

Supporting Information

Transition metal atom doping engineering of two-dimensional pentagonal PtN₂: a theoretical tri-functional electrocatalyst for OER, ORR, and HER

Computational methods

For ORR and OER in acidic electrolyte, the reaction processes can be broken down into a reaction pathway involving four consecutive electron transfers, but the reaction direction is opposite [1]:



Herein, * denotes the active sites on the catalyst surface, while O*, OH* and OOH* correspond to three key intermediates involved throughout the entire reaction pathway.

The adsorption energy of the intermediate was calculated according to the following equation:

$$\Delta E_{O^*} = E_{O^*} - E_* - (E_{H_2O} - E_{H_2}) \quad (S5)$$

$$\Delta E_{OH^*} = E_{OH^*} - E_* - (E_{H_2O} - \frac{1}{2}E_{H_2}) \quad (S6)$$

$$\Delta E_{OOH^*} = E_{OOH^*} - E_* - (2E_{H_2O} - \frac{3}{2}E_{H_2}) \quad (S7)$$

where E_* , E_{OH^*} , E_{O^*} , and E_{OOH^*} represent the total energy of the catalyst separated and when catalyst combined with OH*, O*, and OOH* respectively.

$E_{\text{H}_2\text{O}}$ and E_{H_2} denote the total energies of H_2O in the liquid and H_2 molecules in the gas phase respectively.

The free energies ΔG_i ($\text{i}=\text{O}^*$, OH^* , OOH^*) of key intermediates were calculated based on theoretical hydrogen electrode (CHE) model [2]:

$$\Delta G_i = \Delta E_i + \Delta E_{\text{ZPE}} - T\Delta S + \Delta G_{\text{pH}} + \Delta G_U \quad (\text{S8})$$

where ΔE_i represents the adsorption energy of the intermediate, ΔE_{ZPE} denotes the zero-point energy correction, T is fixed at 298.15 K, and ΔS corresponds to the entropy variation during the reaction process. $\Delta G_{\text{pH}} = -k\text{B}T\ln(10) \cdot \text{pH}$, We applies a PH value of 0, where ΔG_{pH} denotes the free energy correction for H^+ considering concentration effects. Additionally, the applied electrode potential contributes to the system via $\Delta G_U = -eU$. The free energy change of each step can be described as:

$$\Delta G_1 = \Delta G_{\text{OH}^*} \quad (\text{S9})$$

$$\Delta G_2 = \Delta G_{\text{O}^*} - \Delta G_{\text{OH}^*} \quad (\text{S10})$$

$$\Delta G_3 = \Delta G_{\text{OOH}^*} - \Delta G_{\text{O}^*} \quad (\text{S11})$$

$$\Delta G_4 = 4.92 - \Delta G_{\text{OOH}^*} \quad (\text{S12})$$

$$\Delta G_5 = \Delta G_{\text{OOH}^*} - 4.92 \quad (\text{S13})$$

$$\Delta G_6 = \Delta G_{\text{O}^*} - \Delta G_{\text{OOH}^*} \quad (\text{S14})$$

$$\Delta G_7 = \Delta G_{\text{OH}^*} - \Delta G_{\text{O}^*} \quad (\text{S15})$$

$$\Delta G_8 = -\Delta G_{\text{OH}^*} \quad (\text{S16})$$

Using the free energy data presented above, the overpotential for ORR and OER can be calculated by applying Equations (S17) and (S18):

$$\eta^{OER} = \frac{\max [\Delta G_1, \Delta G_2, \Delta G_3, \Delta G_4]}{e} - 1.23V \quad (S17)$$

$$\eta^{ORR} = \frac{\max [-\Delta G_1, -\Delta G_2, -\Delta G_3, -\Delta G_4]}{e} \quad (S18)$$

Define η to evaluate OER and ORR bifunctional electrocatalytic performance:

$$\eta^{OER + ORR} = \eta^{OER} + \eta^{ORR} \quad (S19)$$

In an acidic environment at pH=0, the HER reaction process is defined as:



Gibbs free energy of hydrogen adsorption (ΔG_{H^*}) is a key indicator for evaluating HER, defined as:

$$\Delta G_H = \Delta E_{H^*} + \Delta E_{ZPE} - T\Delta S \quad (S22)$$

where ΔE_{H^*} is the adsorption energy of hydrogen, with its definition given by:

$$\Delta E_{H^*} = E_{H^*} - E_* - \frac{1}{2}E_{H_2} \quad (S23)$$

where E_{H^*} , E_* and E_{H_2} represent the total energy of H atoms adsorbed on the catalyst, the original catalyst and the H_2 molecule respectively.

the overpotential of HER can be obtained using equation (20):

$$\eta^{HER} = \frac{-|\Delta G_{H^*}|}{e} \quad (S24)$$

To determine the stability of the doped system, the binding energy (E_{bind}) and the cohesive energy (E_{coh}) are calculated [3-4]:

$$E_{bind} = E_d - E_V - xE_{single} \quad (S25)$$

$$E_{coh} = (E_d - E_{TM} - aE_{Pt} - bE_N)/n \quad (S26)$$

Specifically, E_d , E_v and E_{Single} are defined as the energies of the doped system, vacancy system, and individual dopant atom, x herein refers to the quantity of dopant atoms.

E_{TM} , E_{Pt} , E_N are the energy of transition metal atoms, Pt atom and N atom, with n standing for the overall number of atoms in the studied system.

We define the dissolution potential (U_{diss}) [5]:

$$U_{diss} = U_{diss}^0(metal,bulk) - \frac{E_{bind}}{ne} \quad (S27)$$

References

- [1] T. Liu, J. Lu, Z. Chen, Z. Luo, Y. Ren, X. Zhuge, K. Luo, G. Ren, W. Lei, D. Liu, Chem. Eng. J. 496 (2024) 153719.
- [2] H. Xu, D. Cheng, D. Cao, X.C. Zeng, Nat. Catal. 1 (2018) 339–348.
- [3] X. Liu, Z. Gao, V. Wang, Z. Luo, B. Lv, Z. Ding, Z. Zhang, ACS Appl. Mater. Interfaces, 12 (2020) 17055–17061.
- [4] J. Hao, Y. Ma, B. Jia, X. Zhang, C. Zhang, Ge Wu, W. Chen, Y. Li, P. Lu, Int. J. Hydrogen Energy. 62 (2024) 462-272.
- [5] X. Guo, J. Gu, S. Lin, S. Zhang, Z. Chen, S. Huang, J. Am. Chem. Soc. 142 (2020) 5709–5721.

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Fig. S5 The volcano diagrams of OER corresponding to the TM/V_{Pt}-PtN₂ systems.

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Table S7 Binding energies (E_{bind}) of TM/V_{Pt}-PtN₂, cohesive energies (E_{coh}) of TM atoms in bulk, the standard dissolution potentials ($U_{\text{diss-bulk}}$) of TM bulk, the number of transferred electrons (n) during the process of dissolution, and the calculated dissolution potentials (U_{diss}) of TM atoms on TM/V_{Pt}-PtN₂.

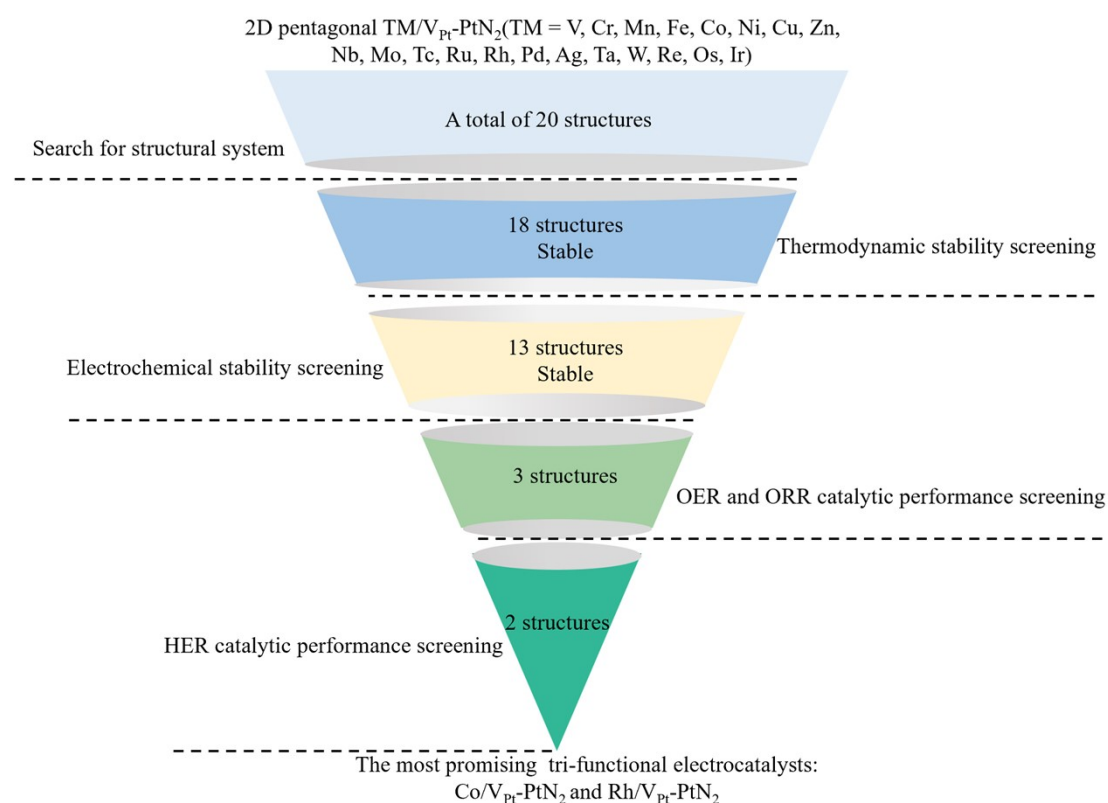


Fig. S1 Schematic diagram of using first principles calculations to screen potential tri-functional electrocatalysts

