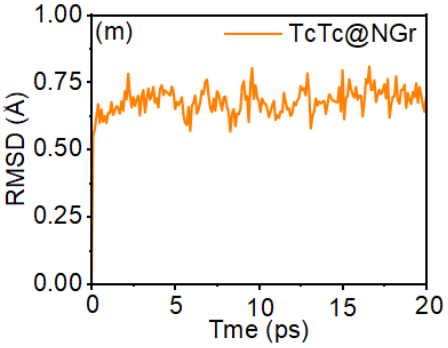

(h)
WMo@NGr
RMSD (Å)
Time (ps)

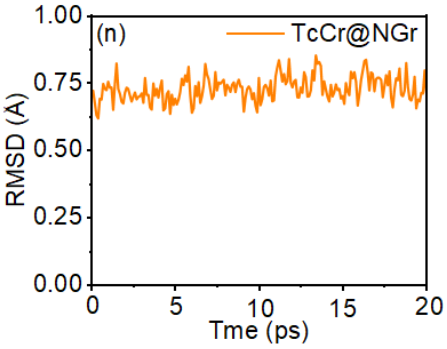

(i)
WCo@NGr
RMSD (A)
Time (ps)

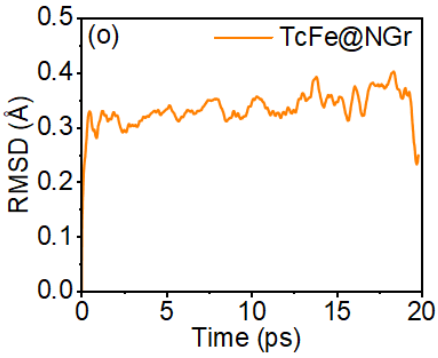

(j)
WNi@NGr
RMSD (Å)
Time (ps)

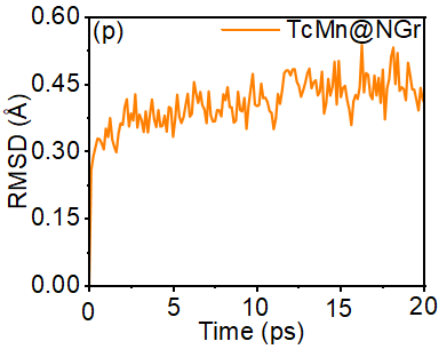

(k)
WIr@NGr
RMSD (A°)
Time (ps)


(l)
WW@NGr
RMS (A°)
Time (ps)


(m)
TcTc@NGr
RMSD (A)
Tme (ps)


(n)
TcCr@NGr
RMSD (A)
Tme (ps)


(o)
TcFe@NGr
RMSD (Å)
Time (ps)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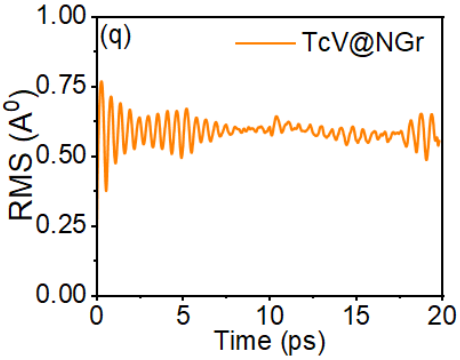
RMSD (Å)
Time (ps)


(q)
TcV@NGr
RMS (A°)
Time (ps)

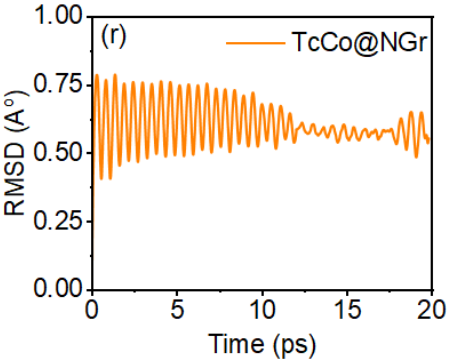

(r)
TcCo@NGr
RMSD (A°)
Time (ps)

Fig. S5 The NVT AIMD simulation at 300 K for (a)ZnNi@NGr, (b) ZnCo@NGr, (c) ZnMn@NGr, (d) ZnCr@NGr, (e) ZnV@NGr, (f) ZnTi@NGr, (g) ZnSc@NGr, (h) WMo@NGr, (i) WCo@NGr, (j) WNi@NGr, (k) WIr@NGr, (l) WW@NGr, (m) TcTc@NGr, (n) TcCr@NGr, (o) TcFe@NGr, (p) TcMn@NGr, (q) TcV@NGr and (r) TcCo@NGr performed at 300 K.

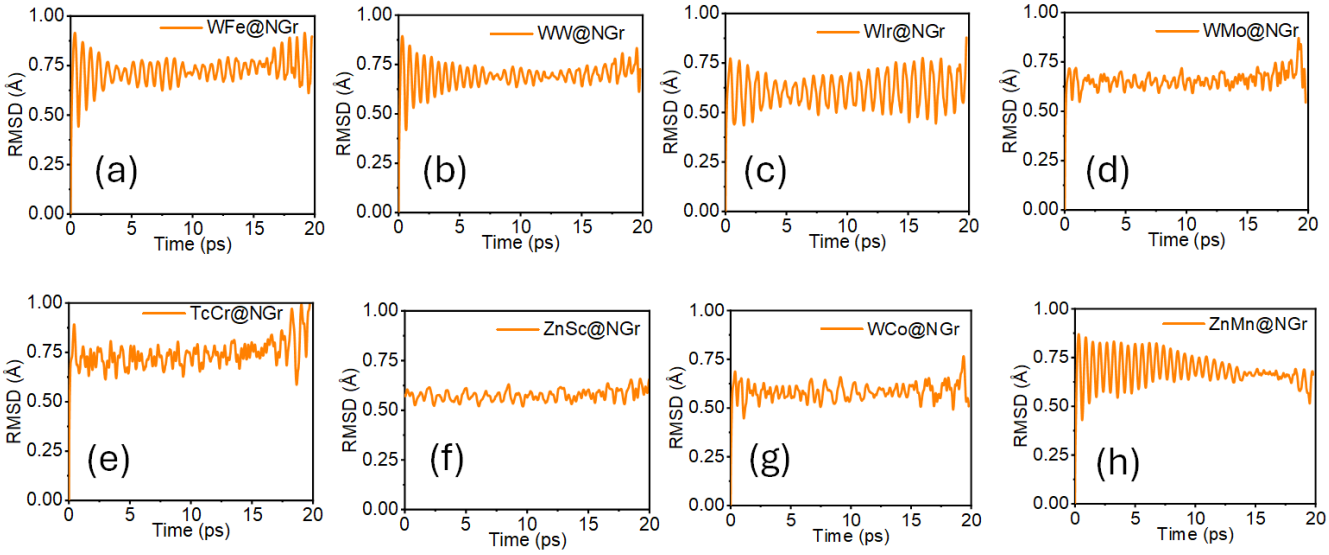
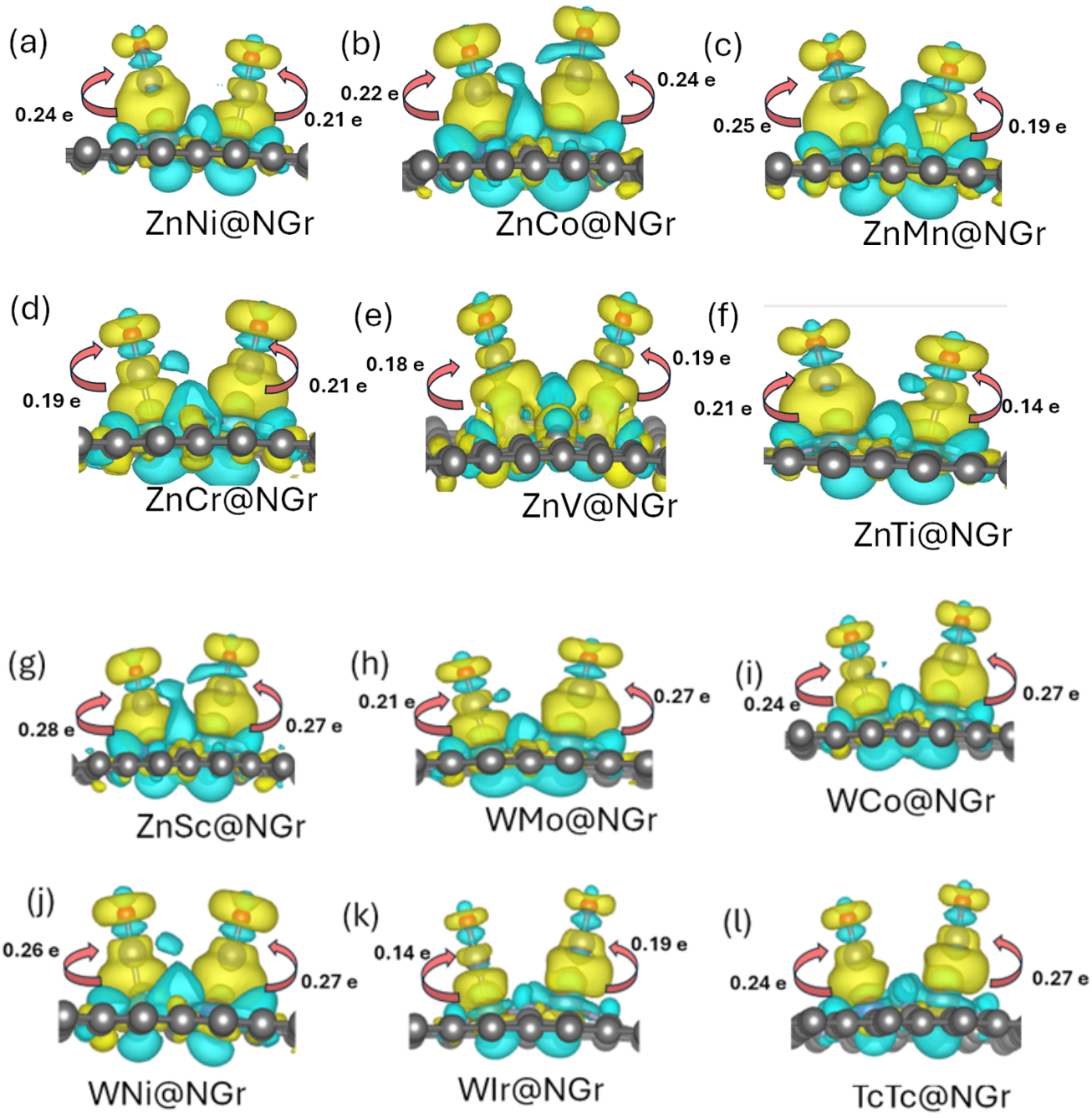


Fig. S6 The AIMD simulation performed at 700 K for (a)WFe@NGr, (b) WW@NGr, (c) WIr@NGr, (d) WMo@NGr, (e) TcCr@NGr, (f) ZnSc@NGr, (g) WCo@NGr and (i) ZnMn@NGr respectively.


