

High-Selectivity Electrocatalytic Ammonia Oxidation on Mo Single-Atom Catalysts Supported on BP@ZrC

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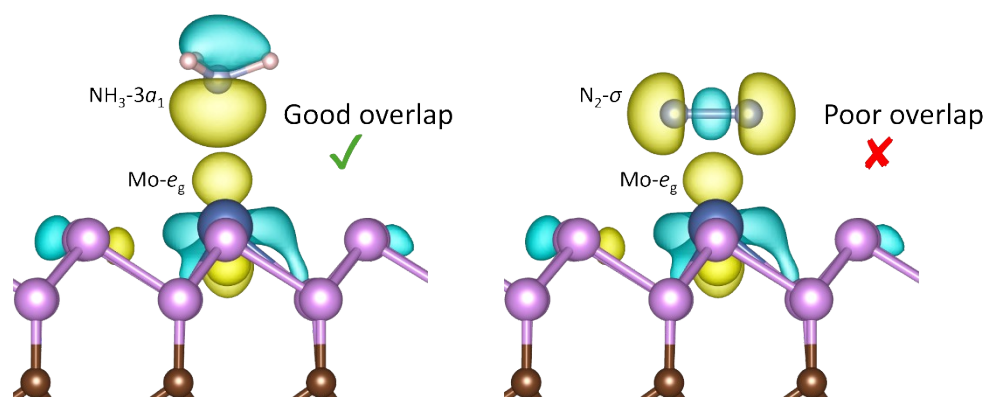


Figure S1. Schematic of the orbital overlap of transition metal SAC, taking Mo-BP@ZrC as an example. The NH_3-3a_1 orbital can better overlap with the $\text{Mo}-e_g$ orbital compared to the orbital of $\text{N}_2-\sigma$.

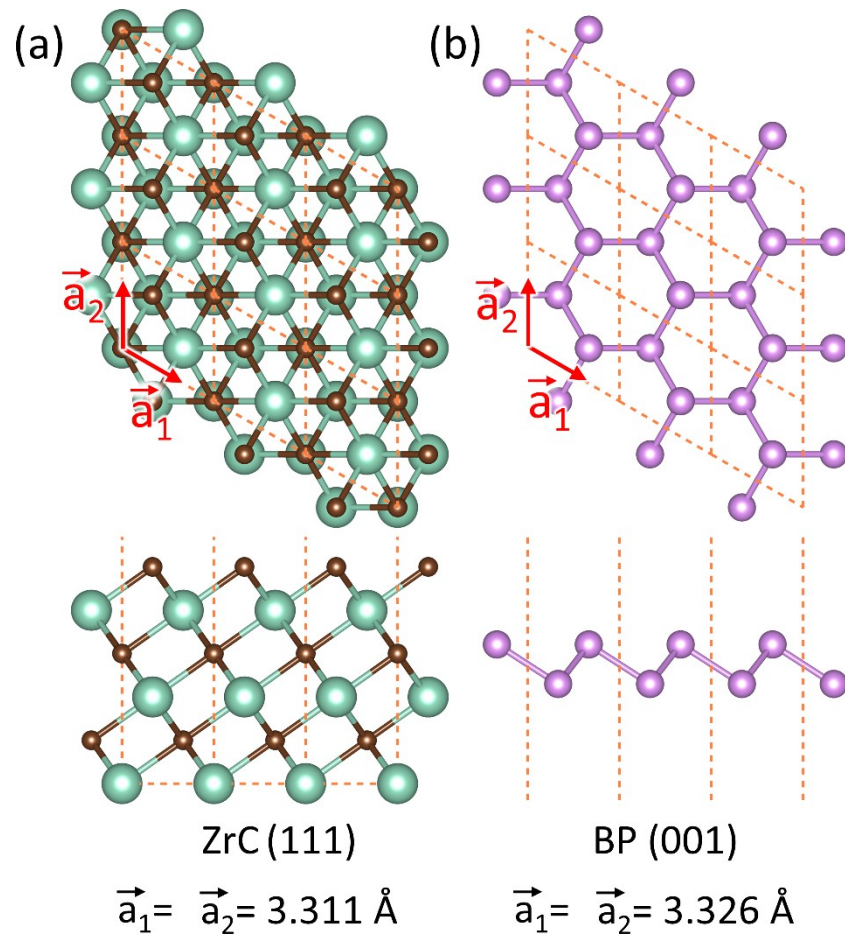


Figure S2. Top and side views of (a) ZrC and (b) monolayer BP, the corresponding lattice constant was mark on the figure. The brown, pink, and turquoise represent C, P, and Zr, respectively.

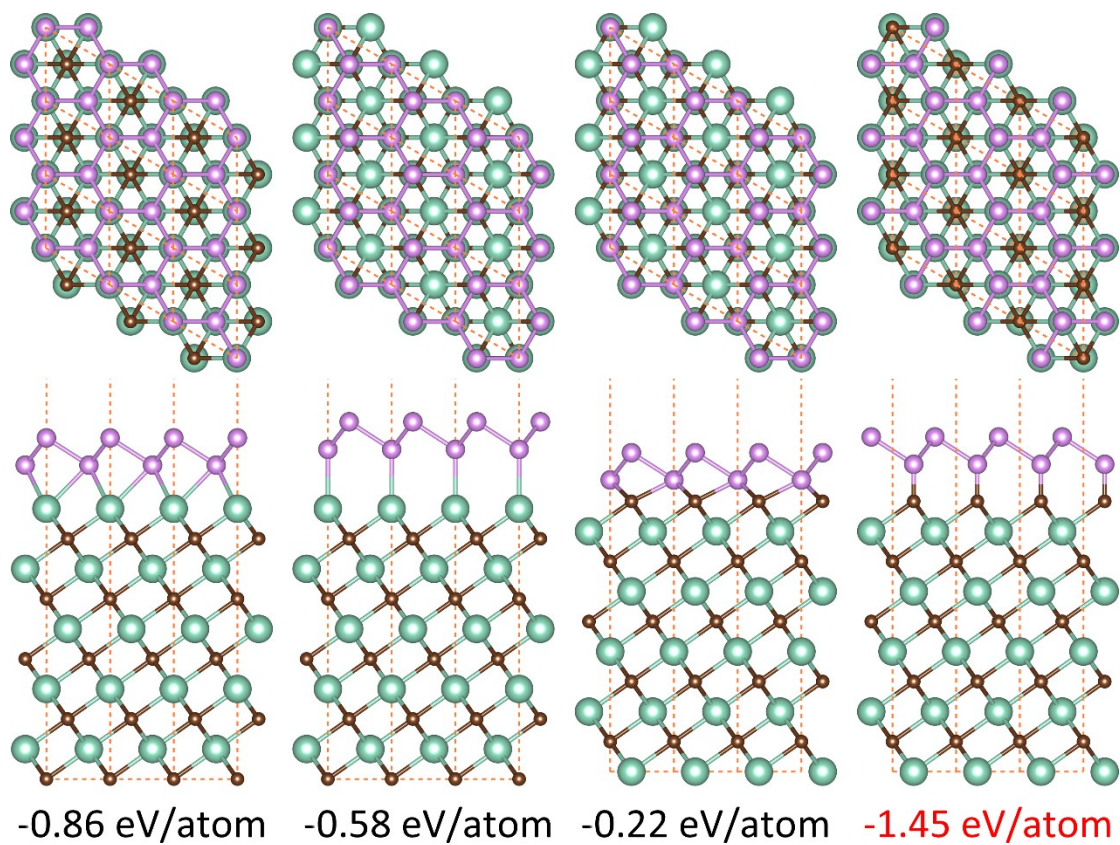


Figure S3. The configurations of the four considered heterogeneous structures of BP@ZrC, the corresponding binding energy between ZrC and BP was mark on the figure.