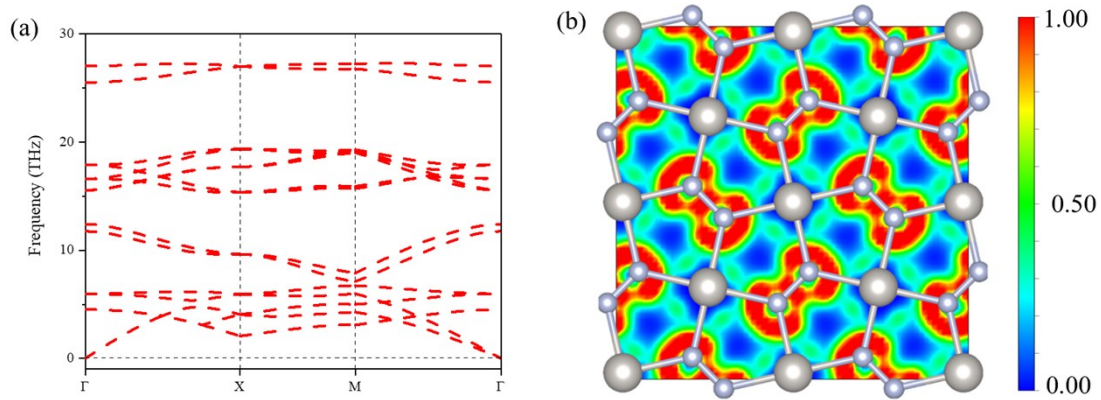
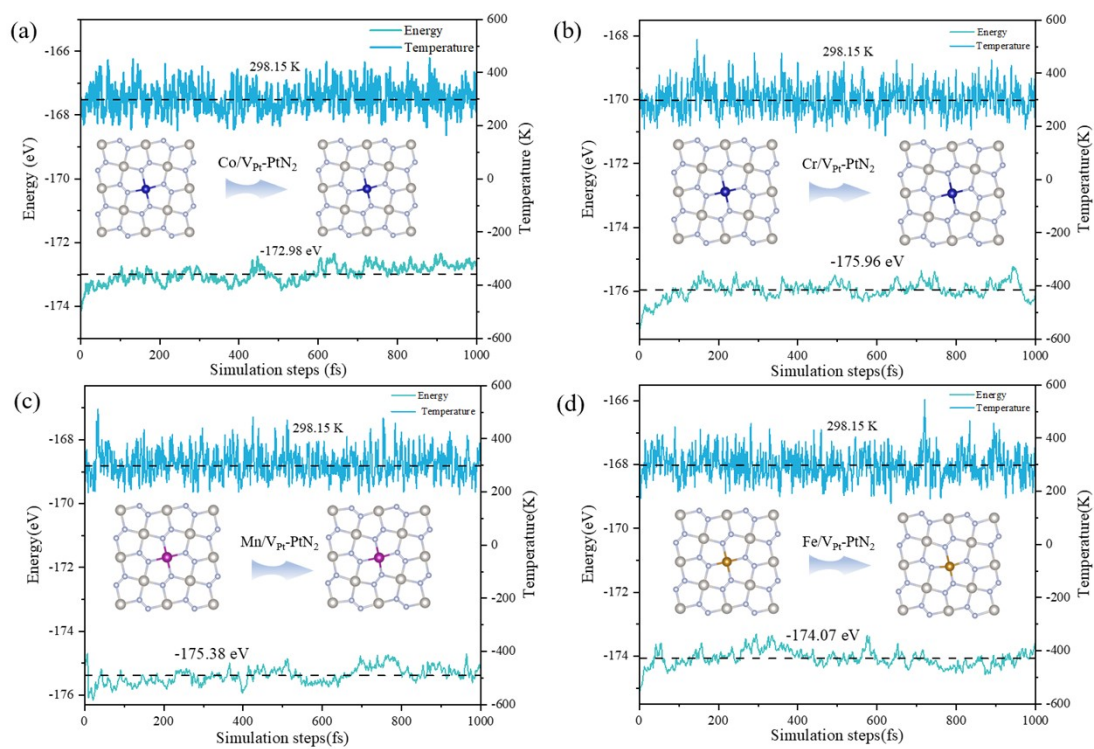
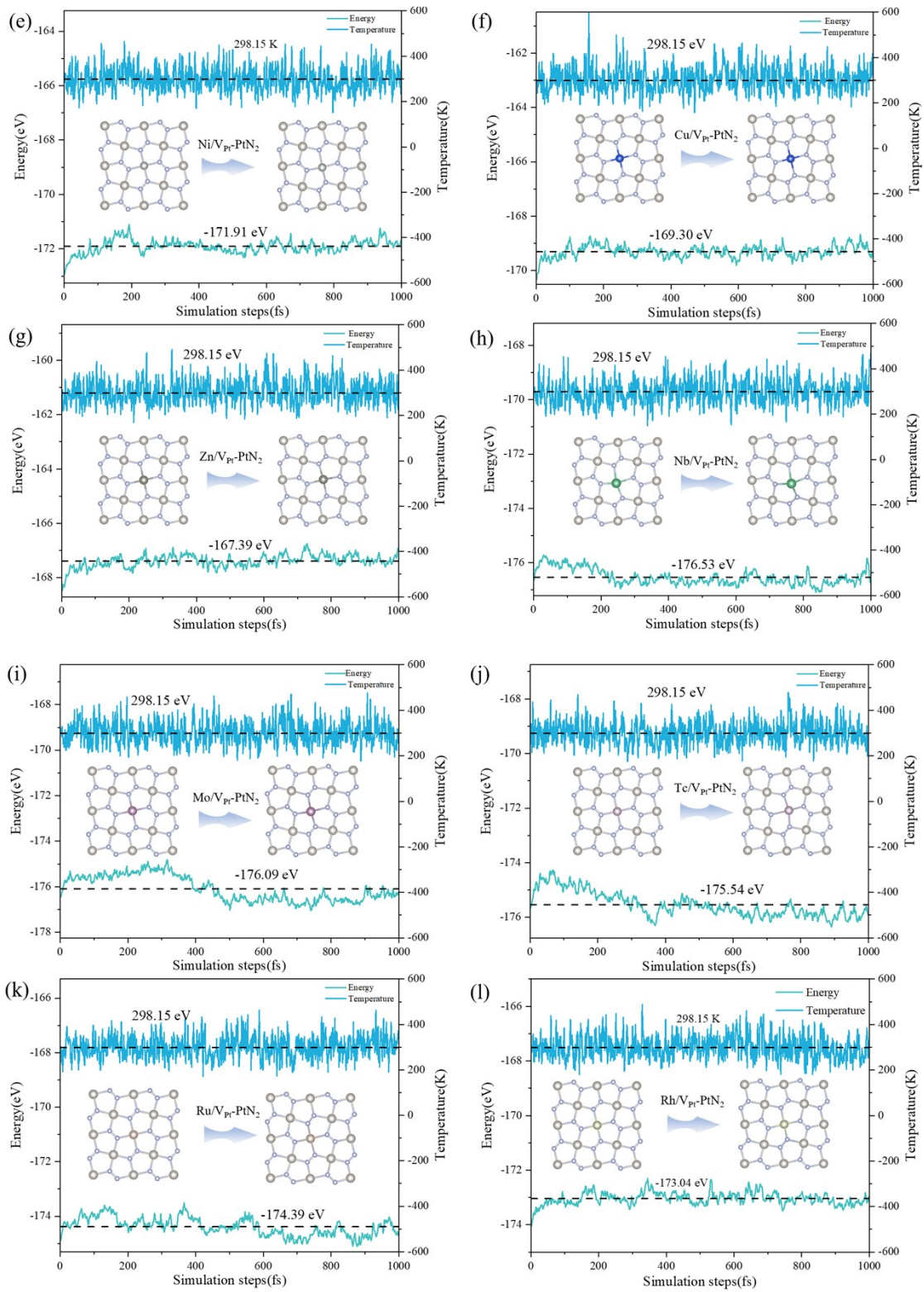


Fig. S2 Phonon spectra and electron local function(ELF) analysis of PtN₂ structure.