(a)
0.24 e
0.21 e
ZnNi@NGr
(b)
0.22 e
0.24 e
ZnCo@NGr
(c)
0.25 e
0.19 e
ZnMn@NGr
(d)
0.19 e
0.21 e
ZnCr@NGr
(e)
0.18 e
0.19 e
ZnV@NGr
(f)
0.21 e
0.14 e
ZnTi@NGr
(g)
0.28 e
0.27 e
ZnSc@NGr
(h)
0.21 e
0.27 e
WMo@NGr
(i)
0.24 e
0.27 e
WCo@NGr
(j)
0.26 e
0.27 e
WNi@NGr
(k)
0.14 e
0.19 e
WIr@NGr
(l)
0.24 e
0.27 e
TcTc@NGr

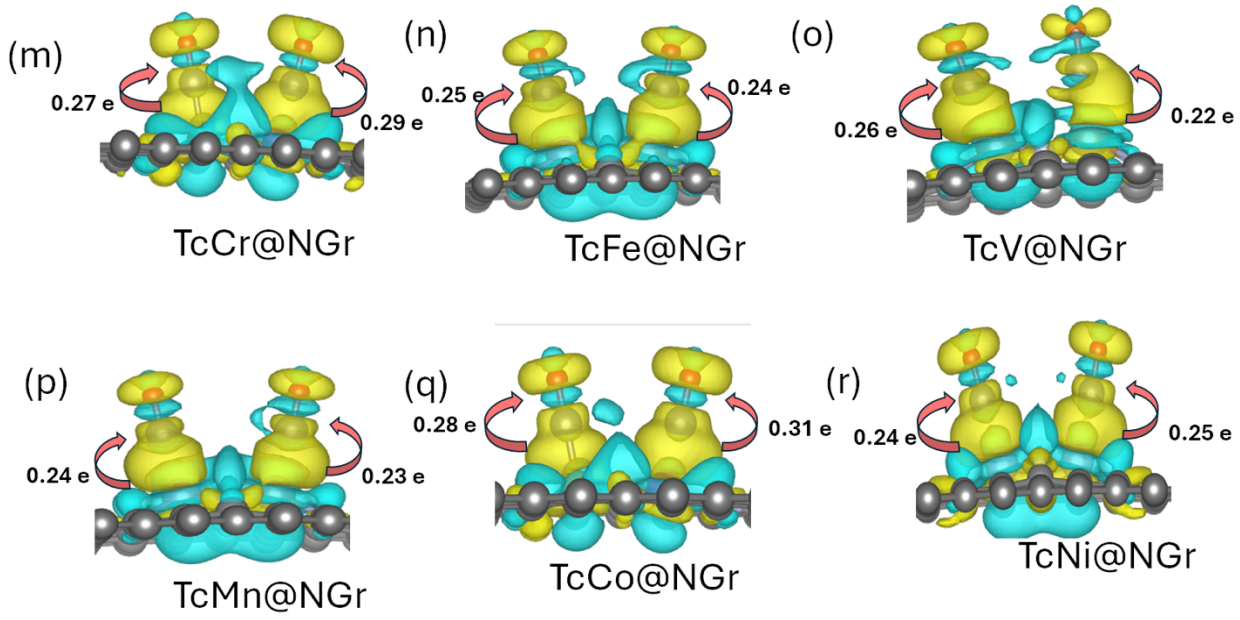
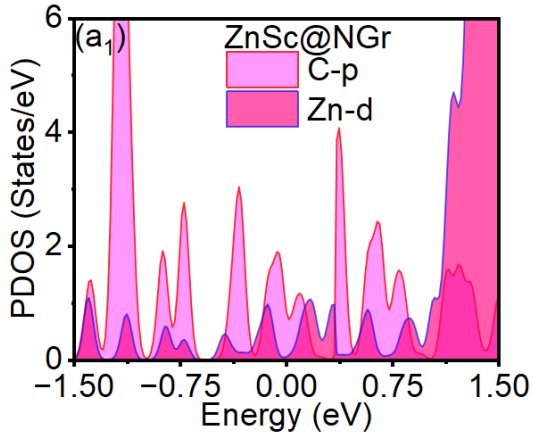
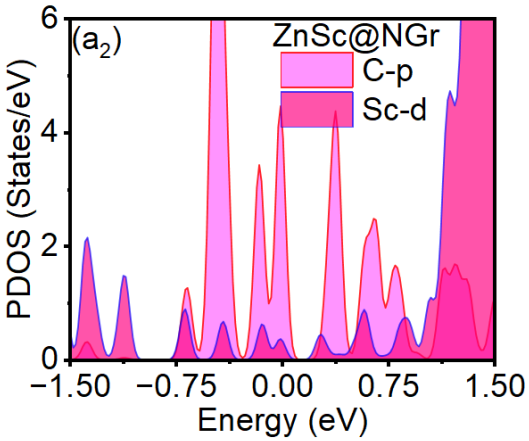
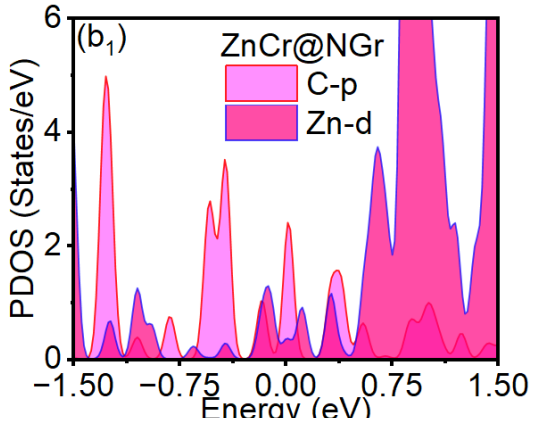
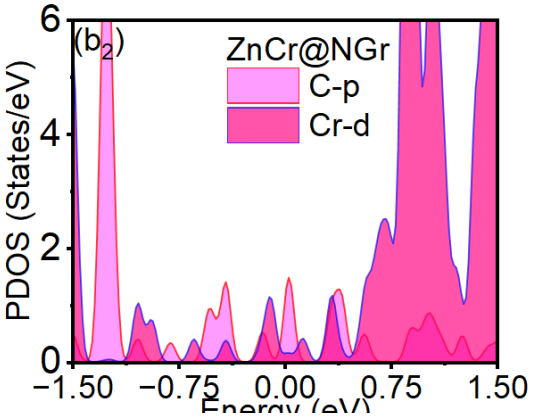


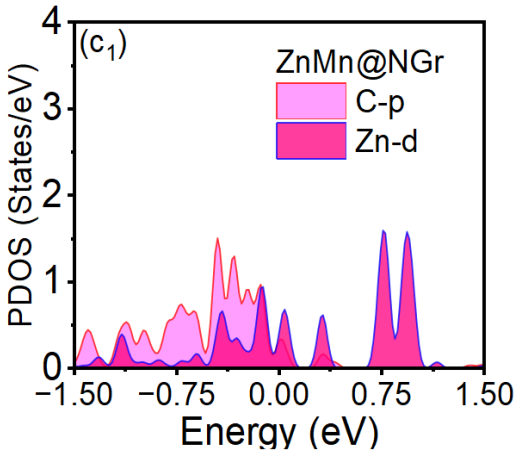
Fig. S7 charge density difference between 2CO and (a)ZnNi@NGr, (b) ZnCo@NGr, (c) ZnMn@NGr, (d) ZnCr@NGr, (e) ZnV@NGr, (f) ZnTi@NGr, (g) ZnSc@NGr, (h) WMo@NGr, (i) WCo@NGr, (j) WNi@NGr, (k) WIr@NGr, (l) WW@NGr, (m) TcTc@NGr, (n) TcCr@NGr, (o) TcFe@NGr, (p) TcMn@NGr, (q) TcV@NGr and (r) TcCo@NGr respectively.

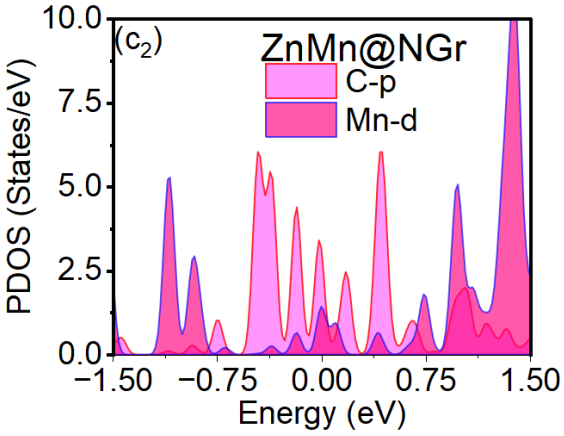

(a1)
ZnSc@NGr
C-p
Zn-d
PDOS (States/eV)
Energy (eV)

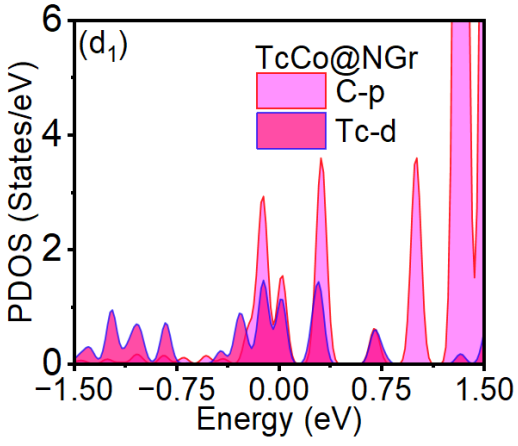

(a2)
ZnSc@NGr
C-p
Sc-d
PDOS (States/eV)
Energy (eV)

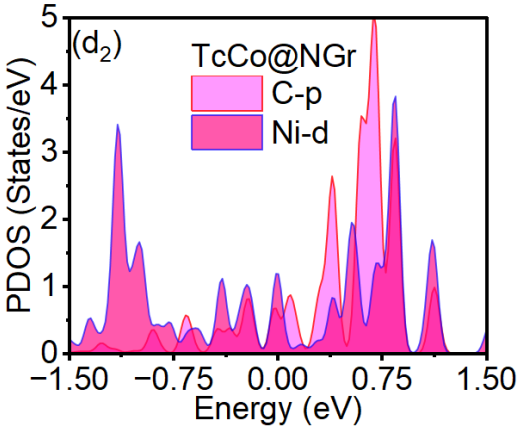

(b1)
ZnCr@NGr
C-p
Zn-d
PDOS (States/eV)
Energy (eV)