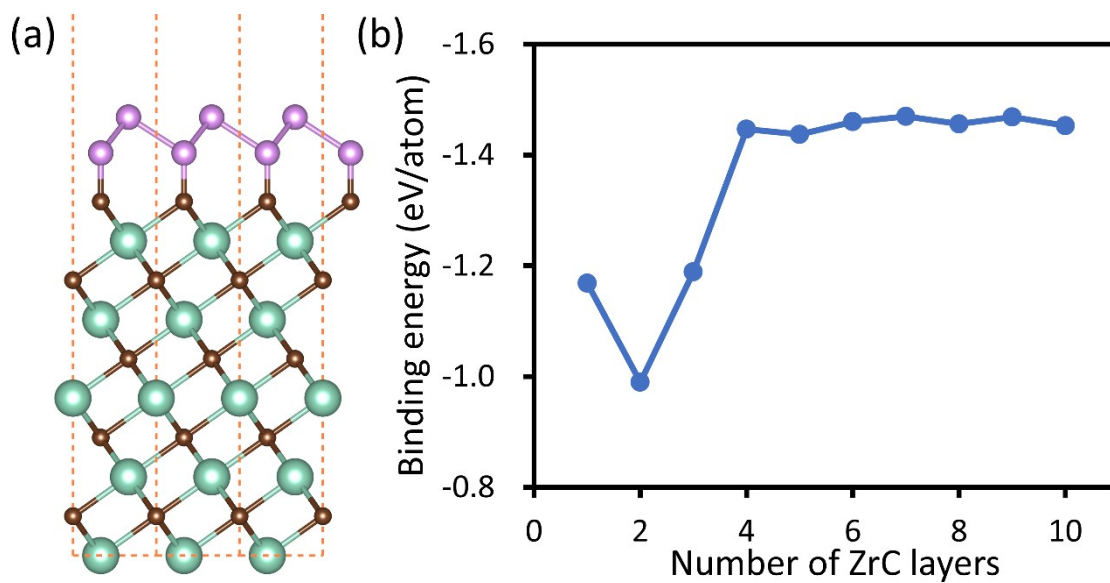


Figure S4. (a) The configurations of BP@ZrC; (b) the convergence test plots of the thickness of ZrC in the BP@ZrC heterostructure on binding energy between ZrC and BP.

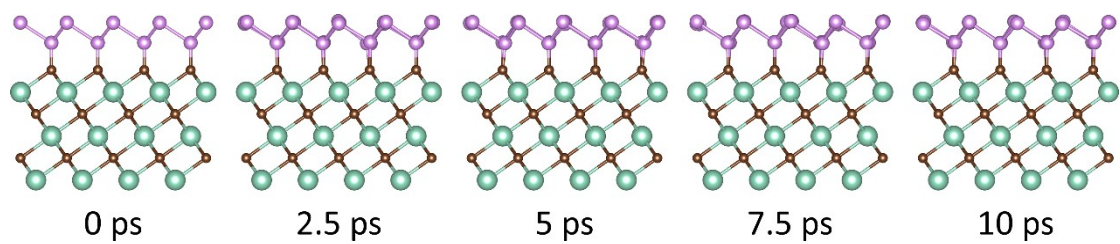


Figure S5. The geometry configuration of BP@ZrC during the 10 ps (10000 dynamics steps) at 1000K.

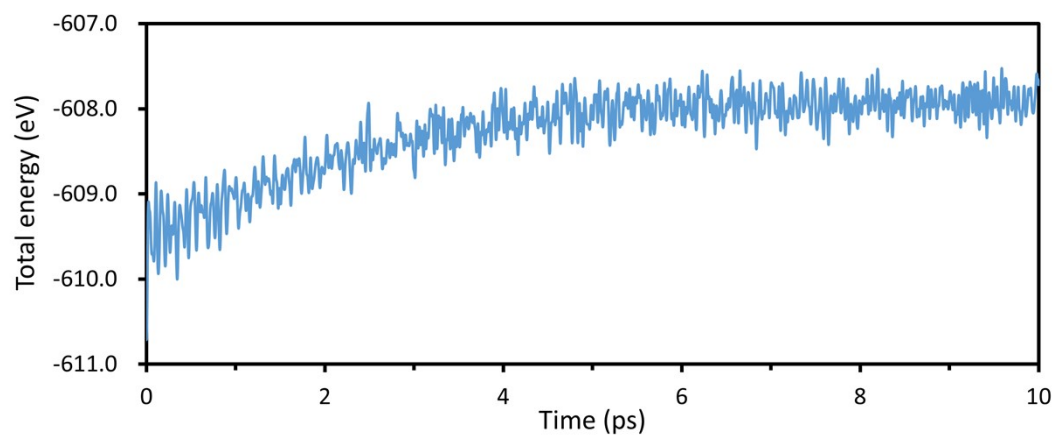


Figure S6. The total energy evolution plots of BP@ZrC during the 10 ps (10000 dynamics steps) at 1000 K.

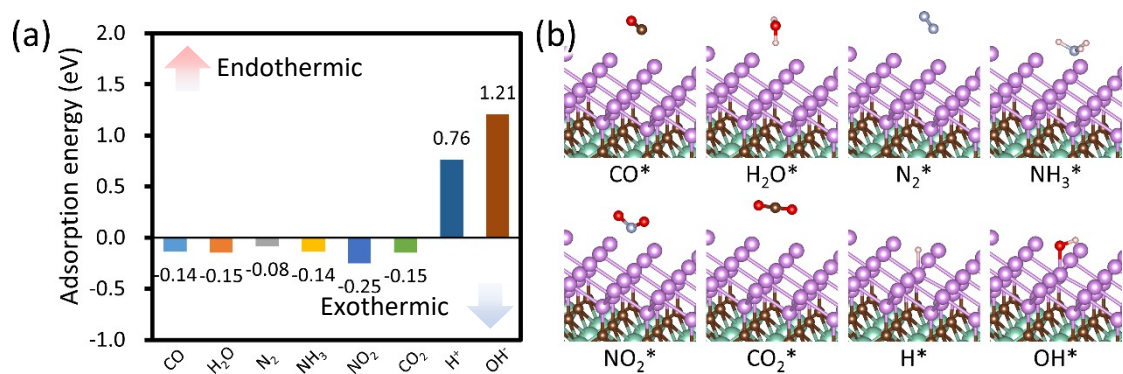


Figure S7. (a) The adsorption energy and (b) the corresponding configuration of small molecules adsorbed on BP@ZrC.

Table S1. The numerical data of N* adsorption energy, limiting potentials of each eAOR steps for TM-BP@ZrC catalysts. The limiting potential of the potential determining step was marked as red. The limit potential of the OH* formation step is provided for comparing.