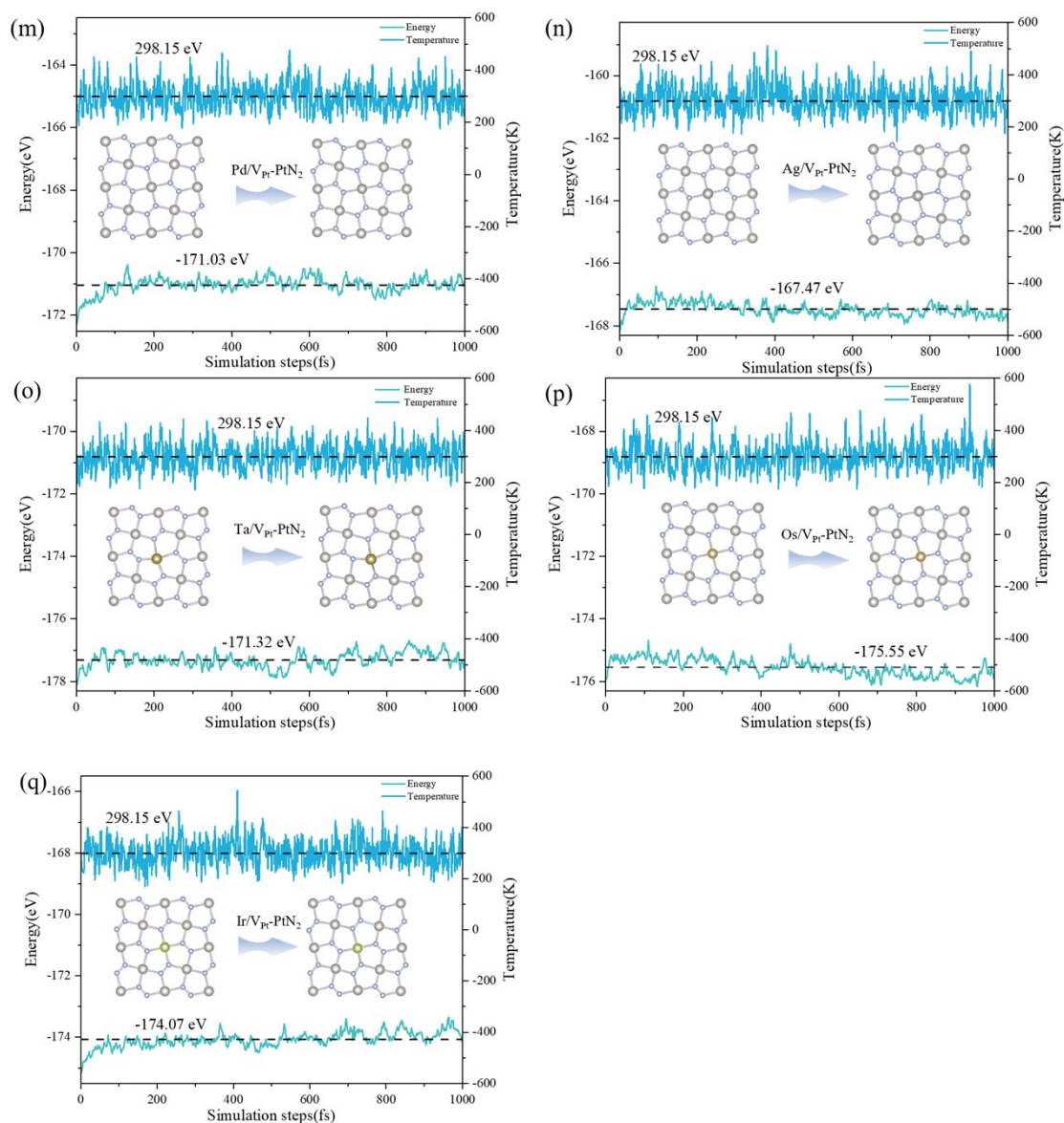


Fig. S3 (a)Co/V_{Pt}-PtN₂, (b) Cr/V_{Pt}-PtN₂, (c)Mn/V_{Pt}-PtN₂, (d)Fe/V_{Pt}-PtN₂, (e) Ni/V_{Pt}-PtN₂, (f)Cu/V_{Pt}-PtN₂, (g)Zn/V_{Pt}-PtN₂, (h) Nb/V_{Pt}-PtN₂, (i)Mo/V_{Pt}-PtN₂, (j)Tc/V_{Pt}-PtN₂, (k) Ru/V_{Pt}-PtN₂, (l)Rh/V_{Pt}-PtN₂, (m)Pd/V_{Pt}-PtN₂, (n) Ag/V_{Pt}-PtN₂, (o)Ta/V_{Pt}-PtN₂, (o)Os/V_{Pt}-PtN₂, and (p)Ir/V_{Pt}-PtN₂ AIMD simulation in 298.15K aqueous solution.

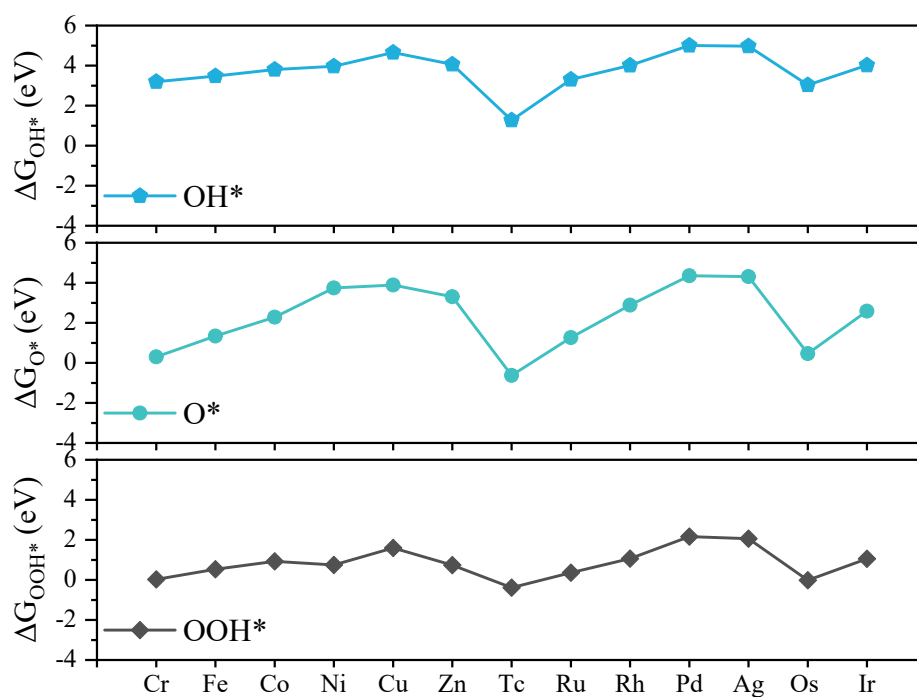


Fig. S4 The adsorption free energies of intermediate species on the TM/V_{Pt}-PtN₂.

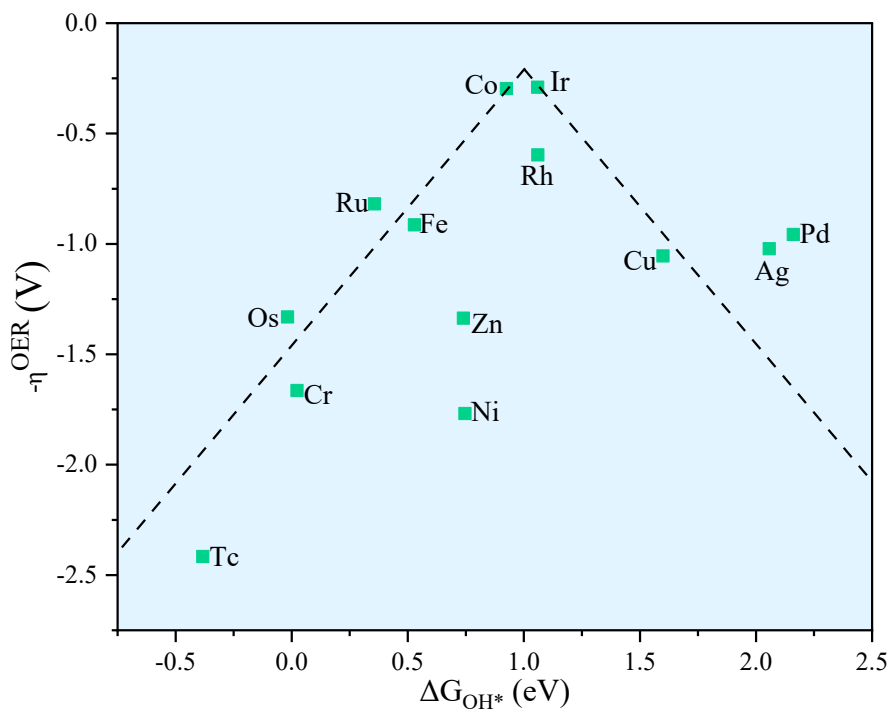


Fig. S5 The volcano diagrams of OER corresponding to the TM/ V_{Pt} -PtN₂ systems.

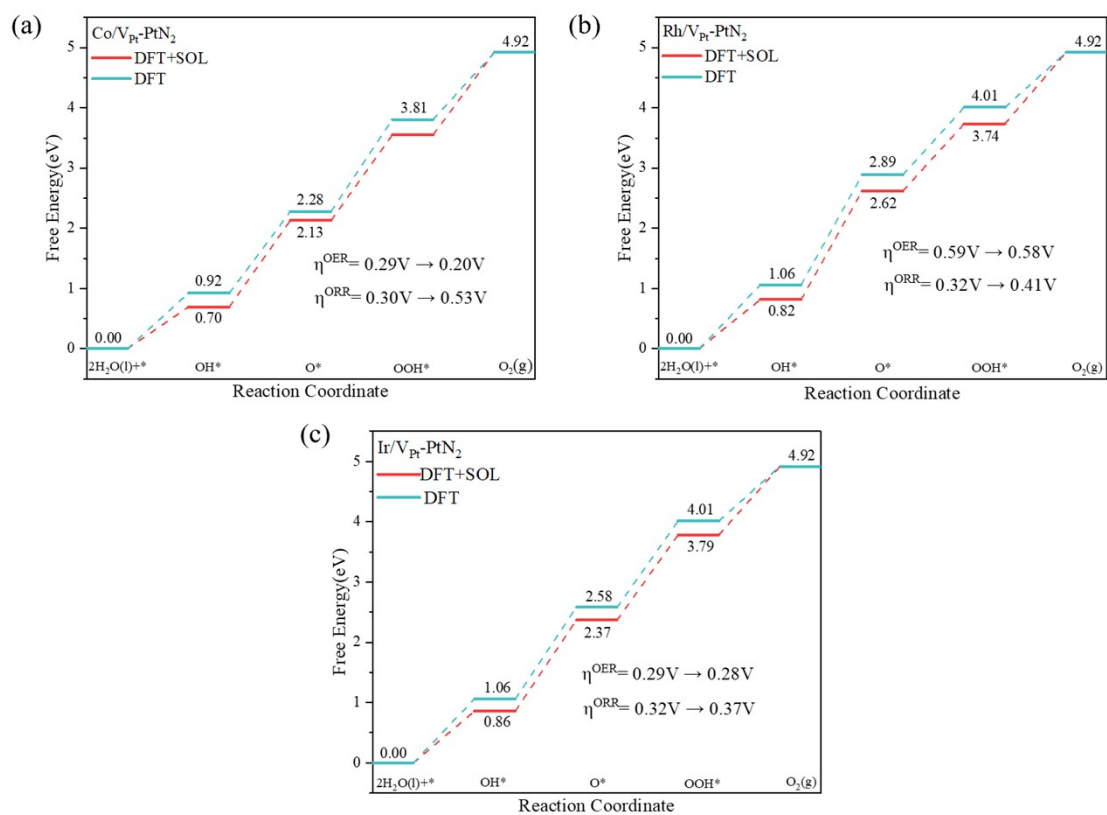


Fig. S6 The OER and ORR free energy diagrams for (a)Co/ V_{Pt} -PtN₂ (b)Rh/ V_{Pt} -PtN₂ ,and (c)Ir/ V_{Pt} -PtN₂ with(red) and without(blue) solvent effects.