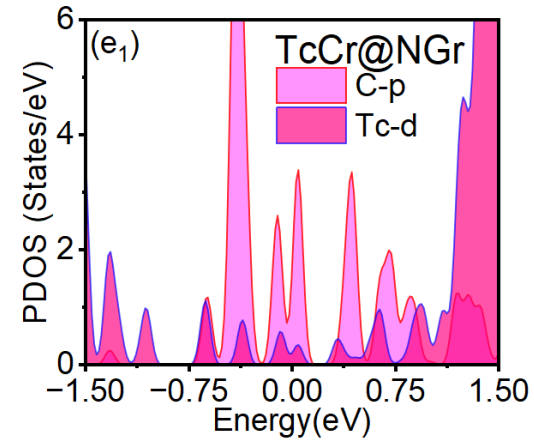

(b2)
ZnCr@NGr
C-p
Cr-d
PDOS (States/eV)

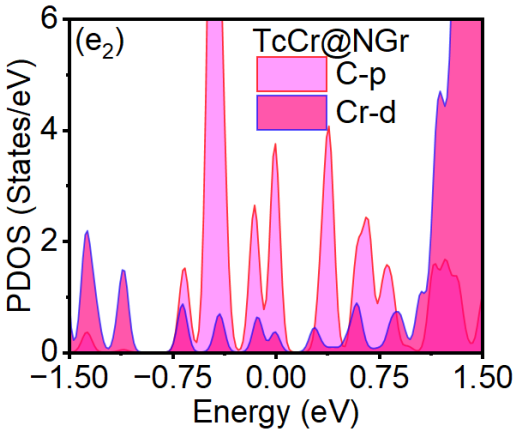

(c1)
ZnMn@NGr
C-p
Zn-d
PDOS (States/eV)
Energy (eV)

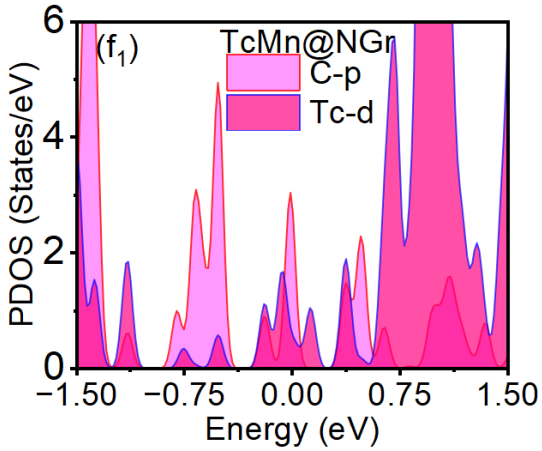

(c2)
ZnMn@NGr
C-p
Mn-d
PDOS (States/eV)
Energy (eV)

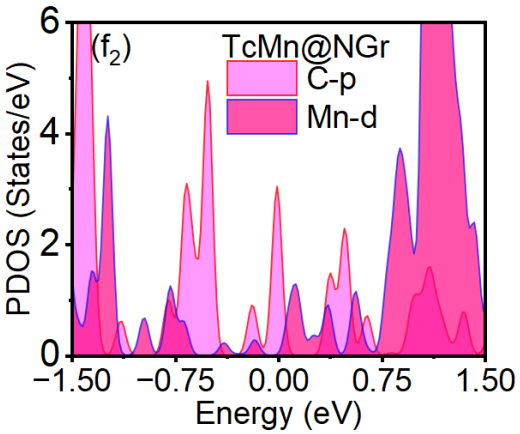

(d1)
TcCo@NGr
C-p
Tc-d
PDOS (States/eV)
Energy (eV)


(d2)
TcCo@NGr
C-p
Ni-d
PDOS (States/eV)
Energy (eV)


(e1)
TcCr@NGr
C-p
Tc-d
PDOS (States/eV)
Energy(eV)


(e2)
TcCr@NGr
C-p
Cr-d
PDOS (States/eV)
Energy (eV)


(f1)
TcMn@NGr
C-p
Tc-d
PDOS (States/eV)
Energy (eV)


(f2)
TcMn@NGr
C-p
Mn-d
PDOS (States/eV)
Energy (eV)

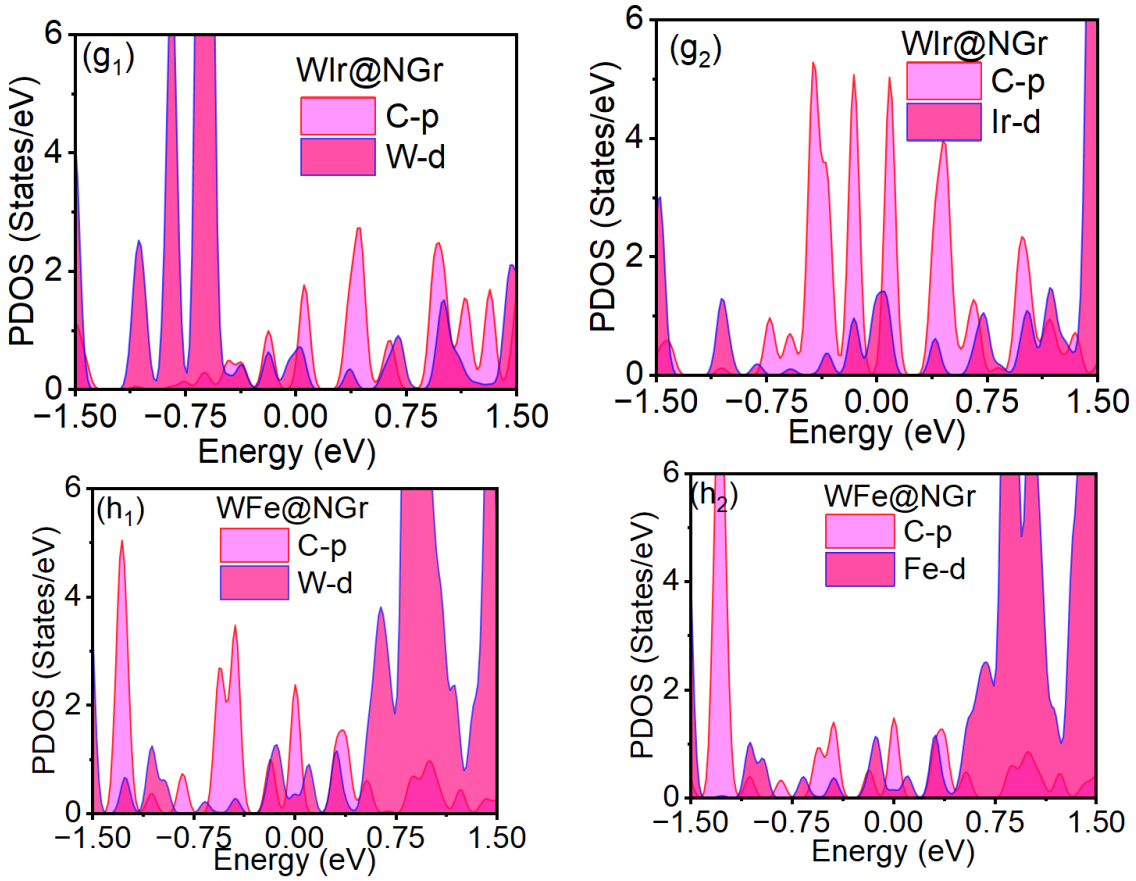


Fig. S8 The p-d hybridization between TM_1 (or TM_2) and C-p for (a_1-a_2) ZnSc@NGr, (b_1-b_2) ZnCr@NGr, (c_1-c_2) ZnMn@NGr, (d_1-d_2) TcCo@NGr, (e_1-e_2) TcCr@NGr, (f_1-f_2) TcMn@NGr, (g_1-g_2) WIr@NGr, and (h_1-h_2) WFe@NGr respectively.

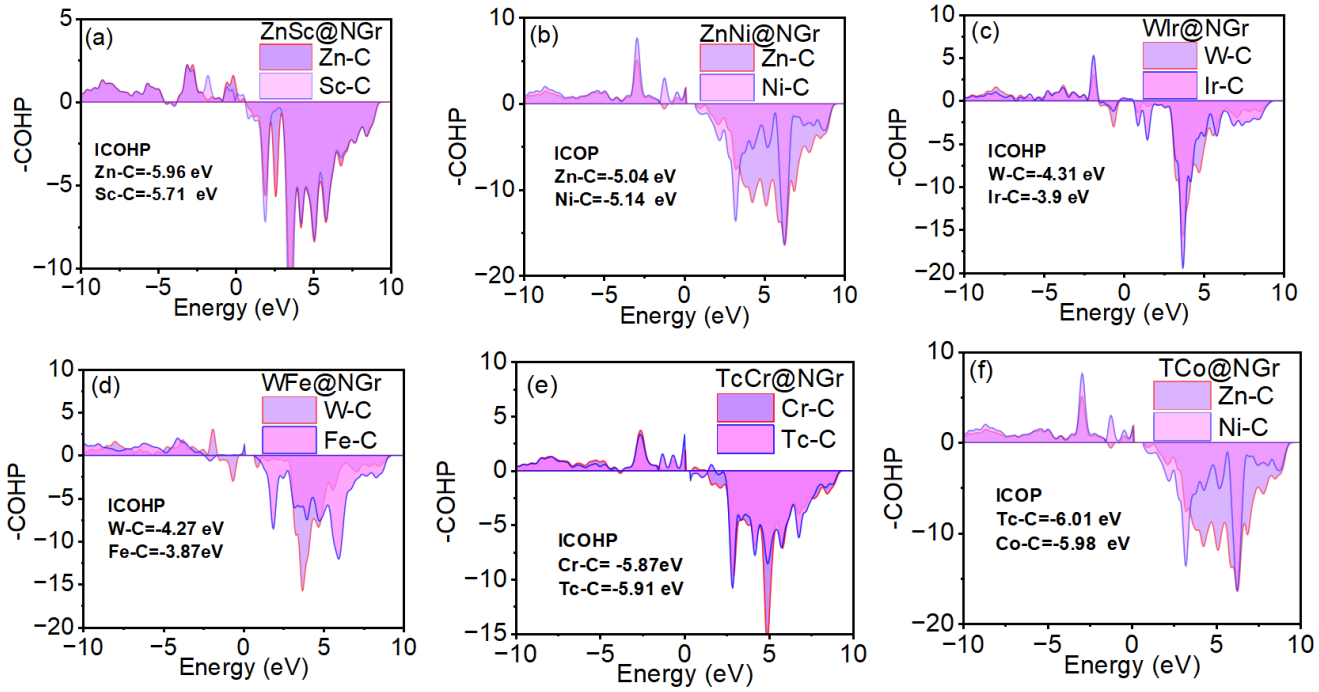


Fig. S9 The COHP plot C of adsorb CO and TM of (a) ZnSc@NGr, (b) ZnNi@NGr, (c)WIr@NGr, (d) WFe@NGr, (e) TcCr@NGr and (f) TcCo@NGr respectively.