SAC	ΔG_{N^*}	Limiting potential (V vs. RHE)						
		NH ₃ (g)→	NH ₂ *→	NH*→	N*→	NNH ₂ *→	NNH*→	H ₂ O(l)→
		NH ₂ *+H ⁺ +e ⁻	NH*+H ⁺ +e ⁻	N*+H ⁺ +e ⁻	NNH ₂ *+H ⁺ +e ⁻	NNH*+H ⁺ +e ⁻	N ₂ +H ⁺ +e ⁻	OH*+H ⁺ +e ⁻
W	-0.654	-1.390	0.189	0.075	0.957	0.189	0.437	-1.179
Re	-0.473	-1.028	0.183	0.000	0.654	0.175	-0.127	-0.732
Cr	-0.399	-1.199	0.348	0.080	0.660	-0.053	0.220	-0.868
Ta	-0.342	-1.421	0.517	0.184	0.809	0.228	0.333	-1.365
V	-0.275	-1.174	0.361	0.065	0.544	0.021	0.238	-1.066
Mo	-0.261	-0.766	0.514	0.019	0.365	0.032	-0.108	-0.595
Mn	-0.188	-0.810	0.724	-0.074	0.194	0.085	-0.063	-0.629
Hf	-0.093	-1.262	0.759	0.438	0.345	-0.019	-0.204	-1.256
Nb	0.082	-1.011	0.719	0.402	-0.063	0.106	-0.098	-0.837
Zr	0.164	-0.850	0.722	0.321	0.366	-0.016	-0.487	-0.835
Tc	0.459	-0.366	0.775	0.078	0.170	0.023	-0.625	-0.145
Os	0.499	-0.524	0.899	0.152	0.132	0.403	-1.006	-0.193
Fe	0.521	-0.570	0.895	0.225	-0.179	0.208	-0.521	-0.354
Ti	0.673	-1.105	0.980	0.327	-0.050	0.010	-0.106	-1.080
Ru	1.466	0.136	1.073	0.286	-0.280	0.196	-1.354	0.332
Co	1.503	-0.368	1.076	0.823	-0.816	0.154	-0.813	-0.095
Ir	1.620	-0.162	1.144	0.666	-0.486	0.344	-1.450	0.207
Ni	2.499	-0.164	1.343	1.348	-1.473	0.246	-1.244	0.150
Pt	2.567	0.154	1.373	1.068	-1.038	0.311	-1.812	0.553
Rh	2.627	0.341	1.393	0.922	-1.065	0.088	-1.622	0.596
Au	3.284	0.298	1.613	1.401	-1.532	0.247	-1.971	0.676
Zn	3.412	-0.365	1.927	1.878	-2.015	0.355	-1.724	-0.104
Cu	3.451	0.096	1.760	1.624	-2.027	0.354	-1.750	0.320
Pd	3.635	0.500	1.675	1.489	-1.839	0.135	-1.903	0.780
Ag	4.175	0.431	1.974	1.798	-2.394	0.200	-1.953	0.646

Table S2. The ΔG of all possible intermediates of eAOR and OER on Mo-BP@ZrC. The row of the intermediate with lowest ΔG for each step is marked as red. The “@Mo” represents that the intermediate is bond to the Mo site, and “@P” represents that the intermediate is bond to the P site adjacent to the Mo atom. The ΔG was calculated at temperature of 298.15 K and the potential of 0 V vs. RHE.

Reaction step	Intermediate	ΔG (eV)
0	NH₃*@Mo	-1.18
	NH ₃ *@Mo+NH ₃ *@P	-1.00
	H ₂ O*@Mo	-0.27
	H ₂ O*@P	Relax to H ₂ O*@Mo
1	NH ₂ NH ₃ *@Mo	1.06
	NH ₃ *@Mo+NH ₂ *@P	-0.22
	NH ₂ *@Mo +NH ₃ *@P	Relax to NH ₃ *@Mo+NH ₂ *@P
	NH₂*@Mo	-0.77
	OH*@Mo	-0.52
	OH*@P	1.07
2	NH ₃ *@Mo+NH*@P	0.07
	NH ₂ NH ₂ *@Mo	0.40
	NH ₂ *@Mo+NH ₂ *@P	0.20
	NH*@Mo	-0.25
	NH*@Mo+NH ₃ *@P	Relax to NH ₂ *@Mo+NH ₂ *@P
	O*@Mo	0.01
	O*@P	0.67
3	NH ₃ *@Mo+N*@P	0.83
	NH ₂ *@Mo+NH*@P	0.56
	NHNH ₂ *@Mo	0.25
	NH*@Mo+NH ₂ *@P	0.63
	N*@Mo	-0.23
	N*@Mo+NH ₃ *@P	1.26
	OOH*@Mo	3.16
	OOH*@P	Relax to O*@Mo+OH*@P
	O*@Mo+OH*@P	0.69
4	NH ₂ *@Mo+N*@P	0.60
	NH*@Mo+NH*@P	0.91
	NNH₂*@Mo	0.13
	N*@Mo+NH ₂ *@P	0.60
5	NH*@Mo+N*@P	Relax to NNH*@Mo
	NNH*@Mo	0.16
	N*@Mo+NH*@P	1.01
6	N₂*@Mo	-0.20
	N*@Mo+N*@P	2.03

Table S3. The ΔG of eAOR pathway on Pt(100), Pt-BP@ZrC, and Mo-N4 catalyst. The reaction mechanism is considered to be the same as Mo-BP@ZrC for comparison.

Reaction coordinate	ΔG (eV)		
	Pt(100)	Pt-BP@ZrC	Mo-N4
*	0.000	0.000	0.000
NH ₃ *	-1.043	-1.137	-1.385
NH ₂ *	-0.540	0.155	-1.859
NH*	0.703	1.754	-2.072
N*	1.002	3.004	-1.446
NNH ₂ *	1.266	1.485	-1.290
NNH*	0.671	1.534	-0.573
N ₂ *	0.009	0.302	-1.004
*+N ₂ (g)	0.059	0.059	0.059

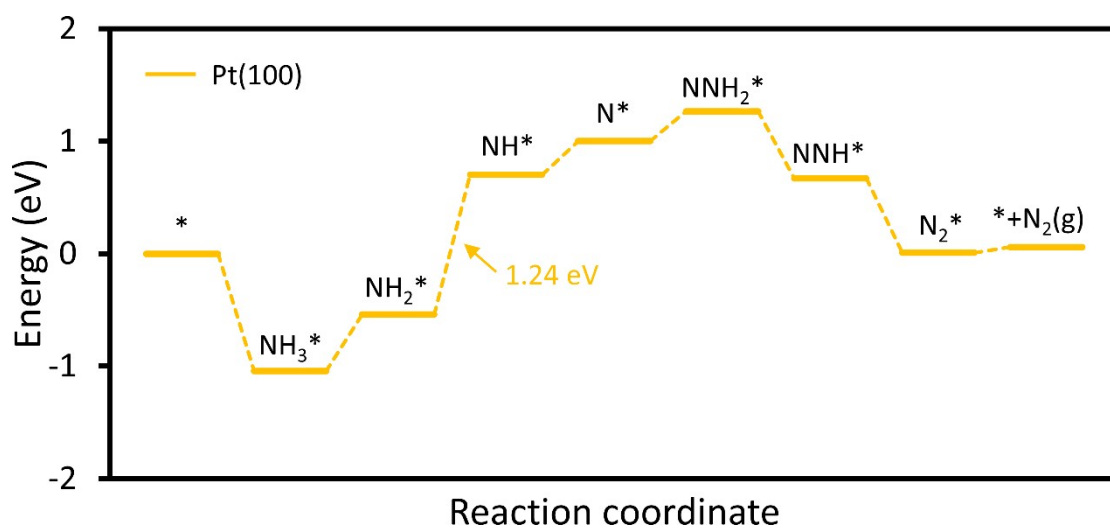


Figure S8. The relative energy plots of eAOR on Pt(100), the potential determining step and corresponding reaction energy were mark on the figure. The corresponding numerical data is presented in Table S3.

Table S4. Summary of ΔG of potential determining step (ΔG_{PDS}) on various eAOR catalysts.