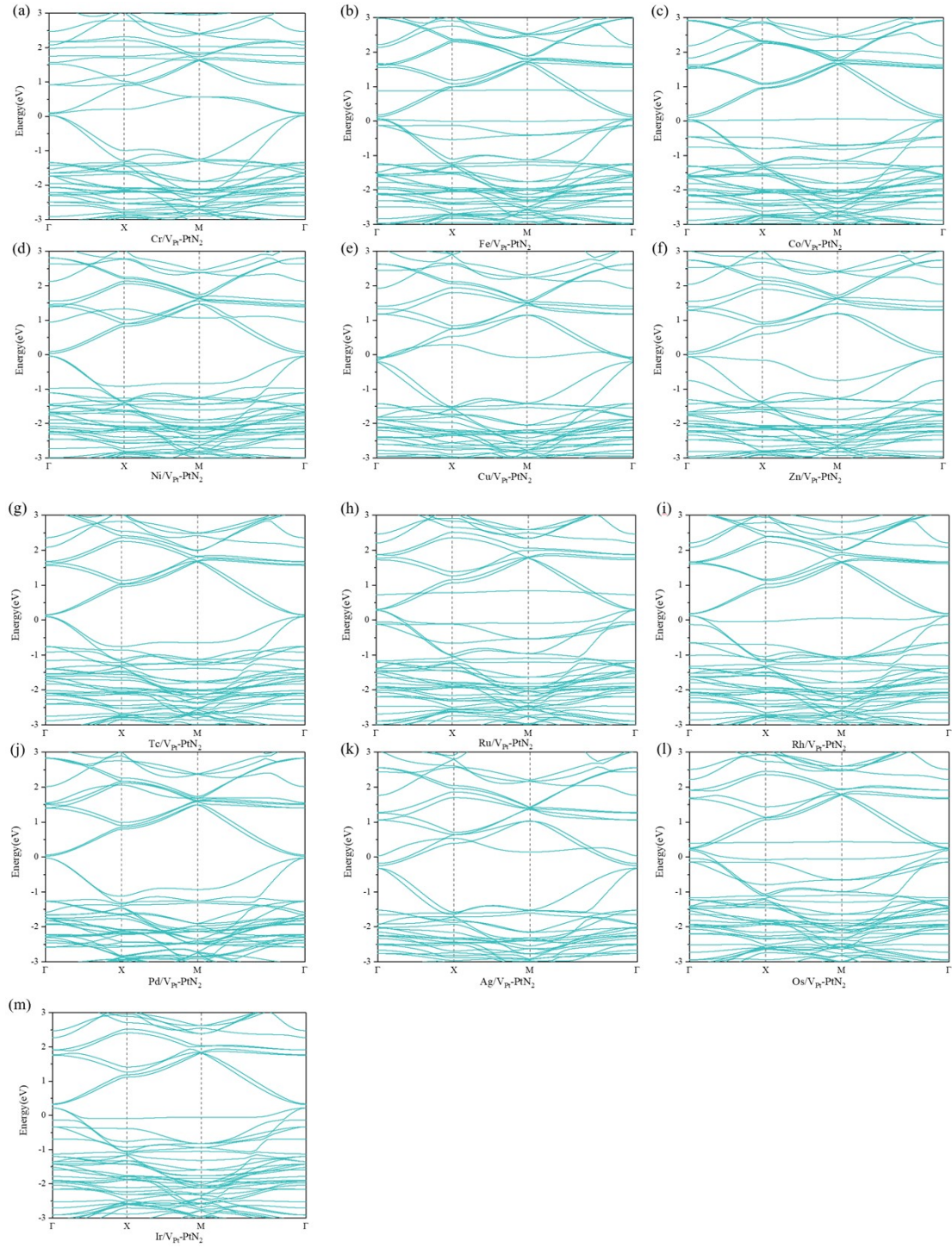


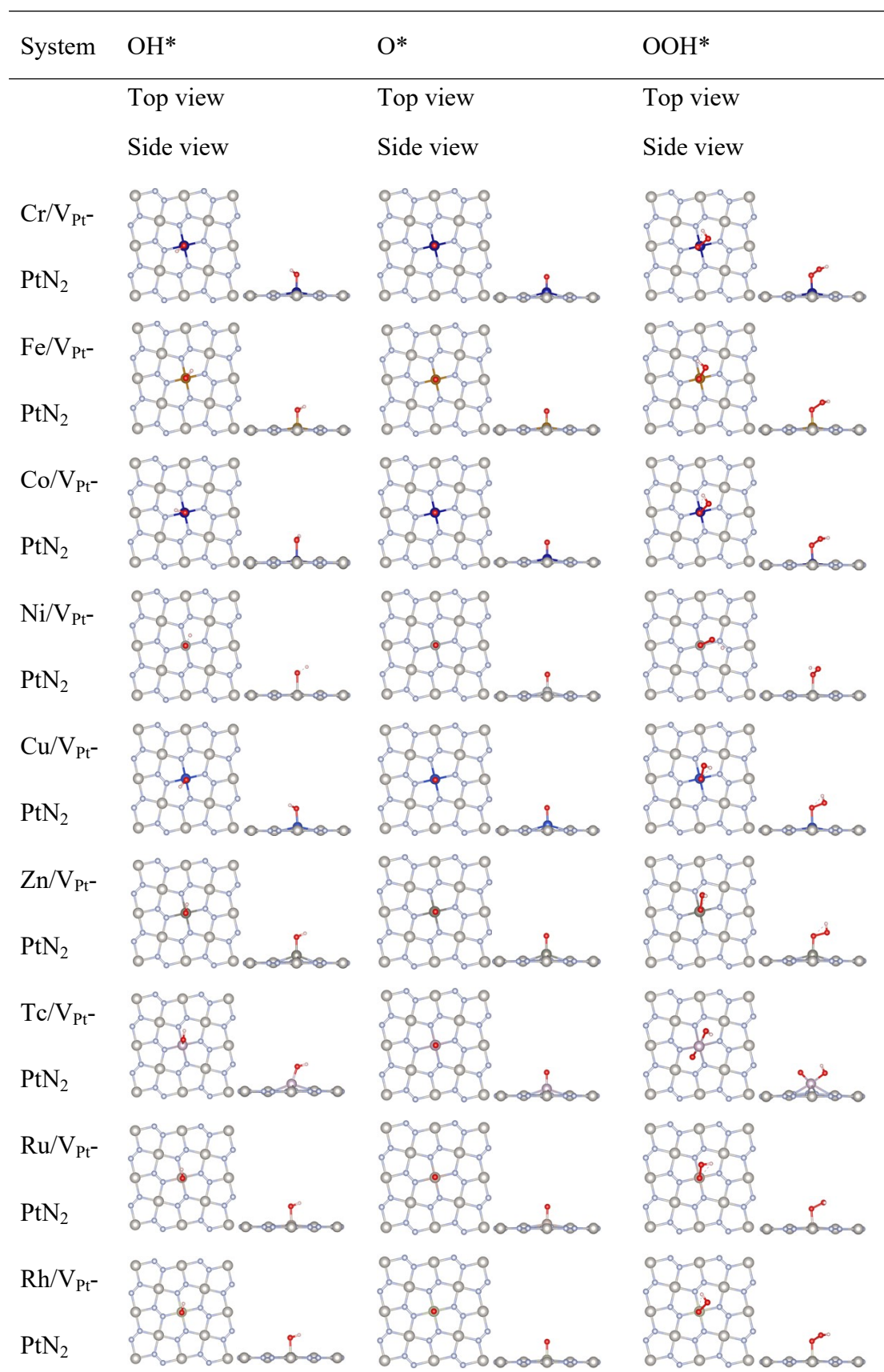
Fig. S7 The band structures of TM/V_{Pt}-PtN₂ (TM = Cr, Fe, Co, Ni, Cu, Zn, Tc, Ru, Rh, Pd, Ag, Os, Ir).

Table S1 Optimized lattice parameters of TM/V_{Pt}-PtN₂ and different TM/V_{Pt}-PtN₂ systems.

System	$a_0(\text{\AA})$	$b_0(\text{\AA})$	Average bond length(\AA)
PtN ₂	9.65	9.65	2.02
V/V _{Pt} -PtN ₂	9.68	9.65	2.03
Cr/V _{Pt} -PtN ₂	9.66	9.65	2.02
Mn/V _{Pt} -PtN ₂	9.62	9.65	1.99
Fe/V _{Pt} -PtN ₂	9.60	9.65	1.95
Co/V _{Pt} -PtN ₂	9.58	9.65	1.93
Ni/V _{Pt} -PtN ₂	9.58	9.65	1.94
Cu/V _{Pt} -PtN ₂	9.63	9.65	2.00
Zn/V _{Pt} -PtN ₂	9.69	9.65	2.05
Nb/V _{Pt} -PtN ₂	9.72	9.65	2.09
Mo/V _{Pt} -PtN ₂	9.73	9.65	2.07
Tc/V _{Pt} -PtN ₂	9.69	9.65	2.04
Ru/V _{Pt} -PtN ₂	9.68	9.65	2.01
Rh/V _{Pt} -PtN ₂	9.66	9.65	2.01
Pd/V _{Pt} -PtN ₂	9.66	9.65	2.03
Ag/V _{Pt} -PtN ₂	9.68	9.65	2.09
Ta/V _{Pt} -PtN ₂	9.71	9.65	2.08
Os/V _{Pt} -PtN ₂	9.68	9.65	2.00
Ir/V _{Pt} -PtN ₂	9.65	9.65	1.99

Table S2 The optimized structures of OH*, O* and OOH* intermediates on different

TM/V_{Pt}-PtN₂ systems.