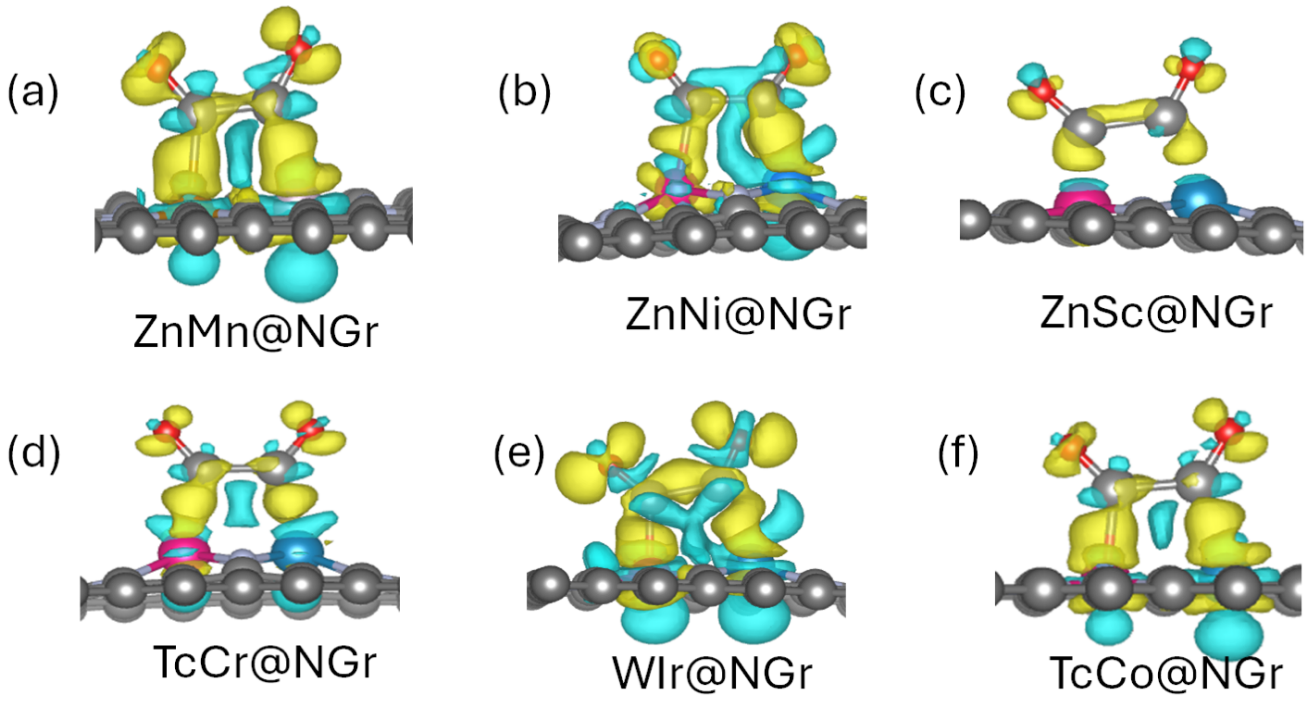


Fig. S10 the charge density difference between the COdimer and (a) ZnMn@NGr, (b) ZnNi@NGr, (c) ZnSc@NGr, (d) TcCr@NGr, (e) WIr@NGr and (f) TcCo@NGr respectively.

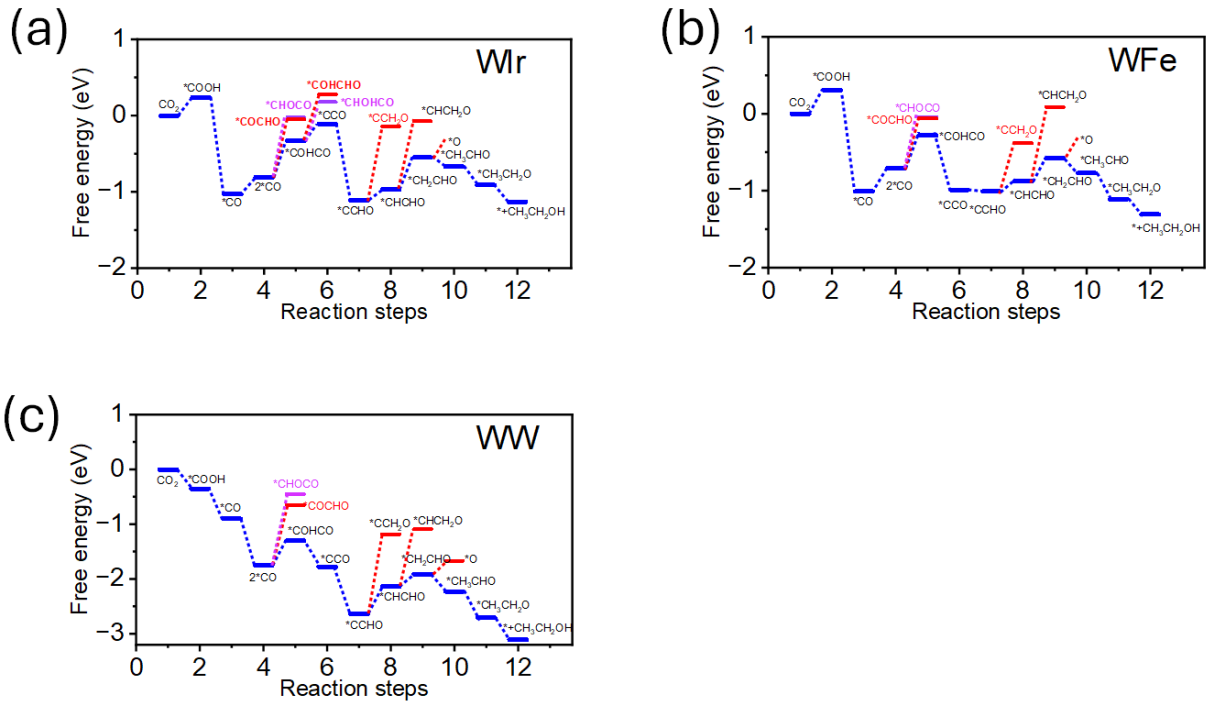
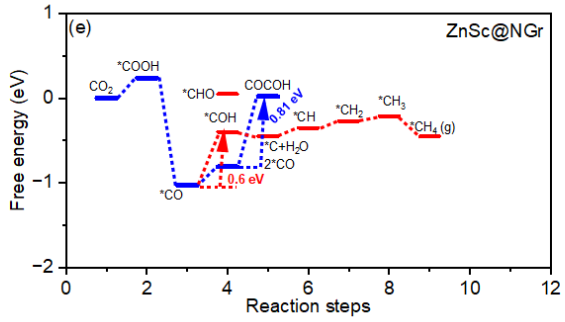
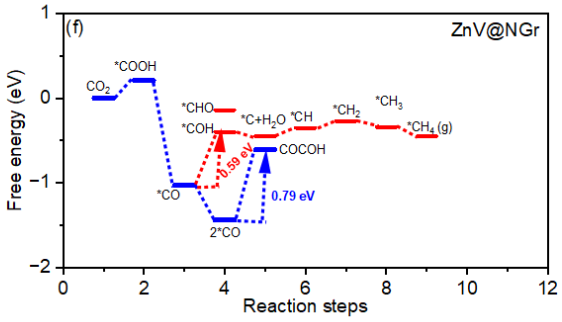
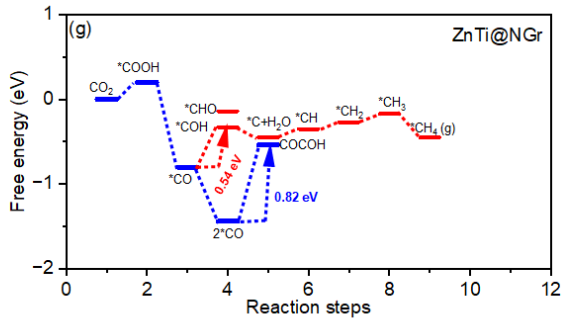
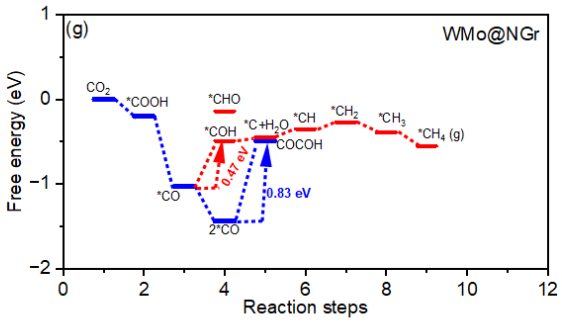


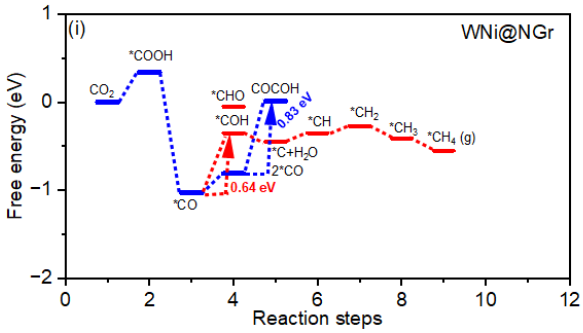
Fig. S11 (a-c) Free energy profile for CO_2ER towards ethanol production with comparison of different possible alternative intermediates on WIr@NGr, WFe@NGr and WW@NGr respectively.

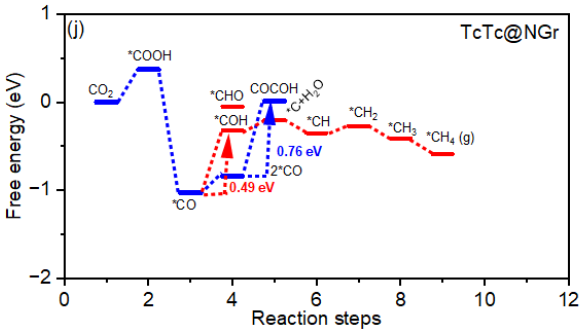

(e)
ZnSc@NGr
Free energy (eV)
Reaction steps
*COOH
CO2
*CHO
COCOH
*COH
0.81 eV
*CH
*CH2
*CH3
*CH4 (g)
*C+H2O
2*CO
0.6 eV
*CO

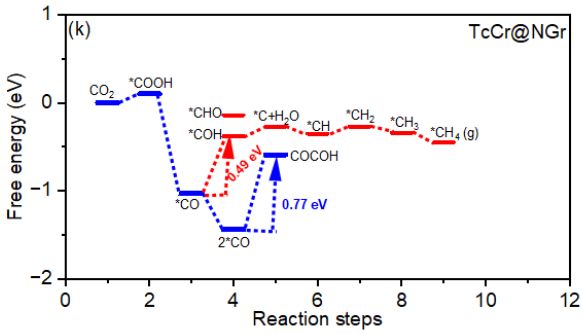

(f)
ZnV@NGr
Free energy (eV)
Reaction steps
*COOH
CO2
*CHO
*COH
*C+H2O
*CH
*CH2
*CH3
*CH4 (g)
COCOH
0.59 eV
0.79 eV
*CO
2*CO