System	Potential determining step	ΔG_{PDS} (eV)	Reference
Mo-BP@ZrC	$\text{NH}_2^* \rightarrow \text{NH}^*$	0.49	This work
Pt-BP@ZrC	$\text{NH}_2^* \rightarrow \text{NH}^*$	1.60	This work
Mo-N ₄	$\text{NNH}_2^* \rightarrow \text{NNH}^*$	0.72	This work
NiOOH	$\text{NH}_3^* \rightarrow \text{NH}_2^*$	1.25	S1
Pt _{0.88} Ir _{0.12} alloy	$\text{NH}^* + \text{NH}_2^* \rightarrow \text{NHNH}_2^*$	0.90	S2
Ir-de4corated Pt	$\text{NH}_2^* \rightarrow \text{NH}^*$	0.74	S3
Pt ₁₃ /NDG	$\text{NH}_3^* \rightarrow \text{NH}_2^*$	0.62	S4
PtZn alloy	$2\text{NH}_2^* \rightarrow \text{NH}_2^* + \text{NH}^*$	0.56	S5

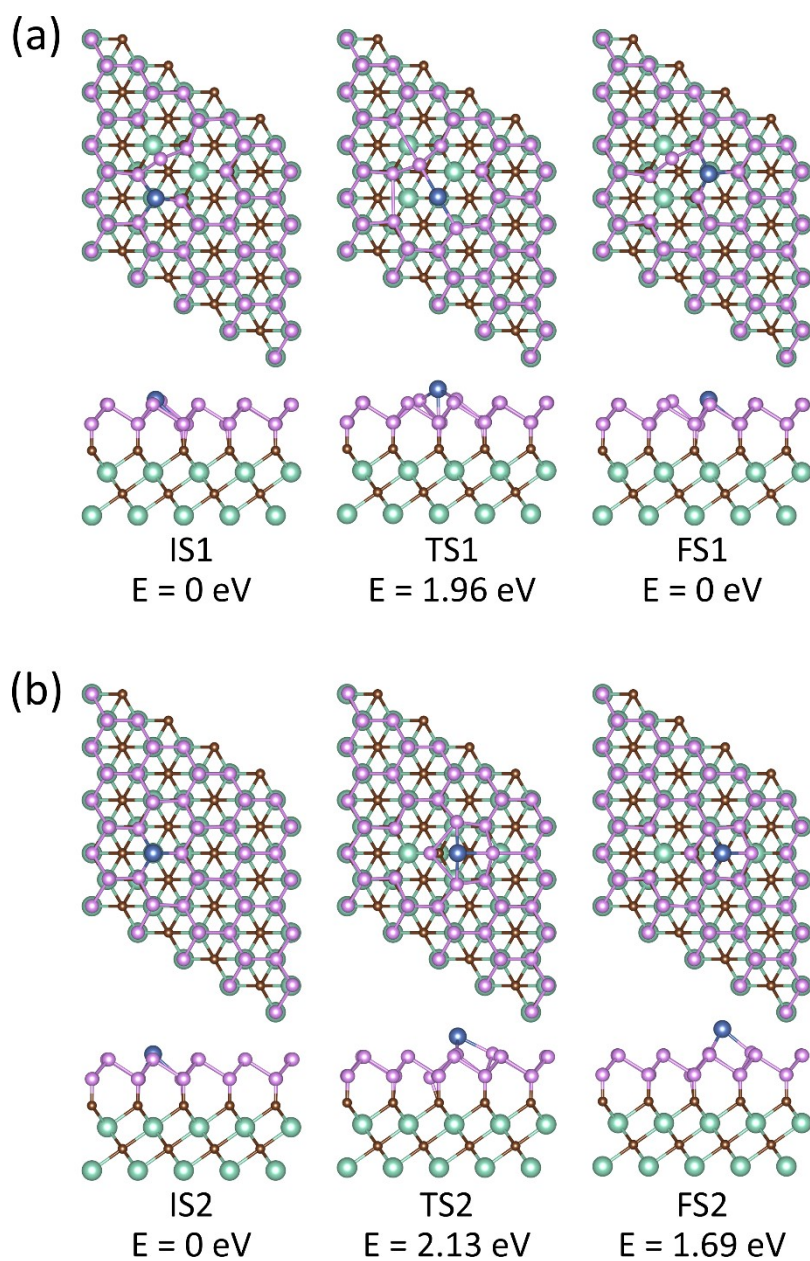


Figure S9. The migration pathway configuration of (a) Mo atom migrates to the nearest neighbor P vacancy on the BP@ZrC with P vacancy, and (b) Mo atom migrates to neighbor P-P-P hollow site on the BP@ZrC without P vacancy, the energy relative to the migration initial state was mark on the figure.

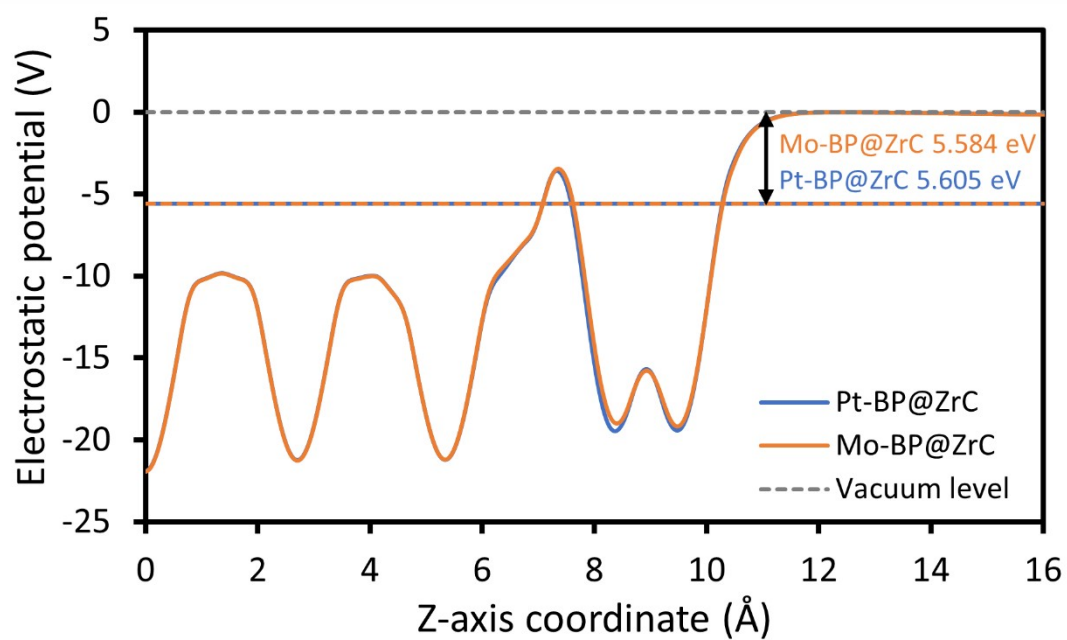


Figure S10. The electrostatic potential plots of Mo-BP@ZrC and Pt-BP@ZrC, with the corresponding work function marked on the figure.