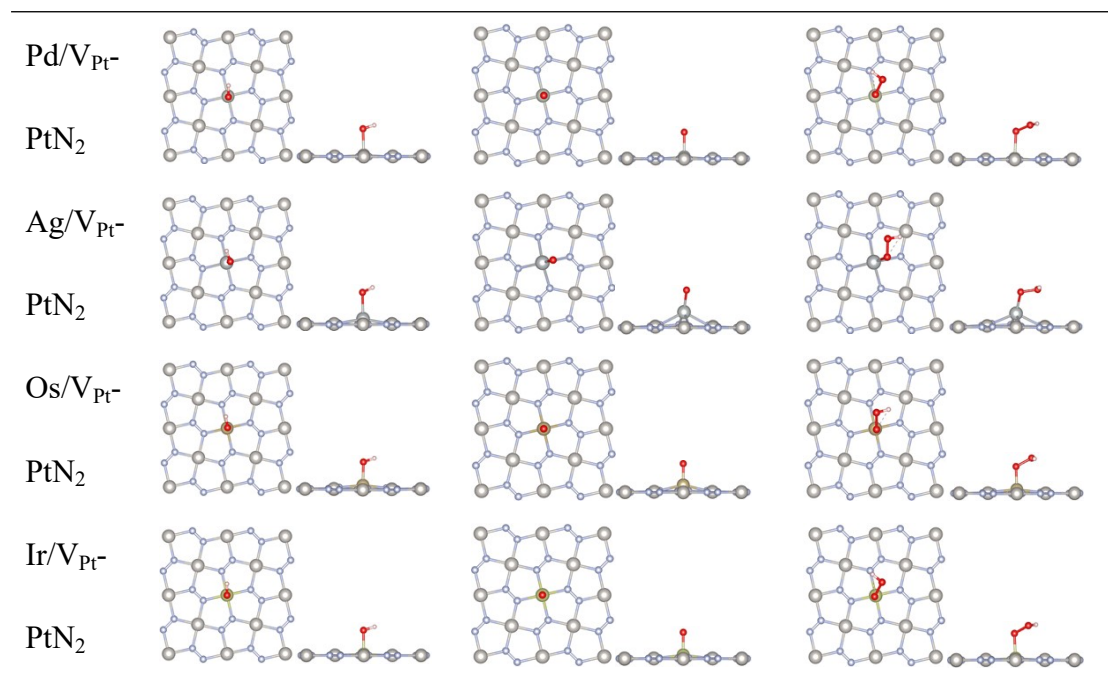


Table S3 The Gibbs free energy of OH*, O* and OOH* (ΔG_{OH^*} , ΔG_{O^*} and ΔG_{OOH^*}) on the different TM/V_{Pt}-PtN₂ systems.

System	ΔG_{OH^*} (eV)	ΔG_{O^*} (eV)	ΔG_{OOH^*} (eV)
Cr/V _{Pt} -PtN ₂	0.02	0.30	3.19
Fe/V _{Pt} -PtN ₂	0.53	1.34	3.48
Co/V _{Pt} -PtN ₂	0.92	2.28	3.81
Ni/V _{Pt} -PtN ₂	0.75	3.74	3.97
Cu/V _{Pt} -PtN ₂	1.60	3.88	4.65
Zn/V _{Pt} -PtN ₂	0.74	3.31	4.06
Tc/V _{Pt} -PtN ₂	-0.38	-0.63	1.27
Ru/V _{Pt} -PtN ₂	0.36	1.26	3.31
Rh/V _{Pt} -PtN ₂	1.06	2.89	4.01
Pd/V _{Pt} -PtN ₂	2.16	4.35	5.01

Ag/V _{Pt} -PtN ₂	2.06	4.31	4.97
Os/V _{Pt} -PtN ₂	-0.02	0.47	3.03
Ir/V _{Pt} -PtN ₂	1.06	2.58	4.01

Table S4 The Gibbs free energy change between two intermediate processes, slab to OH* (ΔG_1), OH* to O* (ΔG_2), O* to OOH* (ΔG_3) and OOH* to O₂ (ΔG_4) of TM/V_{Pt}-PtN₂ systems, as well as the corresponding OER overpotential (η_{OER}) and ORR overpotential (η_{ORR}).

System	$\Delta G_1(\text{eV})$	$\Delta G_2(\text{eV})$	$\Delta G_3(\text{eV})$	$\Delta G_4(\text{eV})$	$\eta_{\text{OER}}(\text{V})$	$\eta_{\text{ORR}}(\text{V})$
Cr/V _{Pt} -PtN ₂	0.02	0.27	2.89	1.73	1.66	1.21
Fe/V _{Pt} -PtN ₂	0.53	0.81	2.14	1.44	0.91	0.70
Co/V _{Pt} -PtN ₂	0.92	1.36	1.53	1.11	0.29	0.30
Ni/V _{Pt} -PtN ₂	0.75	3.00	0.22	0.95	1.77	1.01
Cu/V _{Pt} -PtN ₂	1.60	2.29	0.77	0.27	1.06	0.96
Zn/V _{Pt} -PtN ₂	0.74	2.57	0.76	0.86	1.34	0.49
Tc/V _{Pt} -PtN ₂	-0.38	-0.25	1.90	3.65	2.42	1.61

PtN ₂						
Ru/V _{Pt} -	0.36	0.90	2.05	1.61	0.82	0.87
PtN ₂						
Rh/V _{Pt} -	1.06	1.83	1.12	0.91	0.59	0.31
PtN ₂						
Pd/V _{Pt} -	2.16	2.19	0.66	-0.09	0.96	1.32
PtN ₂						
Ag/V _{Pt} -	2.06	2.25	0.66	-0.05	1.02	1.28
PtN ₂						
Os/V _{Pt} -	-0.02	0.48	2.56	1.89	1.33	1.25
PtN ₂						
Ir/V _{Pt} -	1.06	1.52	1.43	0.91	0.29	0.32
PtN ₂						

Table S5 The η of different TM/V_{Pt}-PtN₂ structures.

System	η
Cr/V _{Pt} -PtN ₂	2.87
Mn/V _{Pt} -PtN ₂	3.42
Fe/V _{Pt} -PtN ₂	1.61
Co/V _{Pt} -PtN ₂	0.59
Ni/V _{Pt} -PtN ₂	2.78
Cu/V _{Pt} -PtN ₂	2.01

Zn/V _{Pt} -PtN ₂	1.83
Tc/V _{Pt} -PtN ₂	4.03
Ru/V _{Pt} -PtN ₂	1.69
Rh/V _{Pt} -PtN ₂	0.9
Pd/V _{Pt} -PtN ₂	2.28
Ag/V _{Pt} -PtN ₂	2.3
Os/V _{Pt} -PtN ₂	2.58
Ir/V _{Pt} -PtN ₂	0.61

Table S6 The Gibbs free energy (G) of gas O₂(g), H₂(g) and H₂O (l) at 1/0.035 bar and 298.15 K, E presents the free energy calculated from DFT, and ΔE is the Frequency correction energy.

Molecular	Pressure/bar	Temperature/ K	E	$\Delta E/eV$	G/eV
O ₂ (g)	1	298.15	--	--	-9.91
H ₂ (g)	1	298.15	-6.76	-0.045	-6.8
H ₂ O(l)	0.035	298.15	-14.22	-0.001	-14.22

Table S7 Binding energies (E_{bind}) of TM/V_{Pt}-PtN₂, cohesive energies (E_{coh}) of TM atoms in bulk, the standard dissolution potentials ($U_{\text{diss-bulk}}$) of TM bulk, the number of transferred electrons (n) during the process of dissolution, and the calculated dissolution potentials (U_{diss}) of TM atoms on TM/V_{Pt}-PtN₂.

System	E_{bind} (eV)	E_{coh} (eV)	$U_{\text{diss-bulk}}$ (V)	n	U_{diss} (V)
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Cr/V _{Pt} -PtN ₂	-2.16	-1.10	-0.91	2	0.17
Fe/V _{Pt} -PtN ₂	-1.76	-1.08	-0.45	2	0.43
Co/V _{Pt} -PtN ₂	-2.06	-1.10	-0.28	2	0.75
Ni/V _{Pt} -PtN ₂	-2.26	-1.10	-0.26	2	0.87
Cu/V _{Pt} -PtN ₂	-1.18	-1.06	0.34	2	0.93
Zn/V _{Pt} -PtN ₂	-1.93	-1.09	-0.76	2	0.20
Tc/V _{Pt} -PtN ₂	-0.01	-1.01	0.30	2	0.30
Ru/V _{Pt} -PtN ₂	-0.84	-1.04	0.46	2	0.88
Rh/V _{Pt} -PtN ₂	-1.79	-1.08	0.60	2	1.50
Pd/V _{Pt} -PtN ₂	-2.13	-1.10	0.95	2	2.02
Ag/V _{Pt} -PtN ₂	-0.53	-1.03	0.80	1	1.33
W/V _{Pt} -PtN ₂	0.14	-	-	-	-
Os/V _{Pt} -PtN ₂	-0.07	-1.01	0.84	8	0.85
Ir/V _{Pt} -PtN ₂	-1.63	-1.08	1.16	3	1.70

Table S8 Atomic lattices in VASP POSCAR format

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0.0000000000000000	0.0000000000000000	20
Pt	N	
8	16	
Direct		
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0.7038571363162259	0.5461429233331972	0.5000000000000000

V/VPt-PtN2

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0.0000000000000000	9.6506996155000007	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Pt N V
7 16 1

Direct

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Cr/VPt-PtN2

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0.0000000000000000	9.6506996155000007	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Pt N Cr
7 16 1

Direct

0.0000711683932516	-0.0004644038781549	0.5000000000000000
0.0000702406341942	0.4995290785017888	0.5000000000000000
0.5000515530214193	-0.0005465353693864	0.5000000000000000
0.2503751787499570	0.2500404071275091	0.5000000000000000
0.2503894645787240	0.7493179848132394	0.5000000000000000
0.7496414409212390	0.2499786582982026	0.5000000000000000
0.7497120829981783	0.7492814021281625	0.5000000000000000
0.4543659609001524	0.2029176449490450	0.5000000000000000
0.4538861699327486	0.7035165493307638	0.5000000000000000
0.9541585360797749	0.2034671441895524	0.5000000000000000
0.9537425240106603	0.7035370224277415	0.5000000000000000
0.0463488776456917	0.2956832783287508	0.5000000000000000
0.0459393872380922	0.7957418150026623	0.5000000000000000
0.5461759730204075	0.2955229265532498	0.5000000000000000
0.5457056495617181	0.7961147963591636	0.5000000000000000
0.2960738459573143	0.4535135149845174	0.5000000000000000
0.2961542223063752	0.9533357747409771	0.5000000000000000
0.7967462128161127	0.4539530004877652	0.5000000000000000
0.7962194885248127	0.9537703000420291	0.5000000000000000
0.2039021104634626	0.0455216795253165	0.5000000000000000
0.2034035835397658	0.5452869989004597	0.5000000000000000
0.7039395841315484	0.0459242964035139	0.5000000000000000
0.7040868857037406	0.5457348586073889	0.5000000000000000
0.5000998413006090	0.4994618136291140	0.5000000000000000