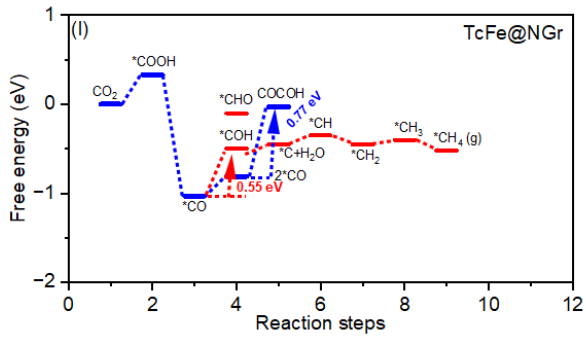

(g)
ZnTi@NGr
Free energy (eV)
Reaction steps
*COOH
CO2
*CHO
*COH
*C+H2O
*CH
*CH2
*CH3
*CH4 (g)
COCOH
0.54 eV
0.82 eV
*CO
2*CO


(g)
WMo@NGr
Free energy (eV)
Reaction steps
CO2
*COOH
*CHO
*COH
*C+H2O
*CH
*CH2
*CH3
*CH4 (g)
COCOH
0.47 eV
0.83 eV
*CO
2*CO


(i)
WNi@NGr
Free energy (eV)
Reaction steps
*COOH
CO2
*CHO
COCOH
*COH
0.83 eV
*CH
*CH2
*CH3
*CH4 (g)
*C+H2O
2*CO
0.64 eV
*CO


(j)
TcTc@NGr
Free energy (eV)
Reaction steps
*COOH
CO2
*CHO
COCOH
*C+H2O
*COH
*CH
*CH2
*CH3
*CH4 (g)
0.76 eV
2*CO
0.49 eV
*CO


(k)
TcCr@NGr
Free energy (eV)
Reaction steps
CO2
*COOH
*CHO
*C+H2O
*CH
*CH2
*CH3
*CH4 (g)
*COH
0.49 eV
COCOH
0.77 eV
*CO
2*CO


(l)
TcFe@NGr
Free energy (eV)
Reaction steps
*COOH
CO2
*CHO
COCOH
0.77 eV
*CH
*COH
*C+H2O
*CH3
*CH4 (g)
*CH2
2*CO
0.55 eV
*CO

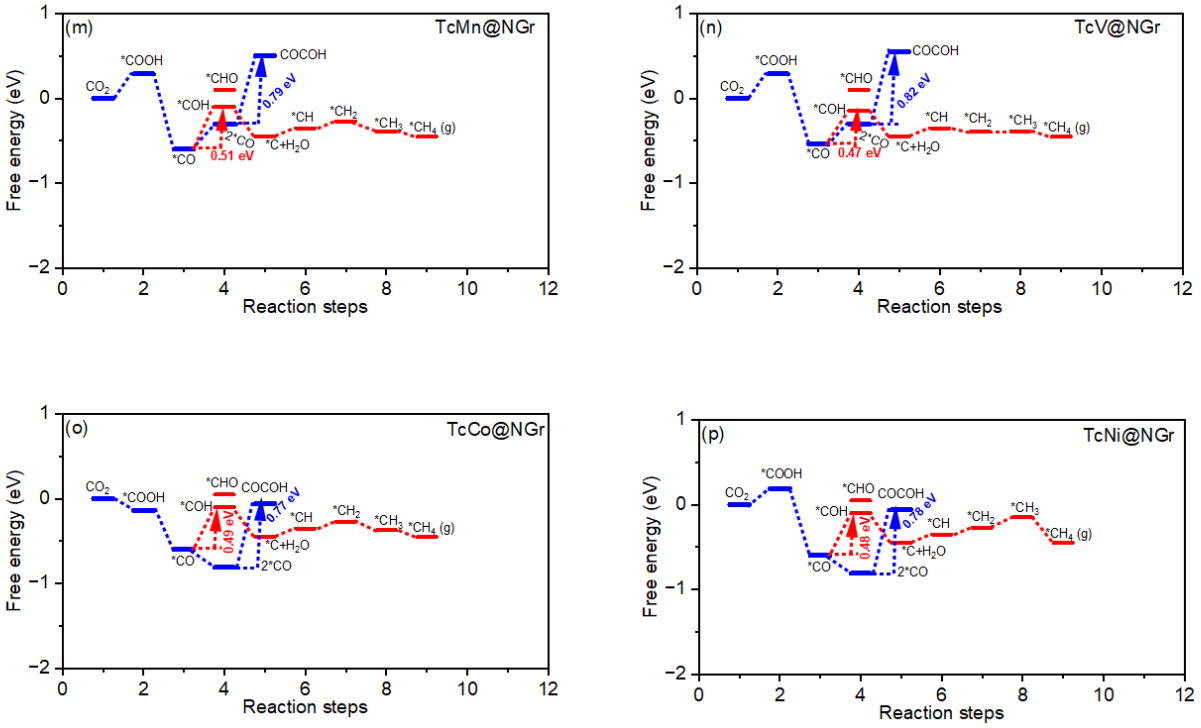


Fig. S12 Free energy profile of (a)ZnNi@NGr, (b) ZnCo@NGr, (c) ZnMn@NGr, (d) ZnCr@NGr, (e) ZnSc@NGr, (f) ZnV@NGr, (g) ZnTi@NGr, (h) WMo@NGr, (i) WCo@NGr, (j) TcTc@NGr, (k) TcCr@NGr, (l) TcFe@NGr, (m) TcMn@NGr, (n) TcV@NGr, (o) TcCo@NGr, and (p) TcNi@NGr respectively.

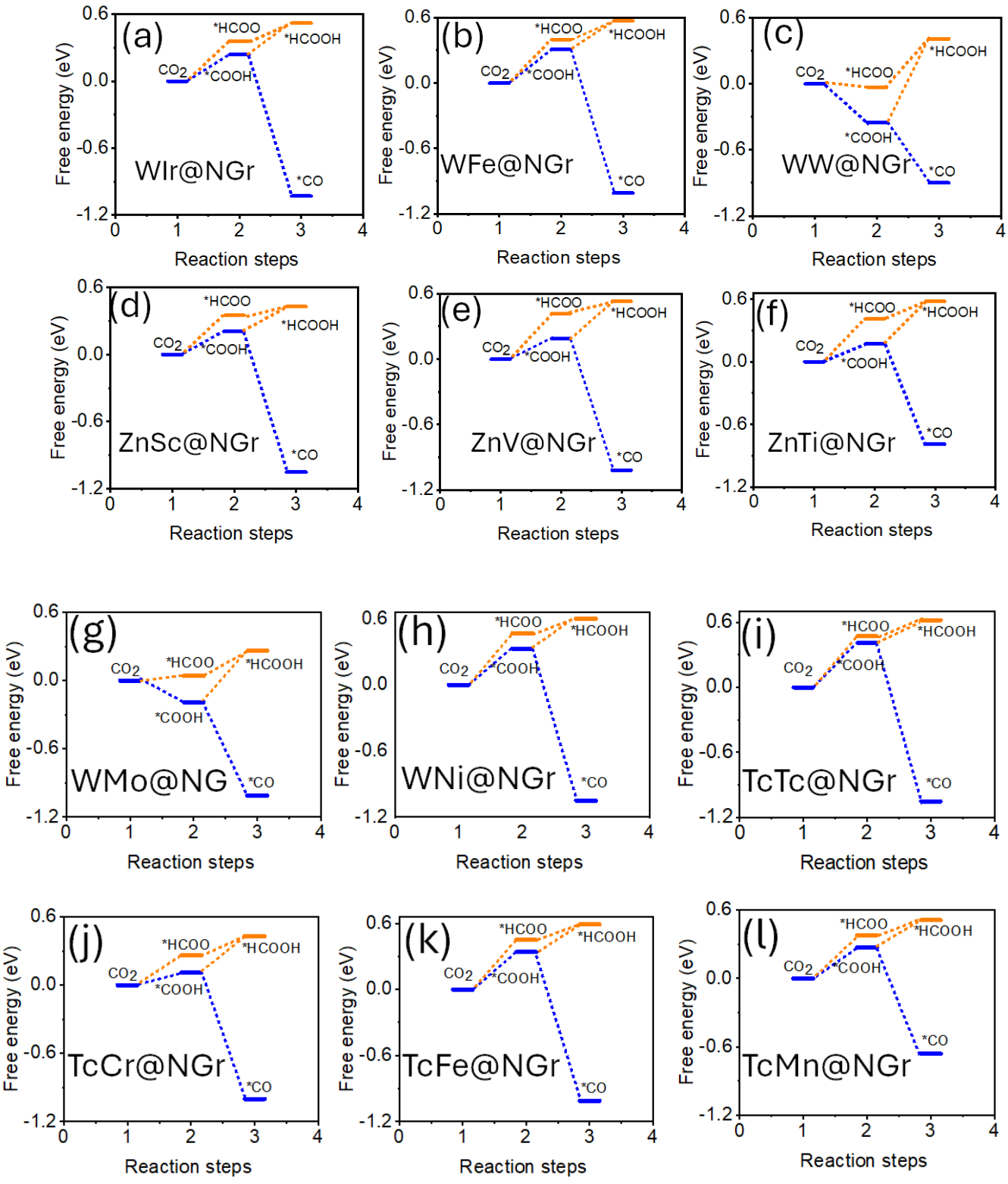


Fig. S13 For energy profile for the comparison of HCOOH and Co selectivity on (a) WIr@NGr, (b) WFe@NGr, (c) WW@NGr, (d) ZnSc@NGr, (e) ZnV@NGr, (f) ZnTi@NGr, (g) WMo@NGr, (h) WNi@NGr, (i) TcTc@NGr, (j) TcCr@NGr, (k) TcFe@NGr, and (l) TcMn@NGr respectively.

The details of electronic parameters calculation through python code

General Structure of DOSCAR File in VASP

When you perform a DOS calculation in VASP with projected DOS (PDOS), the DOSCAR file is structured to include contributions from various orbitals for each atom in the system. The format of the DOSCAR file depends on:

Whether the calculation is spin-polarized (ISPIN=2) or not (ISPIN=1).

The value of LORBIT, which controls the level of detail in the DOS output.

For LORBIT=11 or LORBIT=12, VASP outputs PDOS with orbital projections, and the DOSCAR file includes multiple columns corresponding to different orbitals.

For LORBIT =10, The DOS Files have 7 Columns

Columns and Corresponding Orbitals

When your DOS files have 7 columns, and the calculation is spin-polarized (ISPIN=2), the columns typically represent the following:

Column 1 (dos_data.iloc[:, 0]): Energy (E)

Column 2 (dos_data.iloc[:, 1]): Total DOS spin-up

Column 3 (dos_data.iloc[:, 2]): Total DOS spin-down

Column 4 (dos_data.iloc[:, 3]): Integrated DOS spin-up

Column 5 (dos_data.iloc[:, 4]): Integrated DOS spin-down

Column 6 (dos_data.iloc[:, 5]): Projected DOS of a specific orbital (spin-up)

Column 7 (dos_data.iloc[:, 6]): Projected DOS of the same orbital (spin-down)

Specific Orbital Projections

Given that your code extracts dos_pz_up and dos_pz_down from columns 5 and 6:

python code

```
dos_pz_up = dos_data.iloc[:, 5].values  # Column 6

dos_pz_down = dos_data.iloc[:, 6].values  # Column 7
```

This suggests that columns 6 and 7 correspond to the projected DOS of the p_z orbital for spin-up and spin-down electrons, respectively.