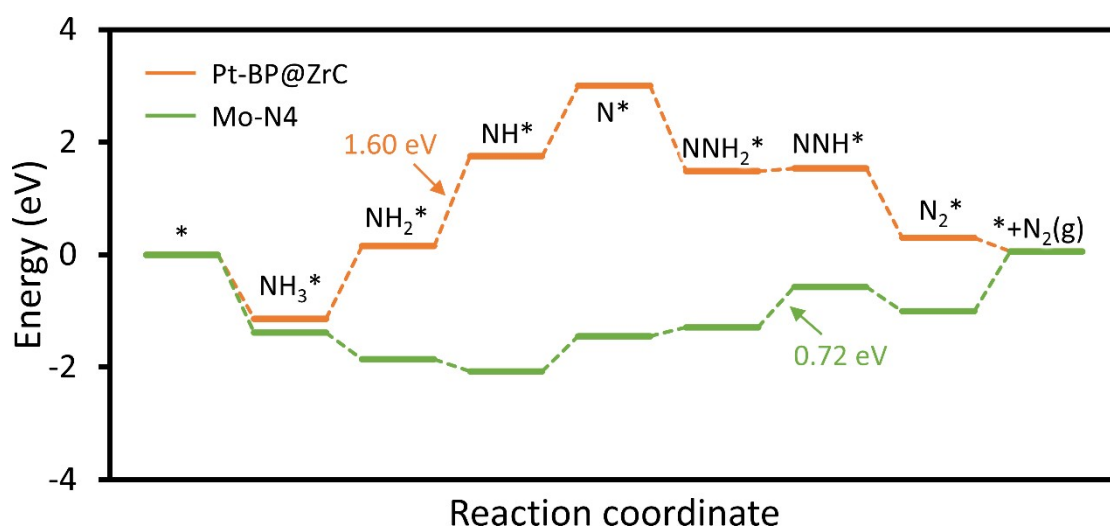


Figure S11. The relative energy plots of eAOR on Pt-BP@ZrC and Mo-N₄, the potential determining step and corresponding reaction energy were mark on the figure. The corresponding numerical data is presented in Table S3.

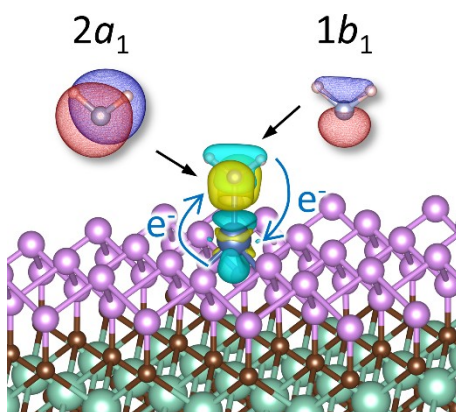


Figure S12. The charge density difference distribution plots of NH_2^* adsorbed on Mo-BP@ZrC . The $2a_1$ and $1b_1$ orbital of NH_2^* was marked on the figure.

Table S5. The Bader charge analysis of Mo-BP@ZrC, NH₂, and NH₂*@Mo-BP@ZrC. The Δq represents the change in Bader charge before and after NH₂* bonding. The “Mo and NH₂” represent the un-adsorbed catalysts and NH₂, “NH₂*@Mo” represent the NH₂* bonding to the Mo atom.

Atom	Bader charge (e)		Δq (e)
	Mo and NH ₂	NH ₂ *@Mo	
Mo	0.561	0.915	0.354
N of NH ₂	-0.764	-1.145	-0.381
H1 of NH ₂	0.382	0.441	0.059
H2 of NH ₂	0.382	0.441	0.059

Table S6. The integral DOS of Mo, N, H atom in Mo-BP@ZrC, NH₂, and NH₂*@Mo-BP@ZrC. The Δ_{IDOS} represents the change in integral DOS before and after NH₂* bonding. The “Mo and NH₂” represent the un-adsorbed catalysts and NH₂, “NH₂*@Mo” represent the NH₂* bonding to the Mo atom.

Orbital	integral DOS (states)		Δ_{IDOS} (states)
	Mo and NH ₂	NH ₂ *@Mo	
N_s	1.31	1.24	-0.06
N_py	0.77	0.85	0.08
N_px	0.93	0.89	-0.04
N_pz	0.64	0.86	0.22
H_s	1.41	1.41	0.00
Mo_s	2.28	2.36	0.08
Mo_dxy	0.85	0.95	0.10
Mo_dyz	0.81	0.87	0.07
Mo_dz ²	0.99	0.68	-0.31
Mo_dxz	0.80	0.71	-0.10
Mo_dx ² -y ²	0.85	1.00	0.15

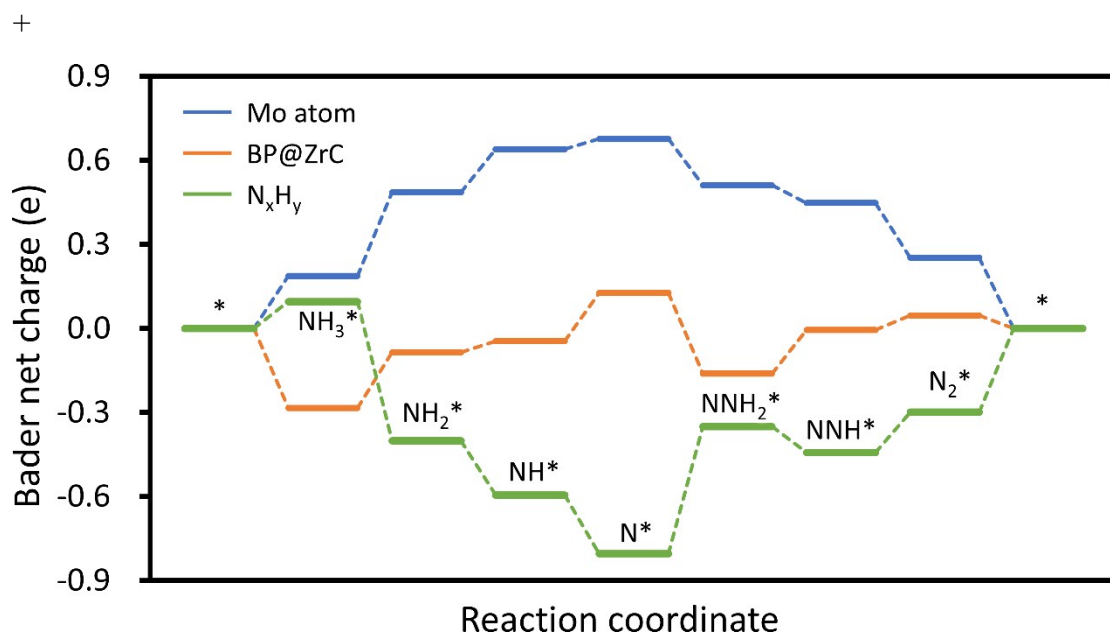


Figure S13. The Bader charge of the intermediate (N_xH_y), substrate (BP@ZrC) and Mo atom during eAOR process. The corresponding numerical data is presented in Table S7.

Table S7. The Bader charge of the intermediate (N_xH_y), substrate (BP@ZrC) and Mo atom during eAOR process.

Reaction coordinate	Bader charge (e)		
	Mo atom	BP@ZrC	N_xH_y
*	0.000	0.000	0.000
NH_3^*	0.188	-0.284	0.096
NH_2^*	0.486	-0.085	-0.401
NH^*	0.640	-0.045	-0.595
N^*	0.677	0.127	-0.804
NNH_2^*	0.511	-0.161	-0.350
NNH^*	0.448	-0.005	-0.443
N_2^*	0.253	0.046	-0.299
$^*+N_2(g)$	0.000	0.000	0.000

Reference

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- [S2] M.-D. Zhang, T. Wang, X.-M. Du, Y. Mao, A.-N. Zhu, A.-X. Du, L.-B. Tong, W. Xie. *J. Am. Chem. Soc.*, 2025, 147,28331.
- [S3] K. Siddharth, Y.-M. Hong, X.-P. Qin, H.J. Lee, Y.T. Chan, S.-Q. Zhu, G.-H. Chen, S.I. Choi, M.-H. Shao. *Appl. Catal. B*, 2020, 269, 118821.
- [S4] H.-G. Shi, J.-Y. Tang, W.-Q. Yu, M.O. Tadé, Z.-P. Shao. *Chem. Eng. J.*, 2024, 488, 150896.
- [S5] J.-Y. Zhang, T.-Q. Yu, L. Chen, Y.-X. Li, L.-Q. Yang, H.-X. He, S.-B. Yin. *Appl. Surf. Sci.* 2025, 683, 161731.