Mn/VPt-PtN2

1.0000000000000000

9.6191382395667411	0.0000000000000000	0.0000000000000000
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0.0000000000000000	9.650699615500007	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000
Pt	N	Mn
7	16	1
Direct		
0.0000795605534246	-0.0002770920221862	0.5000000000000000
0.0001133945437928	0.4995171291082887	0.5000000000000000
0.4999980421504163	-0.0006802254250258	0.5000000000000000
0.2511838625910668	0.2496941720079210	0.5000000000000000
0.2499446473528487	0.74853144468691012	0.5000000000000000
0.7499672570651800	0.2507253310749158	0.5000000000000000
0.7490062103845762	0.7496294486260708	0.5000000000000000
0.4546637776595724	0.2034317749455007	0.5000000000000000
0.4542402389897982	0.7005308539131536	0.5000000000000000
0.9541209157553997	0.2034669269873604	0.5000000000000000
0.9535425287624456	0.7035120161821078	0.5000000000000000
0.0466734806993951	0.2958299733338349	0.5000000000000000
0.0459485708460830	0.7960085503555453	0.5000000000000000
0.5457926256484091	0.2984381309930594	0.5000000000000000
0.5454075249615070	0.7954842532811406	0.5000000000000000
0.2991447632971386	0.4537715208047687	0.5000000000000000
0.2960690459084628	0.9528660635290676	0.5000000000000000
0.7959364023361045	0.4541584236478378	0.5000000000000000
0.7963040499683989	0.9536395277235029	0.5000000000000000
0.2038856720336628	0.0456172797634987	0.5000000000000000
0.2041626397843133	0.5450258479977936	0.5000000000000000
0.7039118111126375	0.0461696992510080	0.5000000000000000
0.7010728252159073	0.5455158058330420	0.5000000000000000
0.5000901348094080	0.4995331473020648	0.5000000000000000

Fe/VPt-PtN2

1.0000000000000000

9.6017120604568156	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.650699615500007	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Pt N Fe
7 16 1

Direct

-0.0000220263122417	-0.0002224108195338	0.5000000000000000
0.0001678689341835	0.4996684304689245	0.5000000000000000
0.5000091691455232	-0.0007228636732179	0.5000000000000000
0.2517298326064185	0.2503387853735466	0.5000000000000000
0.2507960508292803	0.7479315340191335	0.5000000000000000
0.7492057257360734	0.2513496610885277	0.5000000000000000

0.7484315714764753	0.7488377736452513	0.5000000000000000
0.4552690557575282	0.2057031150438248	0.5000000000000000
0.4553044034974255	0.6972630081600147	0.5000000000000000
0.9539435424575325	0.2038911297207914	0.5000000000000000
0.9538178509720480	0.7035546685968683	0.5000000000000000
0.0463689242361700	0.2959787779914022	0.5000000000000000
0.0461308581276843	0.7957551440298768	0.5000000000000000
0.5446467330933851	0.3014139551343671	0.5000000000000000
0.5447171443812543	0.7929344741809377	0.5000000000000000
0.3023056259770834	0.4549743843689280	0.5000000000000000
0.2960857228578250	0.9532099344407826	0.5000000000000000
0.7935721732818607	0.4548438986169611	0.5000000000000000
0.7958651513248103	0.9534928337219275	0.5000000000000000
0.2041689051203529	0.0458255395015785	0.5000000000000000
0.2066754804358035	0.5444960366952141	0.5000000000000000
0.7038406432380943	0.0460072764006755	0.5000000000000000
0.6980559527791440	0.5445307902110671	0.5000000000000000
0.5001736224762348	0.4990841291655231	0.5000000000000000

Co/VPt-PtN2

1.0000000000000000

9.5823576041283509	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.6506996155000007	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Pt N Co
7 16 1

Direct

-0.0000157088339321	-0.0003373964630557	0.5000000000000000
0.0001622893284223	0.4996413571489052	0.5000000000000000
0.4999406771379450	-0.0006362787933139	0.5000000000000000
0.2522253090204233	0.2511222115999678	0.5000000000000000
0.2514468536152487	0.7473438383937980	0.5000000000000000
0.7486997285383399	0.2517889671653027	0.5000000000000000
0.7478700808610923	0.7480833425651797	0.5000000000000000
0.4559726534626290	0.2075380302768277	0.5000000000000000
0.4555252289482897	0.6952849395104240	0.5000000000000000
0.9539096826104697	0.2041656655731781	0.5000000000000000
0.9538334286003821	0.7033762287396623	0.5000000000000000
0.0463426760781639	0.2960314251187283	0.5000000000000000
0.0462102742571458	0.7952911559158979	0.5000000000000000
0.5445717302938434	0.3036638658497571	0.5000000000000000
0.5440935718534334	0.7914282706832532	0.5000000000000000
0.3044500458646815	0.4550631408621230	0.5000000000000000
0.2960524106161344	0.9531939829235289	0.5000000000000000

0.7919297374760667	0.4553711913026148	0.5000000000000000
0.7954624163743294	0.9532799439098621	0.5000000000000000
0.2045098889071404	0.0459699788196683	0.5000000000000000
0.2083494890621902	0.5438801189848383	0.5000000000000000
0.7038182127195094	0.0459381265873531	0.5000000000000000
0.6958029429273593	0.5441536108297257	0.5000000000000000
0.5000963627106414	0.4995042885791450	0.5000000000000000

Ni/VPt-PtN2

1.0000000000000000

9.5801736802307893	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.6506996155000007	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Pt N Ni
7 16 1

Direct

0.0000240707995993	-0.0004186014807950	0.5000000000000000
0.0001386658769515	0.4995593691205065	0.5000000000000000
0.5000054169780638	-0.0005088022118347	0.5000000000000000
0.2520399332067624	0.2504639620871885	0.5000000000000000
0.2508536309329574	0.7475732892714854	0.5000000000000000
0.7492100057491765	0.2515868296110562	0.5000000000000000
0.7480430979589312	0.7487301046692937	0.5000000000000000
0.4555776219463138	0.2075563485558512	0.5000000000000000
0.4546654224745469	0.6967161623478076	0.5000000000000000
0.9538862296689418	0.2034831128219836	0.5000000000000000
0.9537095529971943	0.7030915285328176	0.5000000000000000
0.0464013734973897	0.2961348093373241	0.5000000000000000
0.0461910140447430	0.7957764747793545	0.5000000000000000
0.5454426787784930	0.3023692969337713	0.5000000000000000
0.5444906995888286	0.7915614612656536	0.5000000000000000
0.3031587588555674	0.4541922937945245	0.5000000000000000
0.2963323914622378	0.9531681175456963	0.5000000000000000
0.7918138609900480	0.4549862577232412	0.5000000000000000
0.7960352429811323	0.9532922101721016	0.5000000000000000
0.2040081522564609	0.0459840532188119	0.5000000000000000
0.2084056672362952	0.5442430996145405	0.5000000000000000
0.7036777679974350	0.0460661973199697	0.5000000000000000
0.6970479587986258	0.5449994362362099	0.5000000000000000
0.5001007673532556	0.4995329948168120	0.5000000000000000

Cu/VPt-PtN2

1.0000000000000000

9.6255736969971899	0.0000000000000000	0.0000000000000000
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0.0000000000000000	9.650699615500007	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000
Pt	N	Cu
7	16	1
Direct		
0.0000119696313932	-0.0003091176885948	0.5000000000000000
0.0001742395882813	0.4996129533452585	0.5000000000000000
0.5000183619634605	-0.0007615138359078	0.5000000000000000
0.2507819410678852	0.2496482032542561	0.5000000000000000
0.2499985512891679	0.7490141187438829	0.5000000000000000
0.7500425706466973	0.2504320630913210	0.5000000000000000
0.7493575245672247	0.7496036330903717	0.5000000000000000
0.4548527726995892	0.2054635105185008	0.5000000000000000
0.4532679986981614	0.7019267408417144	0.5000000000000000
0.9542266311446160	0.2032003840365954	0.5000000000000000
0.9537743315515813	0.7030768590419010	0.5000000000000000
0.0464360018969086	0.2963315701575807	0.5000000000000000
0.0458663914040049	0.7963230629039746	0.5000000000000000
0.5467224867829804	0.2969263851549916	0.5000000000000000
0.5452232032007108	0.7932978547593524	0.5000000000000000
0.2977769681487952	0.4528674626110240	0.5000000000000000
0.2965244043431919	0.9531674625699859	0.5000000000000000
0.7938354710224682	0.4544068011048958	0.5000000000000000
0.7965678078572496	0.9536856699704243	0.5000000000000000
0.2035213449931850	0.0455522228311503	0.5000000000000000
0.2063974626040040	0.5448955291799898	0.5000000000000000
0.7034299506408148	0.0459239166342628	0.5000000000000000
0.7024021957381061	0.5463754727067530	0.5000000000000000
0.5000494009494727	0.4994787610596881	0.5000000000000000

Zn/VPt-PtN2

1.0000000000000000

9.6945267714270411	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.650699615500007	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Pt N Zn
7 16 1

Direct

0.0000841449366626	-0.0003937233292184	0.5000000000000000
0.0000644566374186	0.4994533720020184	0.5000000000000000
0.5000525303932454	-0.0005831458672788	0.5000000000000000
0.2496725703416349	0.2504265607366916	0.5000000000000000
0.2507518956658664	0.7498547904979999	0.5000000000000000
0.7492395661972031	0.2493742149103495	0.5000000000000000

0.7505836959222609	0.7488397480766142	0.5000000000000000
0.4548270832093814	0.2028742645509768	0.5000000000000000
0.4529335725119105	0.7057756546803636	0.5000000000000000
0.9540888562205738	0.2035083381059949	0.5000000000000000
0.9539723424839984	0.7036067056031439	0.5000000000000000
0.0461620821374738	0.2955698632949105	0.5000000000000000
0.0459569881612818	0.7957633068889125	0.5000000000000000
0.5470724848637413	0.2933770795975269	0.5000000000000000
0.5452298024387022	0.7962242410817606	0.5000000000000000
0.2933894763497407	0.4526554400496316	0.5000000000000000
0.2961740691358185	0.9534881909250233	0.5000000000000000
0.7971839378362692	0.4543992231922646	0.5000000000000000
0.7962537612244414	0.9538788691793995	0.5000000000000000
0.2039879042909134	0.0453772421471555	0.5000000000000000
0.2028455306055776	0.5447494162182178	0.5000000000000000
0.7039575496428497	0.0456416140109921	0.5000000000000000
0.7067383111559615	0.5465929026197517	0.5000000000000000
0.5000373700670230	0.4996858369101705	0.5000000000000000