Summary of Columns in the 7-Column DOS File

Column 0: Energy (E)

Column 1: Total DOS spin-up

Column 2: Total DOS spin-down

Column 3: Integrated DOS spin-up

Column 4: Integrated DOS spin-down

Column 5: Projected DOS of p_z orbital spin-up (dos_pz_up)

Column 6: Projected DOS of p_z orbital spin-down (dos_pz_down)

Relation to Your Code

In your code, when num_columns == 7, you are specifically analyzing the p_z orbital contributions:

Python code

```
if num_columns == 7:
    energy = dos_data.iloc[:, 0].values  # Energy
    dos_pz_up = dos_data.iloc[:, 5].values  # p_z spin-up
    dos_pz_down = dos_data.iloc[:, 6].values  # p_z spin-down
    pz = dos_pz_up - dos_pz_down  # Net p_z DOS
    # Further calculations...
```

For LORBIT =11 The DOS Files have 19 Columns

Columns and Corresponding Orbitals

When your DOS files have 19 columns, and the calculation is spin-polarized (ISPIN=2), the columns represent projections onto different atomic orbitals for both spin channels.

Here is the typical arrangement:

Column 1 (dos_data.iloc[:, 0]): Energy (E)

Columns 2-3 (dos_data.iloc[:, 1:3]): s orbital DOS (spin-up and spin-down)

Columns 4-5 (dos_data.iloc[:, 3:5]): p_y orbital DOS (spin-up and spin-down)

Columns 6-7 (dos_data.iloc[:, 5:7]): p_z orbital DOS (spin-up and spin-down)

Columns 8-9 (dos_data.iloc[:, 7:9]): p_x orbital DOS (spin-up and spin-down)

Columns 10-11 (dos_data.iloc[:, 9:11]): d_xy orbital DOS (spin-up and spin-down)

Columns 12-13 (dos_data.iloc[:, 11:13]): d_yz orbital DOS (spin-up and spin-down)

Columns 14-15 (dos_data.iloc[:, 13:15]): d_{z^2} orbital DOS (spin-up and spin-down)

Columns 16-17 (dos_data.iloc[:, 15:17]): d_xz orbital DOS (spin-up and spin-down)

Columns 18-19 (dos_data.iloc[:, 17:19]): $d_{x^2-y^2}$ orbital DOS (spin-up and spin-down)

Summary of Columns in the 19-Column DOS File

Column 0: Energy (E)

Column 1: s orbital DOS spin-up

Column 2: s orbital DOS spin-down

Column 3: p_y orbital DOS spin-up

Column 4: p_y orbital DOS spin-down

Column 5: p_z orbital DOS spin-up

Column 6: p_z orbital DOS spin-down

Column 7: p_x orbital DOS spin-up

Column 8: p_x orbital DOS spin-down

Column 9: d_xy orbital DOS spin-up

Column 10: d_xy orbital DOS spin-down

Column 11: d_yz orbital DOS spin-up

Column 12: d_yz orbital DOS spin-down

Column 13: d_{z^2} orbital DOS spin-up

Column 14: d_{z^2} orbital DOS spin-down

Column 15: d_xz orbital DOS spin-up

Column 16: d_xz orbital DOS spin-down

Column 17: $d_{x^2-y^2}$ orbital DOS spin-up

Column 18: $d_{x^2-y^2}$ orbital DOS spin-down

Relation to Your Code

In your code, when num_columns == 19, you are analyzing the t2g and eg orbitals:

Python code

```
  if num_columns == 19:
energy = dos_data.iloc[:, 0].values  # Energy
 # t2g orbitals: d_xy, d_yz, d_xz
```

t2g_up = (dos_data.iloc[:, 9] + dos_data.iloc[:, 11] + dos_data.iloc[:, 15]).values t2g_down = (dos_data.iloc[:, 10] + dos_data.iloc[:, 12] + dos_data.iloc[:, 16]).values

eg orbitals: d_z², d_x²−y²

eg_up = (dos_data.iloc[:, 13] + dos_data.iloc[:, 17]).values

eg_down = (dos_data.iloc[:, 14] + dos_data.iloc[:, 18]).values

z-component orbitals (for example, combining d_z² and p_z)

zc_up = (dos_data.iloc[:, 13] + dos_data.iloc[:, 5] + dos_data.iloc[:, 7]).values

zc_down = (dos_data.iloc[:, 14] + dos_data.iloc[:, 6] + dos_data.iloc[:, 8]).values

Further calculations...

t_{2g} orbitals (Columns):

d_xy spin-up (dos_data.iloc[:, 9])

d_yz spin-up (dos_data.iloc[:, 11])

d_xz spin-up (dos_data.iloc[:, 15])

Corresponding spin-down columns are one index higher.

e_g orbitals (Columns):

d_z² spin-up (dos_data.iloc[:, 13])

d_x²−y² spin-up (dos_data.iloc[:, 17])

Corresponding spin-down columns are one index higher.

z-component orbitals (zc):

Combines d_z², p_z, and possibly other orbitals with significant z-character.

Explanation of t2g and eg Orbitals

t2g Orbitals: These are the three d orbitals that have lobes pointing between the axes in a Cartesian coordinate system:

d_xy

d_yz

d_xz

eg Orbitals: These are the two d orbitals that have lobes pointing along the axes:

d_z² (also written as d_3z²−r²)

d_x²−y²

Mapping of Columns to Orbitals (19 Columns)

Column Index	Orbital	Spin Channel
0	Energy (E)	N/A
1	s	Up
2	s	Down
3	p_y	Up
4	p_y	Down
5	p_z	Up
6	p_z	Down
7	p_x	Up
8	p_x	Down
9	d_xy	Up
10	d_xy	Down
11	d_yz	Up
12	d_yz	Down
13	d_{z^2}	Up
14	d_{z^2}	Down
15	d_xz	Up
16	d_xz	Down
17	$d_{x^2-y^2}$	Up
18	$d_{x^2-y^2}$	Down

Orbital Occupancy: By integrating the DOS over the energy range.

Band Centers: Calculated as weighted averages of energy and DOS.

DOS at Fermi Level: The value of DOS at the Fermi energy.

Frontier Orbital Analysis: Considering energy ranges near the Fermi level (e.g., between -1 eV and 1 eV).

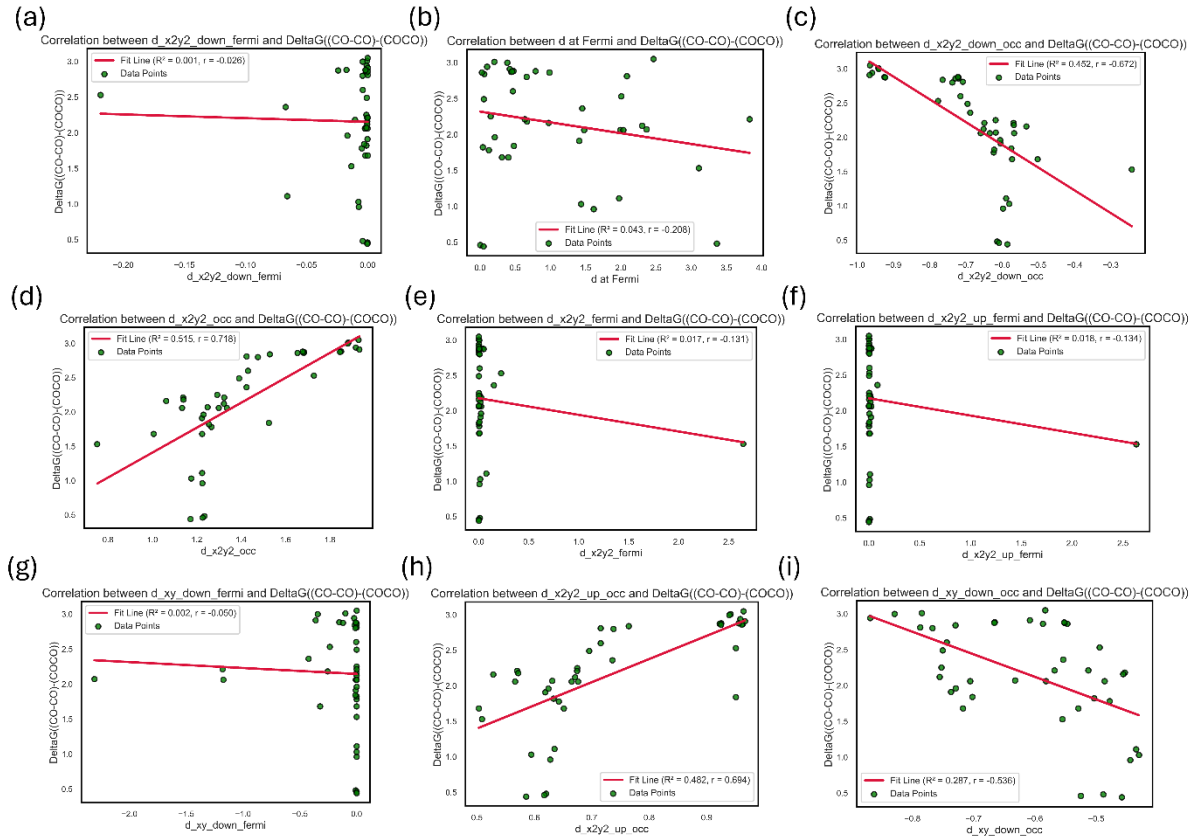


Fig. s14 (a-i) Linear correlation between free energy difference and various electronic parameters.