Optimized Structures of Catalysts with POSCAR format

BP@ZrC

1.00000

9.93360 0.00000 0.00000

-4.96680 8.60275 0.00000

0.00000 0.00000 25.00000

Zr C P

27 27 18

Selective dynamics

Direct

0.22222 0.11111 0.00000 F F F

0.55556 0.11111 0.00000 F F F

0.88889 0.11111 0.00000 F F F

0.22222 0.44445 0.00000 F F F

0.55556 0.44445 0.00000 F F F

0.88889 0.44445 0.00000 F F F

0.22222 0.77778 0.00000 F F F

0.55556 0.77778 0.00000 F F F

0.88889 0.77778 0.00000 F F F

0.00000 0.00000 0.10814 F F F

0.33333 0.00000 0.10814 F F F

0.66667 0.00000 0.10814 F F F

0.00000 0.33333 0.10814 F F F

0.33333 0.33333 0.10814 F F F

0.66667 0.33333 0.10814 F F F

0.00000 0.66667 0.10814 F F F

0.33333 0.66667 0.10814 F F F

0.66667 0.66667 0.10814 F F F

0.11113 0.22224 0.21344 T T T

0.44444 0.22223 0.21344 T T T

0.77778 0.22222 0.21343 T T T

0.11111 0.55555 0.21343 T T T

0.44445 0.55557 0.21343 T T T

0.77777 0.55554 0.21344 T T T

0.11111 0.88888 0.21346 T T T

0.44444 0.88889 0.21343 T T T

0.77775 0.88888 0.21344 T T T

0.11111 0.22222 0.05407 F F F

0.44445 0.22222 0.05407 F F F

0.77778 0.22222 0.05407 F F F

0.11111 0.55556 0.05407 F F F

0.44445 0.55556 0.05407 F F F

0.77778	0.55556	0.05407	F	F	F
0.11111	0.88889	0.05407	F	F	F
0.44445	0.88889	0.05407	F	F	F
0.77778	0.88889	0.05407	F	F	F
0.22222	0.11111	0.16222	F	F	F
0.55556	0.11111	0.16222	F	F	F
0.88889	0.11111	0.16222	F	F	F
0.22222	0.44445	0.16222	F	F	F
0.55556	0.44445	0.16222	F	F	F
0.88889	0.44445	0.16222	F	F	F
0.22222	0.77778	0.16222	F	F	F
0.55556	0.77778	0.16222	F	F	F
0.88889	0.77778	0.16222	F	F	F
-0.00003	0.00000	0.26532	T	T	T
0.33349	1.00006	0.26533	T	T	T
0.66666	1.00003	0.26532	T	T	T
-0.00004	0.33334	0.26532	T	T	T
0.33331	0.33337	0.26532	T	T	T
0.66665	0.33334	0.26532	T	T	T
1.00001	0.66663	0.26533	T	T	T
0.33335	0.66667	0.26532	T	T	T
0.66662	0.66662	0.26533	T	T	T
0.33336	0.00009	0.33169	T	T	T
0.66663	0.00009	0.33169	T	T	T
-0.00003	0.00008	0.33168	T	T	T
0.33336	0.33345	0.33169	T	T	T
0.66666	0.33342	0.33169	T	T	T
-0.00002	0.33343	0.33169	T	T	T
0.33333	0.66677	0.33169	T	T	T
0.66665	0.66674	0.33169	T	T	T
-0.00003	0.66672	0.33169	T	T	T
0.11112	0.22234	0.38028	T	T	T
0.44446	0.22233	0.38029	T	T	T
0.77776	0.22233	0.38029	T	T	T
0.11109	0.55567	0.38029	T	T	T
0.44447	0.55569	0.38029	T	T	T
0.77775	0.55564	0.38030	T	T	T
0.11109	0.88897	0.38027	T	T	T
0.44443	0.88899	0.38029	T	T	T
0.77773	0.88899	0.38028	T	T	T

Mo-BP@ZrC

1.00000					
13.24480	0.00000	0.00000			
-6.62240	11.47033	0.00000			
0.00000	0.00000	30.00000			
Zr	C	P	Mo		
48	48	31	1		
Selective	dynamics				
Direct					
0.16667	0.08333	0.00000	F	F	F
0.41667	0.08333	0.00000	F	F	F
0.66667	0.08333	0.00000	F	F	F
0.91667	0.08333	0.00000	F	F	F
0.16667	0.33333	0.00000	F	F	F
0.41667	0.33333	0.00000	F	F	F
0.66667	0.33333	0.00000	F	F	F
0.91667	0.33333	0.00000	F	F	F
0.16667	0.58333	0.00000	F	F	F
0.41667	0.58333	0.00000	F	F	F
0.66667	0.58333	0.00000	F	F	F
0.91667	0.58333	0.00000	F	F	F
0.16667	0.83333	0.00000	F	F	F
0.41667	0.83333	0.00000	F	F	F
0.66667	0.83333	0.00000	F	F	F
0.91667	0.83333	0.00000	F	F	F
0.00000	0.00000	0.09012	F	F	F
0.25000	0.00000	0.09012	F	F	F
0.50000	0.00000	0.09012	F	F	F
0.75000	0.00000	0.09012	F	F	F
0.00000	0.25000	0.09012	F	F	F
0.25000	0.25000	0.09012	F	F	F
0.50000	0.25000	0.09012	F	F	F
0.75000	0.25000	0.09012	F	F	F
0.00000	0.50000	0.09012	F	F	F
0.25000	0.50000	0.09012	F	F	F
0.50000	0.50000	0.09012	F	F	F
0.75000	0.50000	0.09012	F	F	F
0.00000	0.75000	0.09012	F	F	F
0.25000	0.75000	0.09012	F	F	F
0.50000	0.75000	0.09012	F	F	F
0.75000	0.75000	0.09012	F	F	F
0.08308	0.16669	0.17920	T	T	T
0.33387	0.16704	0.17922	T	T	T
0.58321	0.16687	0.17906	T	T	T

0.83360	0.16681	0.17904	T	T	T
0.08319	0.41631	0.17925	T	T	T
0.33336	0.41684	0.17920	T	T	T
0.58331	0.41647	0.17925	T	T	T
0.83331	0.41657	0.17920	T	T	T
0.08357	0.66641	0.17942	T	T	T
0.33362	0.66678	0.17924	T	T	T
0.58320	0.66704	0.17917	T	T	T
0.83268	0.66630	0.17951	T	T	T
0.08369	0.91731	0.17953	T	T	T
0.33343	0.91682	0.17920	T	T	T
0.58320	0.91649	0.17909	T	T	T
0.83330	0.91681	0.17925	T	T	T
0.08333	0.16667	0.04506	F	F	F
0.33333	0.16667	0.04506	F	F	F
0.58333	0.16667	0.04506	F	F	F
0.83333	0.16667	0.04506	F	F	F
0.08333	0.41667	0.04506	F	F	F
0.33333	0.41667	0.04506	F	F	F
0.58333	0.41667	0.04506	F	F	F
0.83333	0.41667	0.04506	F	F	F
0.08333	0.66667	0.04506	F	F	F
0.33333	0.66667	0.04506	F	F	F
0.58333	0.66667	0.04506	F	F	F
0.83333	0.66667	0.04506	F	F	F
0.08333	0.91667	0.04506	F	F	F
0.33333	0.91667	0.04506	F	F	F
0.58333	0.91667	0.04506	F	F	F
0.83333	0.91667	0.04506	F	F	F
0.16667	0.08333	0.13518	F	F	F
0.41667	0.08333	0.13518	F	F	F
0.66667	0.08333	0.13518	F	F	F
0.91667	0.08333	0.13518	F	F	F
0.16667	0.33333	0.13518	F	F	F
0.41667	0.33333	0.13518	F	F	F
0.66667	0.33333	0.13518	F	F	F
0.91667	0.33333	0.13518	F	F	F
0.16667	0.58333	0.13518	F	F	F
0.41667	0.58333	0.13518	F	F	F
0.66667	0.58333	0.13518	F	F	F
0.91667	0.58333	0.13518	F	F	F
0.16667	0.83333	0.13518	F	F	F
0.41667	0.83333	0.13518	F	F	F
0.66667	0.83333	0.13518	F	F	F