Nb/VPt-PtN2

1.0000000000000000

9.7222426856991646	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.6506996155000007	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Pt N Nb
7 16 1

Direct

0.0037889834368324	0.0025818552543013	0.5000000000000000
-0.0064739871733455	0.5037891049930763	0.5000000000000000
0.5030940206693330	-0.0052832499756192	0.5000000000000000
0.2572488974565555	0.2563596180688296	0.5000000000000000
0.2460001182139529	0.7542825748103865	0.5000000000000000
0.7580618169644681	0.2459400473279884	0.5000000000000000
0.7489913127621727	0.7488119543795306	0.5000000000000000
0.4611578097019787	0.1950629929730829	0.5000000000000000
0.4530287606749311	0.7001243527490661	0.5000000000000000
0.9613377343986041	0.2061495220295884	0.5000000000000000
0.9511711984822320	0.7076917727968635	0.5000000000000000
0.0511247877624522	0.3001604212456303	0.5000000000000000
0.0436109899958915	0.7990023119608434	0.5000000000000000
0.5604696802663917	0.2833082042786240	0.5000000000000000
0.5451030449307770	0.7936301231901700	0.5000000000000000
0.2832793516055748	0.4677478391805587	0.5000000000000000
0.2981464588310280	0.9555920846925027	0.5000000000000000

0.7953092705782715	0.4540303641358349	0.5000000000000000
0.8006412074157926	0.9515341201091748	0.5000000000000000
0.2087536238407231	0.0506152489300202	0.5000000000000000
0.1868913678991167	0.5569541310958764	0.5000000000000000
0.7091112332040072	0.0431302098099694	0.5000000000000000
0.6996120011976757	0.5445879837180597	0.5000000000000000
0.4818002993145334	0.4743364183290136	0.5000000000000000

Mo/VPt-PtN2

1.0000000000000000

9.7262648072224813	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.6506996155000007	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Pt N Mo
7 16 1

Direct

0.0000690389937986	-0.0003598464579234	0.5000000000000000
0.0000057693537079	0.4996291887146488	0.5000000000000000
0.5000579571559057	-0.0006176967611826	0.5000000000000000
0.2491442479939714	0.2493878254814713	0.5000000000000000
0.2492126192305084	0.7506467190716606	0.5000000000000000
0.7508427211007332	0.2485909099491063	0.5000000000000000
0.7510526790481903	0.7498888765655545	0.5000000000000000
0.4535412642799924	0.1995434585116838	0.5000000000000000
0.4534071641293955	0.7082754114696364	0.5000000000000000
0.9547484191907619	0.2036528409409547	0.5000000000000000
0.9536718249554850	0.7041798209742262	0.5000000000000000
0.0464382220423222	0.2952090421360897	0.5000000000000000
0.0453822870911766	0.7957141972258512	0.5000000000000000
0.5465993011737547	0.2906492757150999	0.5000000000000000
0.5465464950612965	0.7993336313416970	0.5000000000000000
0.2912832813498245	0.4539150465968404	0.5000000000000000
0.2955711722065941	0.9535626278766365	0.5000000000000000
0.8004494230966644	0.4529287035802073	0.5000000000000000
0.7962554093421972	0.9541188704199024	0.5000000000000000
0.2039673352944890	0.0451497849378388	0.5000000000000000
0.1995891134742195	0.5463406337517187	0.5000000000000000
0.7045577535156559	0.0455959869485401	0.5000000000000000
0.7088068695236212	0.5453792861097821	0.5000000000000000
0.5000596138256843	0.4994254109833326	0.5000000000000000

Tc/VPt-PtN2

1.0000000000000000

9.6922537735852874	0.0000000000000000	0.0000000000000000
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0.0000000000000000	9.650699615500007	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000
Pt	N	Tc
7	16	1

Direct

0.0001672344598807	-0.0000451060066855	0.5000000000000000
-0.0000027262445648	0.4999428447031504	0.5000000000000000
0.5000422161013482	-0.0010152078549088	0.5000000000000000
0.2499342812268922	0.2495802121715323	0.5000000000000000
0.2497438864924664	0.7500124842796677	0.5000000000000000
0.7503759595372516	0.2494015136930922	0.5000000000000000
0.7502245998454855	0.7498182700951894	0.5000000000000000
0.4536764897926492	0.2002132416558813	0.5000000000000000
0.4545223994487494	0.7049045129370054	0.5000000000000000
0.9544956139585503	0.2040716747166327	0.5000000000000000
0.9538564871134134	0.7042629053518017	0.5000000000000000
0.0463944428931252	0.2957549023056311	0.5000000000000000
0.0457143746766507	0.7959343683345517	0.5000000000000000
0.5455575614830682	0.2930388927265908	0.5000000000000000
0.5461802177323374	0.7977888045991626	0.5000000000000000
0.2942114850391181	0.4549283162673585	0.5000000000000000
0.2957647967918470	0.9535650102587733	0.5000000000000000
0.7989302601562339	0.4535765698078691	0.5000000000000000
0.7961532299931052	0.9540524475378352	0.5000000000000000
0.2041892962338375	0.0454615267305072	0.5000000000000000
0.2010396066098804	0.5461857736716194	0.5000000000000000
0.7043120164963267	0.0456483017288284	0.5000000000000000
0.7057752520430018	0.5448675275560676	0.5000000000000000
0.5000010005492960	0.4981902188162185	0.5000000000000000

Ru/VPt-PtN2

1.0000000000000000

9.6780850925254551	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.650699615500007	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Pt	N	Ru
7	16	1

Direct

-0.0000250079161750	-0.0000496235927323	0.5000000000000000
0.0000730710653685	0.4996652556860230	0.5000000000000000
0.5000549273458674	-0.0009931144668577	0.5000000000000000
0.2500322459591028	0.2504396407943049	0.5000000000000000
0.2505936985144966	0.7498097696328793	0.5000000000000000
0.7492623017032586	0.2495380467819371	0.5000000000000000

0.7502392842668630	0.7490416559197816	0.5000000000000000
0.4546713418941876	0.2026291689153762	0.5000000000000000
0.4554920782981779	0.7020949634939353	0.5000000000000000
0.9544004778861093	0.2045481099465805	0.5000000000000000
0.9542026403221363	0.7041030432836310	0.5000000000000000
0.0460502991169228	0.2955969940167792	0.5000000000000000
0.0456818897845242	0.7953020554805977	0.5000000000000000
0.5446735532495408	0.2959050964145256	0.5000000000000000
0.5452631197890988	0.7955284584229324	0.5000000000000000
0.2971824138971088	0.4556387369689152	0.5000000000000000
0.2957848447831362	0.9538149987622796	0.5000000000000000
0.7965302459255093	0.4545208079942560	0.5000000000000000
0.7954645401365801	0.9540649385682173	0.5000000000000000
0.2045996392153163	0.0453105289438738	0.5000000000000000
0.2034693635329176	0.5450766229353589	0.5000000000000000
0.7041735072512579	0.0455137696212575	0.5000000000000000
0.7032553505203833	0.5445955808866183	0.5000000000000000
0.5001341558882616	0.4984445006729025	0.5000000000000000

Rh/VPt-PtN2

1.0

9.6623001099	0.0000000000	0.0000000000
0.0000000000	9.6506996155	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Pt	N	Rh
7	16	1

Direct

0.000050000	0.999700010	0.500000000
0.000130000	0.499540001	0.500000000
0.499969989	0.999349952	0.500000000
0.250250012	0.250389993	0.500000000
0.250690013	0.749430001	0.500000000
0.749310017	0.249750018	0.500000000
0.749949992	0.749029994	0.500000000
0.454860002	0.203850001	0.500000000
0.455080003	0.702260017	0.500000000
0.954259992	0.204180002	0.500000000
0.954150021	0.703840017	0.500000000
0.046000000	0.295500010	0.500000000
0.045820002	0.795220017	0.500000000
0.545000017	0.296579987	0.500000000
0.545159996	0.795050025	0.500000000
0.297289997	0.454710037	0.500000000
0.295850009	0.953670025	0.500000000

0.795729995	0.454470009	0.500000000
0.795589983	0.953889966	0.500000000
0.204520002	0.045440000	0.500000000
0.204439998	0.544790030	0.500000000
0.704129994	0.045520000	0.500000000
0.702920020	0.544579983	0.500000000
0.500109971	0.499399960	0.500000000

Pd/VPt-PtN2

1.000000000000000

9.6607164967498687	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.6506996155000007	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Pt N Pd
7 16 1

Direct

0.0000611296031294	-0.0004539520585394	0.5000000000000000
0.0000651632984174	0.4995044562628464	0.5000000000000000
0.5000726526615694	-0.0004840210869832	0.5000000000000000
0.2500021322782374	0.2495787299930446	0.5000000000000000
0.2499534542005733	0.7496257796299045	0.5000000000000000
0.7500815932924326	0.2495174539959161	0.5000000000000000
0.7501633062572420	0.7495695972951110	0.5000000000000000
0.4541671268302189	0.2036434776284292	0.5000000000000000
0.4534441433854497	0.7047430354429253	0.5000000000000000
0.9540280856014566	0.2033796690176801	0.5000000000000000
0.9539199947592312	0.7034660954668476	0.5000000000000000
0.0462055491359849	0.2956792731030763	0.5000000000000000
0.0460487112711057	0.7958125619855899	0.5000000000000000
0.5466043246271767	0.2944878822358504	0.5000000000000000
0.5459618814997986	0.7955017432828638	0.5000000000000000
0.2949489264447804	0.4530893063329227	0.5000000000000000
0.2961678358222581	0.9535190789219112	0.5000000000000000
0.7960335380812243	0.4536461076791975	0.5000000000000000
0.7963299349244574	0.9536016052368825	0.5000000000000000
0.2038012394217308	0.0456776991900321	0.5000000000000000
0.2040343128587737	0.5455142561288773	0.5000000000000000
0.7039159337472147	0.0457226300074943	0.5000000000000000
0.7052028659147500	0.5461498579839192	0.5000000000000000
0.5000461465127369	0.4996476824075741	0.5000000000000000