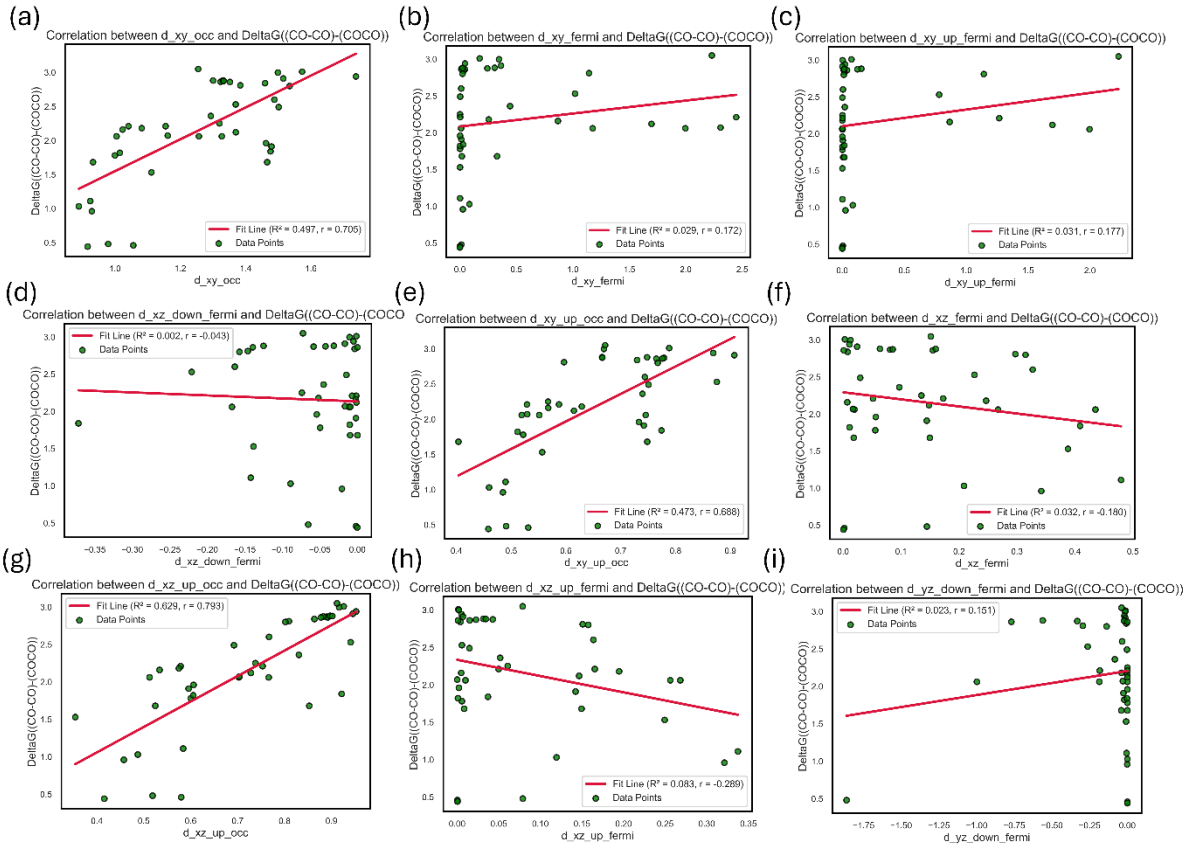


Fig. s15(a-i) Linear correlation between free energy difference and various electronic parameters.

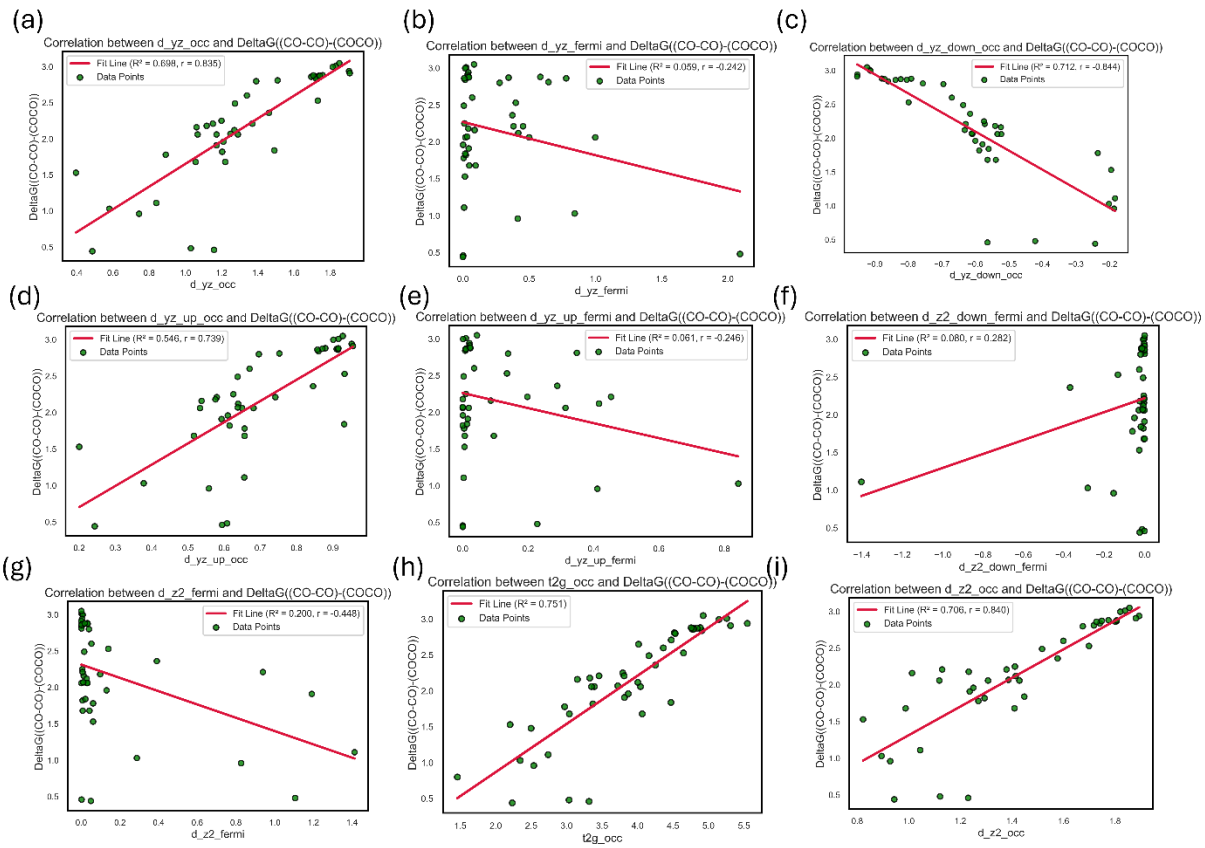


Fig. s16(a-i) Linear correlation between free energy difference and various electronic parameters.

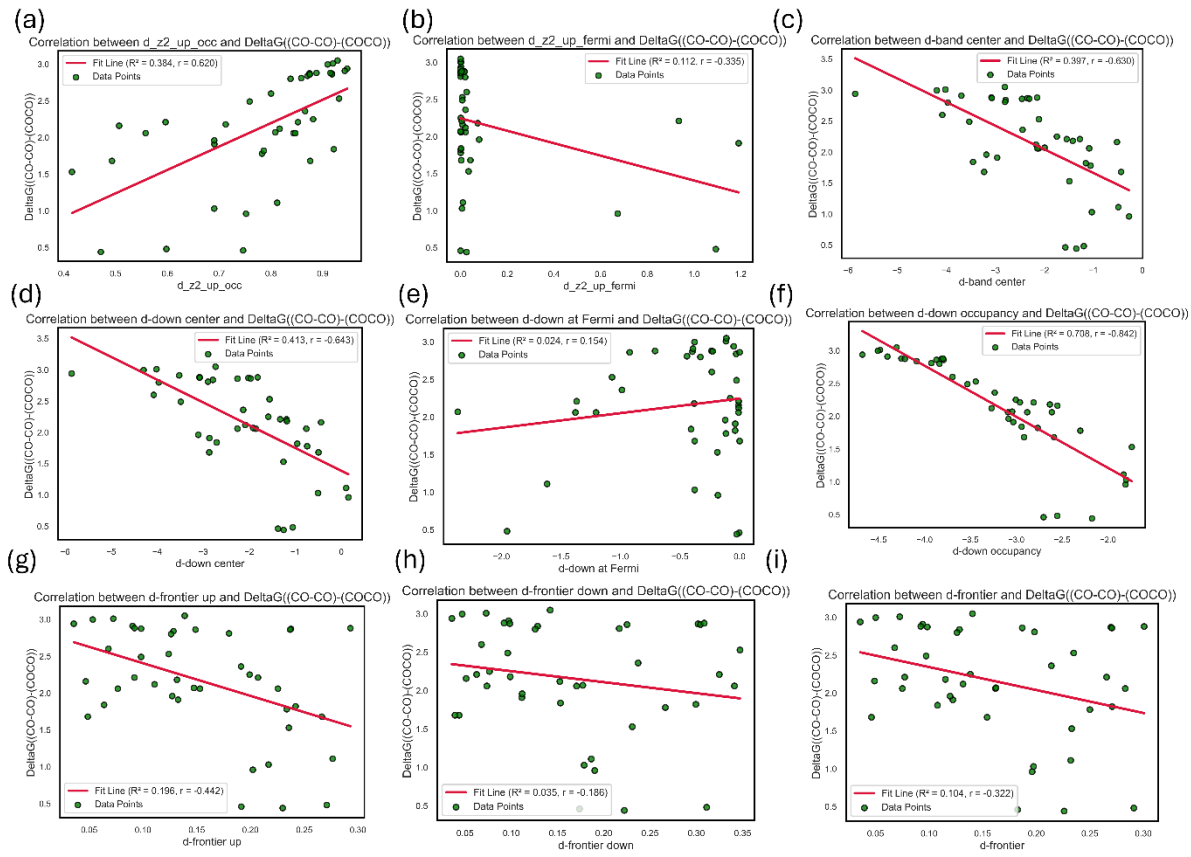


Fig. s17(a-i) Linear correlation between free energy difference and various electronic parameters.