0.91667	0.83333	0.13518	F	F	F
-0.00027	-0.00004	0.22175	T	T	T
0.25026	-0.00019	0.22163	T	T	T
0.50021	0.00013	0.22168	T	T	T
0.74997	-0.00006	0.22166	T	T	T
-0.00115	0.24943	0.22183	T	T	T
0.24895	0.24779	0.22035	T	T	T
0.50057	0.24929	0.22188	T	T	T
0.74998	0.24990	0.22169	T	T	T
-0.00040	0.49978	0.22170	T	T	T
0.24882	0.50121	0.22036	T	T	T
0.50230	0.50112	0.22048	T	T	T
0.75007	0.49966	0.22170	T	T	T
0.00006	0.75006	0.22105	T	T	T
0.25050	0.75044	0.22167	T	T	T
0.50060	0.75131	0.22189	T	T	T
0.75017	0.75034	0.22171	T	T	T
-0.00057	0.00002	0.27711	T	T	T
0.25132	-0.00003	0.27697	T	T	T
0.49987	0.99983	0.27709	T	T	T
0.75085	0.99977	0.27708	T	T	T
0.00290	0.25138	0.27733	T	T	T
0.49945	0.25117	0.27741	T	T	T
0.75086	0.25084	0.27710	T	T	T
-0.00061	0.49929	0.27705	T	T	T
0.75045	0.49916	0.27706	T	T	T
0.00037	0.75015	0.27654	T	T	T
0.25142	0.75121	0.27702	T	T	T
0.49939	0.74799	0.27742	T	T	T
0.75056	0.75111	0.27708	T	T	T
0.25171	0.25212	0.27585	T	T	T
0.25156	0.49936	0.27587	T	T	T
0.49797	0.49887	0.27602	T	T	T
0.08978	0.17135	0.31686	T	T	T
0.33247	0.17042	0.31680	T	T	T
0.58341	0.16743	0.31729	T	T	T
0.83527	0.16747	0.31721	T	T	T
0.08964	0.41834	0.31686	T	T	T
0.57990	0.41816	0.31689	T	T	T
0.83444	0.41810	0.31728	T	T	T
0.08358	0.66715	0.31687	T	T	T
0.33248	0.66160	0.31687	T	T	T
0.57990	0.66141	0.31687	T	T	T
0.83433	0.66702	0.31694	T	T	T

0.08360	0.91629	0.31691	T	T	T
0.33272	0.91637	0.31721	T	T	T
0.58336	0.91568	0.31728	T	T	T
0.83449	0.91617	0.31730	T	T	T
0.33289	0.41641	0.32217	T	T	T

Pt-BP@ZrC

1.00000

13.24480 0.00000 0.00000

-6.62240 11.47033 0.00000

0.00000 0.00000 30.00000

Zr C P Pt

48 48 31 1

Selective dynamics

Direct

0.16667 0.08333 0.00000 F F F

0.41667 0.08333 0.00000 F F F

0.66667 0.08333 0.00000 F F F

0.91667 0.08333 0.00000 F F F

0.16667 0.33333 0.00000 F F F

0.41667 0.33333 0.00000 F F F

0.66667 0.33333 0.00000 F F F

0.91667 0.33333 0.00000 F F F

0.16667 0.58333 0.00000 F F F

0.41667 0.58333 0.00000 F F F

0.66667 0.58333 0.00000 F F F

0.91667 0.58333 0.00000 F F F

0.16667 0.83333 0.00000 F F F

0.41667 0.83333 0.00000 F F F

0.66667 0.83333 0.00000 F F F

0.91667 0.83333 0.00000 F F F

0.00000 0.00000 0.09012 F F F

0.25000 0.00000 0.09012 F F F

0.50000 0.00000 0.09012 F F F

0.75000 0.00000 0.09012 F F F

0.00000 0.25000 0.09012 F F F

0.25000 0.25000 0.09012 F F F

0.50000 0.25000 0.09012 F F F

0.75000 0.25000 0.09012 F F F

0.00000 0.50000 0.09012 F F F

0.25000 0.50000 0.09012 F F F

0.50000 0.50000 0.09012 F F F

0.75000 0.50000 0.09012 F F F

0.00000 0.75000 0.09012 F F F

0.25000 0.75000 0.09012 F F F

0.50000 0.75000 0.09012 F F F

0.75000 0.75000 0.09012 F F F

0.08260 0.16642 0.17897 T T T

0.33388 0.16641 0.17898 T T T

0.58328 0.16676 0.17853 T T T

0.83353	0.16676	0.17853	T	T	T
0.08260	0.41617	0.17897	T	T	T
0.33336	0.41668	0.17864	T	T	T
0.58361	0.41616	0.17897	T	T	T
0.83322	0.41639	0.17899	T	T	T
0.08335	0.66668	0.17934	T	T	T
0.33388	0.66746	0.17898	T	T	T
0.58361	0.66744	0.17897	T	T	T
0.83337	0.66668	0.17936	T	T	T
0.08335	0.91666	0.17934	T	T	T
0.33363	0.91681	0.17900	T	T	T
0.58328	0.91651	0.17853	T	T	T
0.83322	0.91681	0.17900	T	T	T
0.08333	0.16667	0.04506	F	F	F
0.33333	0.16667	0.04506	F	F	F
0.58333	0.16667	0.04506	F	F	F
0.83333	0.16667	0.04506	F	F	F
0.08333	0.41667	0.04506	F	F	F
0.33333	0.41667	0.04506	F	F	F
0.58333	0.41667	0.04506	F	F	F
0.83333	0.41667	0.04506	F	F	F
0.08333	0.66667	0.04506	F	F	F
0.33333	0.66667	0.04506	F	F	F
0.58333	0.66667	0.04506	F	F	F
0.83333	0.66667	0.04506	F	F	F
0.08333	0.91667	0.04506	F	F	F
0.33333	0.91667	0.04506	F	F	F
0.58333	0.91667	0.04506	F	F	F
0.83333	0.91667	0.04506	F	F	F
0.16667	0.08333	0.13518	F	F	F
0.41667	0.08333	0.13518	F	F	F
0.66667	0.08333	0.13518	F	F	F
0.91667	0.08333	0.13518	F	F	F
0.16667	0.33333	0.13518	F	F	F
0.41667	0.33333	0.13518	F	F	F
0.66667	0.33333	0.13518	F	F	F
0.91667	0.33333	0.13518	F	F	F
0.16667	0.58333	0.13518	F	F	F
0.41667	0.58333	0.13518	F	F	F
0.66667	0.58333	0.13518	F	F	F
0.91667	0.58333	0.13518	F	F	F
0.16667	0.83333	0.13518	F	F	F
0.41667	0.83333	0.13518	F	F	F
0.66667	0.83333	0.13518	F	F	F