Ag/VPt-PtN2

1.000000000000000

9.6811438475739333	0.0000000000000000	0.0000000000000000
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0.0000000000000000	9.650699615500007	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000
Pt	N	Ag
7	16	1
Direct		
0.0000562311417341	-0.0005006789577712	0.5000000000000000
0.0000451059235404	0.4994588975307894	0.5000000000000000
0.5001291492889992	-0.0004925538881206	0.5000000000000000
0.2488074059678272	0.2481116790314246	0.5000000000000000
0.2484144857906643	0.7508203048492790	0.5000000000000000
0.7515812082246696	0.2484006395026630	0.5000000000000000
0.7513709785578387	0.7510403069269975	0.5000000000000000
0.4528683183302788	0.2022655082111030	0.5000000000000000
0.4513935921797008	0.7097993239954986	0.5000000000000000
0.9541379831774015	0.2022857662879990	0.5000000000000000
0.9538763010801830	0.7030782331792093	0.5000000000000000
0.0462496986442413	0.2959954941906006	0.5000000000000000
0.0459653702369326	0.7968446794646745	0.5000000000000000
0.5486535408663124	0.2895453047675985	0.5000000000000000
0.5472691144175356	0.7969518773635405	0.5000000000000000
0.2898530525245699	0.4511441636855021	0.5000000000000000
0.2965420988180541	0.9535048377802777	0.5000000000000000
0.7976487877719608	0.4523647122556301	0.5000000000000000
0.7973824290848361	0.9537351911118503	0.5000000000000000
0.2026945851489237	0.0454871153032799	0.5000000000000000
0.2024359694919473	0.5467907220994699	0.5000000000000000
0.7035514080365506	0.0457170088045079	0.5000000000000000
0.7102866692603398	0.5480994700928248	0.5000000000000000
0.5000464984649089	0.4996920024945433	0.5000000000000000

Ta/VPt-PtN2

1.0000000000000000		
9.7116874297154432	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.650699615500007	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Pt N Ta
7 16 1

Direct

0.0037225366995622	0.0025153552872152	0.5000000000000000
-0.0065040880391542	0.5034238302524526	0.5000000000000000
0.5028048675453047	-0.0050368391098525	0.5000000000000000
0.2568560908453396	0.2553645370649253	0.5000000000000000
0.2459023800157530	0.7534302726306217	0.5000000000000000
0.7574928007715850	0.2460247567245364	0.5000000000000000

0.7492330407465684	0.7494053460360208	0.5000000000000000
0.4601063628336340	0.1946262029560413	0.5000000000000000
0.4541166193011730	0.6995836218663667	0.5000000000000000
0.9608047899712909	0.2059258806825454	0.5000000000000000
0.9512788831390706	0.7075084533494153	0.5000000000000000
0.0509168200905193	0.2998400474846373	0.5000000000000000
0.0439933360802028	0.7988474871912924	0.5000000000000000
0.5595055547349048	0.2840592495084583	0.5000000000000000
0.5460195070329412	0.7943829217724151	0.5000000000000000
0.2840742222413419	0.4667890937510126	0.5000000000000000
0.2980549769923485	0.9549938669933583	0.5000000000000000
0.7950704058383983	0.4538905872663653	0.5000000000000000
0.8006141952956208	0.9518088834971671	0.5000000000000000
0.2084146101932887	0.0499902991347606	0.5000000000000000
0.1867479232642482	0.5561815196053647	0.5000000000000000
0.7088817825337248	0.0434968018359911	0.5000000000000000
0.6991247576955584	0.5456032690629912	0.5000000000000000
0.4840276066067259	0.4774845612392705	0.5000000000000000

W/VPt-PtN2

1.0000000000000000

9.6774598454318230	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.6506996155000007	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Pt N W
7 16 1

Direct

0.0035233079058577	0.0031893153896308	0.5000000000000000
-0.0065383931212035	0.5036043038412125	0.5000000000000000
0.5031484255656761	-0.0064541952885534	0.5000000000000000
0.2591439565034021	0.2563205130890291	0.5000000000000000
0.2460342728863556	0.7546421837210394	0.5000000000000000
0.7567375324938784	0.2464535324054681	0.5000000000000000
0.7485901593342992	0.7483520586027055	0.5000000000000000
0.4608939048847954	0.1939780062196424	0.5000000000000000
0.4547326760607068	0.6960404904717150	0.5000000000000000
0.9609004242335483	0.2066678566546758	0.5000000000000000
0.9516898258987074	0.7076386502913721	0.5000000000000000
0.0510302187805888	0.3006323771959989	0.5000000000000000
0.0439870709598893	0.7993988865879269	0.5000000000000000
0.5574735997174858	0.2852462014740875	0.5000000000000000
0.5455165525627859	0.7911161480729402	0.5000000000000000
0.2873787171434317	0.4702883901870895	0.5000000000000000
0.2982355106743674	0.9559402375438846	0.5000000000000000

0.7930193553588354	0.4538954488584511	0.5000000000000000
0.8004570591760948	0.9511763104811189	0.5000000000000000
0.2085341910405224	0.0512078908359949	0.5000000000000000
0.1886461386639904	0.5570334476014078	0.5000000000000000
0.7083205026870762	0.0428216582414015	0.5000000000000000
0.6961887114574318	0.5446591599420602	0.5000000000000000
0.4836162615614251	0.4762911336630723	0.5000000000000000

Re/VPt-PtN2

1.0000000000000000

9.6789562858357421	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.6506996155000007	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Pt N Re
7 16 1

Direct

0.0001485057510738	-0.0003275113720130	0.5000000000000000
0.0000339948755162	0.4997033961690482	0.5000000000000000
0.5000949277600114	-0.0007494350549420	0.5000000000000000
0.2498778277393107	0.2491332552562163	0.5000000000000000
0.2492985350495913	0.7499019078195976	0.5000000000000000
0.7507225464489160	0.2493527508893206	0.5000000000000000
0.7501681324406689	0.7501841291775287	0.5000000000000000
0.4532926938919434	0.1997459520847490	0.5000000000000000
0.4545694213793986	0.7042689310437754	0.5000000000000000
0.9543666974241835	0.2035555269060133	0.5000000000000000
0.9536634198795355	0.7039489991039983	0.5000000000000000
0.0464404579575845	0.2955432801082929	0.5000000000000000
0.0458124180901808	0.7958824879731113	0.5000000000000000
0.5454095698692011	0.2944389919807052	0.5000000000000000
0.5467938222945683	0.7988935144324489	0.5000000000000000
0.2952145056699410	0.4546521035564819	0.5000000000000000
0.2958662377573253	0.9533662676610716	0.5000000000000000
0.7996797273019829	0.4529348301868664	0.5000000000000000
0.7963290977628592	0.9538336184296275	0.5000000000000000
0.2038901904579201	0.0454726479580477	0.5000000000000000
0.2003640854477770	0.5465128286283210	0.5000000000000000
0.7042581212593860	0.0458242874560513	0.5000000000000000
0.7048927918906825	0.5447982390217184	0.5000000000000000
0.5000722540303907	0.4992690066673352	0.5000000000000000

Os/VPt-PtN2

1.0000000000000000

9.6770698556507320	0.0000000000000000	0.0000000000000000
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0.0000000000000000	9.650699615500007	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000
Pt	N	Os
7	16	1
Direct		
-0.0003125872506990	0.0001476969993722	0.5000000000000000
-0.0000188452096510	0.4995032006529444	0.5000000000000000
0.5001218357483401	-0.0011462505466902	0.5000000000000000
0.2500333392707486	0.2504063037609173	0.5000000000000000
0.2502800481782909	0.7502741047250573	0.5000000000000000
0.7492693857792748	0.2494418764380789	0.5000000000000000
0.7505943509843535	0.7491858020870164	0.5000000000000000
0.4541952386802664	0.2017103779150542	0.5000000000000000
0.4560743158535462	0.7010682967818570	0.5000000000000000
0.9541624418859774	0.2046243439499782	0.5000000000000000
0.9543388364178655	0.7040772909357274	0.5000000000000000
0.0460577487085031	0.2955615191260007	0.5000000000000000
0.0457045172917147	0.7954375236705225	0.5000000000000000
0.5446062804532373	0.2959231938344419	0.5000000000000000
0.5458302730232578	0.7956217994980436	0.5000000000000000
0.2980562573642148	0.4568291548410465	0.5000000000000000
0.2957664269340765	0.9540740396275291	0.5000000000000000
0.7967804057654575	0.4541635475304356	0.5000000000000000
0.7954131619026323	0.9538462730993923	0.5000000000000000
0.2044490282388730	0.0455135094828172	0.5000000000000000
0.2028691013402341	0.5458339362318944	0.5000000000000000
0.7041400254869277	0.0455511360477454	0.5000000000000000
0.7028173336984346	0.5450210291371572	0.5000000000000000
0.5000310618840744	0.4974703002570323	0.5000000000000000

Ir/VPt-PN2

1.0000000000000000

9.6542889772417357	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.650699615500007	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Pt N Ir
7 16 1

Direct

0.0000187251866264	-0.0002903706057951	0.5000000000000000
0.0001604321983095	0.4995847602280408	0.5000000000000000
0.4999740157911164	-0.0006937439251317	0.5000000000000000
0.2502885851644003	0.2504396565260970	0.5000000000000000
0.2506775200044565	0.7494721564118159	0.5000000000000000
0.7492464339508029	0.2497407943304957	0.5000000000000000

0.7499390914068893	0.7489554441981399	0.5000000000000000
0.4546555274193286	0.2037163308695483	0.5000000000000000
0.4555795387808840	0.7008893292305138	0.5000000000000000
0.9541823927867370	0.2044792386234558	0.5000000000000000
0.9541561728850650	0.7039226692253353	0.5000000000000000
0.0460113177930515	0.2954712576327888	0.5000000000000000
0.0459162088435154	0.7949886568715490	0.5000000000000000
0.5444683438032180	0.2979266134168408	0.5000000000000000
0.5454112823317486	0.7950949402596570	0.5000000000000000
0.2986777211663497	0.4552583147815542	0.5000000000000000
0.2957676352953422	0.9536919149899461	0.5000000000000000
0.7958037306096898	0.4542385889962420	0.5000000000000000
0.7952922307318038	0.9537700550785401	0.5000000000000000
0.2047762803267346	0.0455293915781620	0.5000000000000000
0.2044098920692759	0.5450169099944489	0.5000000000000000
0.7041802681498992	0.0454777280814303	0.5000000000000000
0.7015713896297840	0.5440374029015943	0.5000000000000000
0.5000952461049198	0.4994219663881042	0.5000000000000000