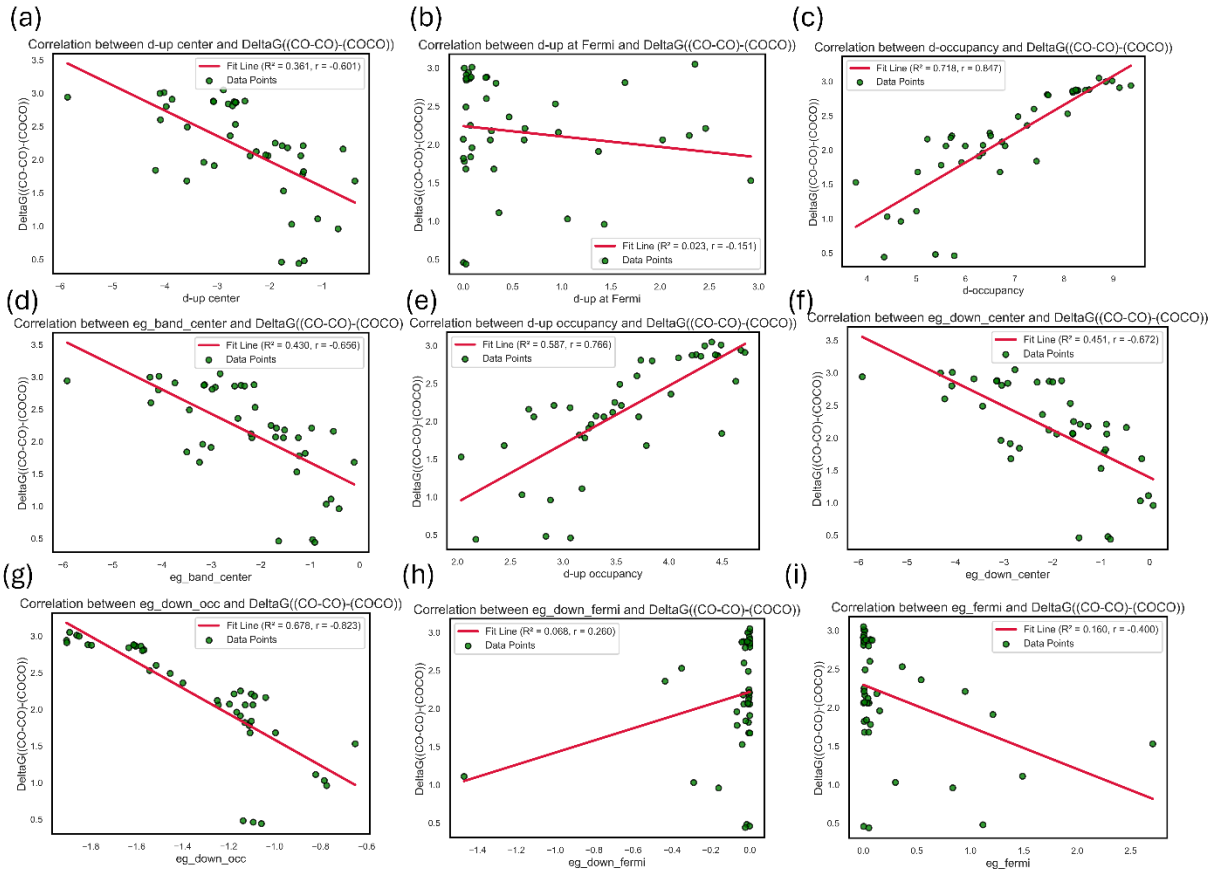


Fig. s18(a-i) Linear correlation between free energy difference and various electronic parameters.

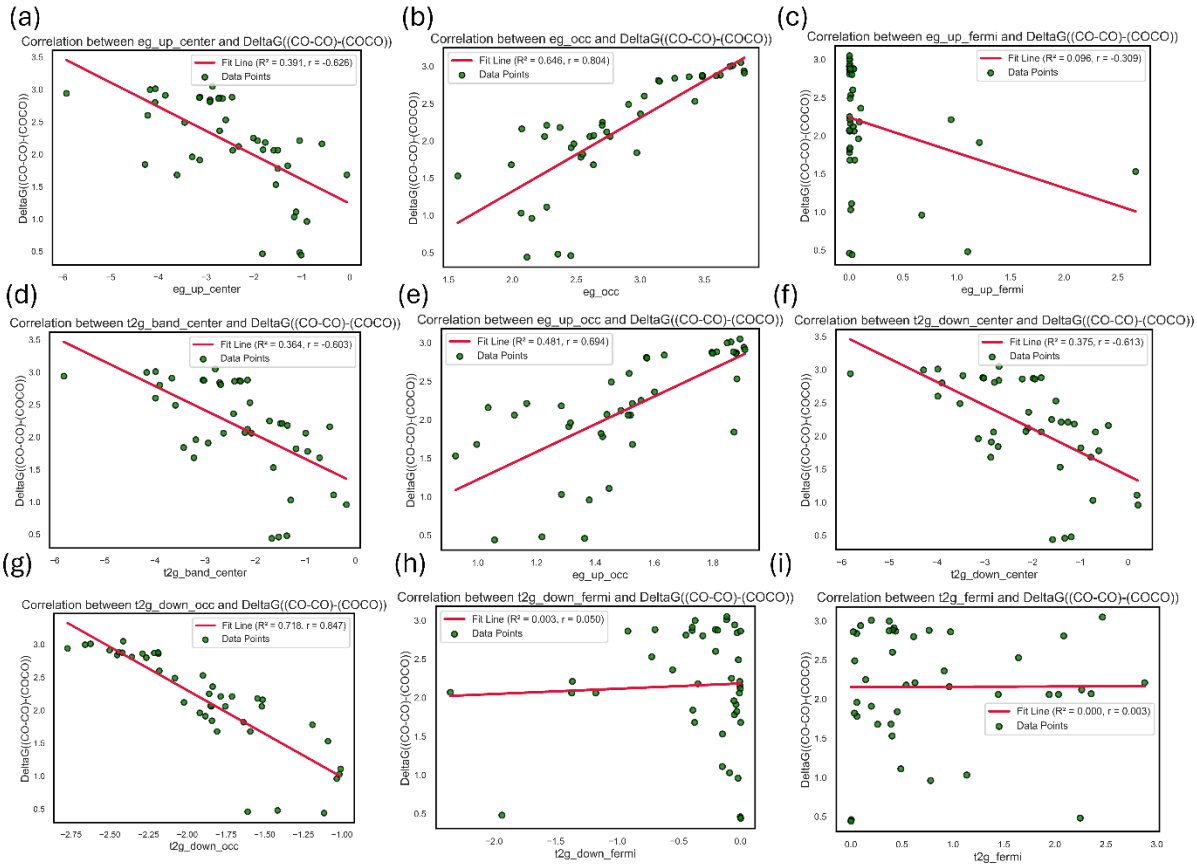


Fig. s19(a-i) Linear correlation between free energy difference and various electronic parameters.

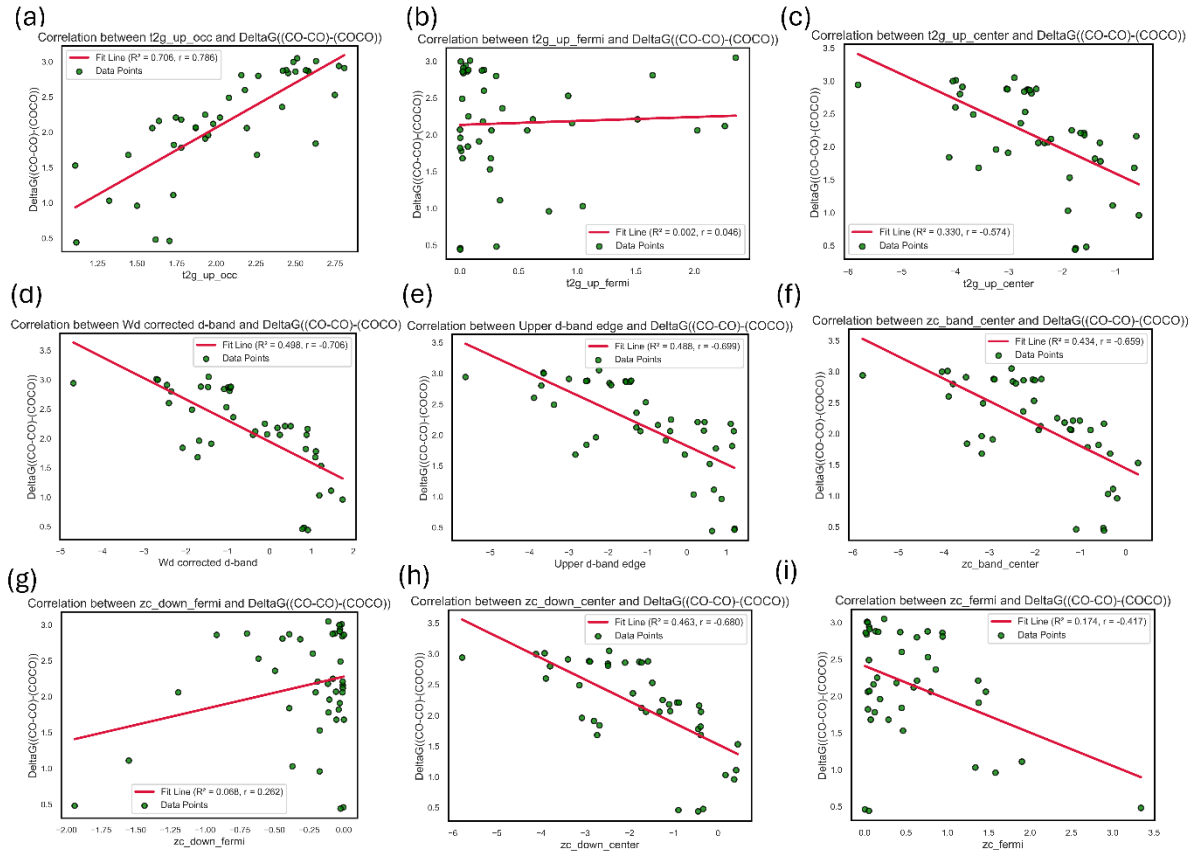


Fig. s20(a-i) Linear correlation between free energy difference and various electronic parameters.

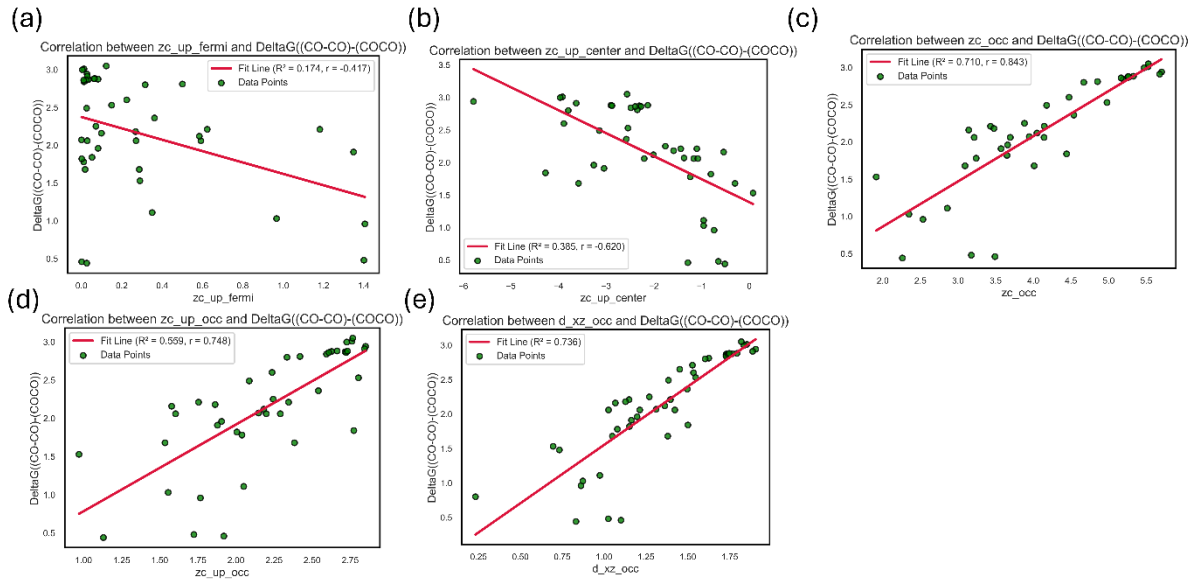


Fig. s21(a-i) Linear correlation between free energy difference and various electronic parameters.