0.91667	0.83333	0.13518	F	F	F
0.00016	0.00009	0.22132	T	T	T
0.25001	0.00008	0.22133	T	T	T
0.50067	0.00033	0.22155	T	T	T
0.74974	0.00033	0.22155	T	T	T
0.99844	0.24921	0.22196	T	T	T
0.24914	0.24818	0.22199	T	T	T
0.50087	0.24922	0.22196	T	T	T
0.74974	0.24939	0.22155	T	T	T
0.00016	0.50006	0.22132	T	T	T
0.24914	0.50095	0.22199	T	T	T
0.50192	0.50095	0.22200	T	T	T
0.74999	0.50004	0.22132	T	T	T
0.00005	0.75002	0.22098	T	T	T
0.25001	0.74991	0.22133	T	T	T
0.50087	0.75163	0.22196	T	T	T
0.74999	0.74993	0.22132	T	T	T
0.99891	0.99902	0.27643	T	T	T
0.25057	0.99902	0.27644	T	T	T
0.50030	0.00013	0.27685	T	T	T
0.75028	0.00013	0.27685	T	T	T
0.00089	0.25042	0.27740	T	T	T
0.49999	0.25042	0.27740	T	T	T
0.75028	0.25011	0.27685	T	T	T
0.99890	0.49984	0.27643	T	T	T
0.75137	0.49983	0.27643	T	T	T
0.00028	0.75011	0.27638	T	T	T
0.25057	0.75150	0.27644	T	T	T
0.49999	0.74952	0.27740	T	T	T
0.75137	0.75149	0.27643	T	T	T
0.24714	0.24383	0.27684	T	T	T
0.24715	0.50326	0.27684	T	T	T
0.50653	0.50324	0.27684	T	T	T
0.08390	0.16611	0.31758	T	T	T
0.33276	0.16615	0.31757	T	T	T
0.58372	0.16678	0.31743	T	T	T
0.83359	0.16676	0.31742	T	T	T
0.08390	0.41773	0.31758	T	T	T
0.58433	0.41773	0.31758	T	T	T
0.83356	0.41661	0.31738	T	T	T
0.08334	0.66713	0.31696	T	T	T
0.33276	0.66656	0.31757	T	T	T
0.58433	0.66654	0.31758	T	T	T
0.83428	0.66711	0.31696	T	T	T

0.08334	0.91616	0.31696	T	T	T
0.33389	0.91692	0.31738	T	T	T
0.58372	0.91688	0.31743	T	T	T
0.83356	0.91690	0.31738	T	T	T
0.33360	0.41677	0.31559	T	T	T

Mo-N ₄					
1.00000					
14.76000	0.00000	0.00000			
0.00000	17.04340	0.00000			
0.00000	0.00000	25.00000			
C	N	Mo			
90	4	1			
Selective	dynamics				
Direct					
0.00000	0.04179	0.50021	T	T	T
0.16703	0.04193	0.49997	T	T	T
0.33403	0.04218	0.49969	T	T	T
0.50000	0.04206	0.49973	T	T	T
0.66597	0.04218	0.49969	T	T	T
0.83297	0.04193	0.49997	T	T	T
0.08360	0.08297	0.50013	T	T	T
0.25058	0.08347	0.49968	T	T	T
0.41710	0.08434	0.49965	T	T	T
0.58290	0.08434	0.49965	T	T	T
0.74942	0.08347	0.49968	T	T	T
0.91640	0.08297	0.50013	T	T	T
0.08350	0.16675	0.50004	T	T	T
0.25046	0.16742	0.49940	T	T	T
0.41717	0.16871	0.49963	T	T	T
0.58283	0.16871	0.49963	T	T	T
0.74954	0.16742	0.49940	T	T	T
0.91650	0.16675	0.50004	T	T	T
0.00000	0.20788	0.50007	T	T	T
0.16672	0.20807	0.49964	T	T	T
0.33381	0.20952	0.49936	T	T	T
0.50000	0.21206	0.49997	T	T	T
0.66619	0.20952	0.49936	T	T	T
0.83328	0.20807	0.49964	T	T	T
0.00000	0.29157	0.49970	T	T	T
0.16628	0.29178	0.49935	T	T	T
0.33317	0.29366	0.49972	T	T	T
0.50000	0.29700	0.50155	T	T	T
0.66683	0.29366	0.49972	T	T	T
0.83372	0.29178	0.49935	T	T	T
0.08284	0.33306	0.49931	T	T	T
0.24847	0.33345	0.49918	T	T	T
0.41471	0.33728	0.50208	T	T	T
0.58529	0.33728	0.50208	T	T	T
0.75153	0.33345	0.49918	T	T	T

0.91716	0.33306	0.49931	T	T	T
0.08236	0.41639	0.49872	T	T	T
0.24687	0.41691	0.49842	T	T	T
0.75313	0.41691	0.49842	T	T	T
0.91764	0.41639	0.49872	T	T	T
0.00000	0.45821	0.49882	T	T	T
0.16437	0.45847	0.49795	T	T	T
0.32841	0.45820	0.50101	T	T	T
0.67159	0.45820	0.50101	T	T	T
0.83563	0.45847	0.49795	T	T	T
0.00000	0.54179	0.49882	T	T	T
0.16437	0.54153	0.49795	T	T	T
0.32841	0.54180	0.50101	T	T	T
0.67159	0.54180	0.50101	T	T	T
0.83563	0.54153	0.49795	T	T	T
0.08236	0.58361	0.49872	T	T	T
0.24687	0.58309	0.49842	T	T	T
0.75313	0.58309	0.49842	T	T	T
0.91764	0.58361	0.49872	T	T	T
0.08284	0.66694	0.49931	T	T	T
0.24847	0.66655	0.49918	T	T	T
0.41471	0.66272	0.50208	T	T	T
0.58529	0.66272	0.50208	T	T	T
0.75153	0.66655	0.49918	T	T	T
0.91716	0.66694	0.49931	T	T	T
0.00000	0.70843	0.49970	T	T	T
0.16628	0.70822	0.49935	T	T	T
0.33317	0.70634	0.49972	T	T	T
0.50000	0.70300	0.50155	T	T	T
0.66683	0.70634	0.49972	T	T	T
0.83372	0.70822	0.49935	T	T	T
0.00000	0.79212	0.50007	T	T	T
0.16672	0.79193	0.49964	T	T	T
0.33381	0.79048	0.49936	T	T	T
0.50000	0.78794	0.49997	T	T	T
0.66619	0.79048	0.49936	T	T	T
0.83328	0.79193	0.49964	T	T	T
0.08350	0.83325	0.50004	T	T	T
0.25046	0.83258	0.49940	T	T	T
0.41717	0.83129	0.49963	T	T	T
0.58283	0.83129	0.49963	T	T	T
0.74954	0.83258	0.49940	T	T	T
0.91650	0.83325	0.50004	T	T	T
0.08360	0.91703	0.50013	T	T	T

0.25058	0.91653	0.49968	T	T	T
0.41710	0.91566	0.49965	T	T	T
0.58290	0.91566	0.49965	T	T	T
0.74942	0.91653	0.49968	T	T	T
0.91640	0.91703	0.50013	T	T	T
0.00000	0.95821	0.50021	T	T	T
0.16703	0.95807	0.49997	T	T	T
0.33403	0.95782	0.49969	T	T	T
0.50000	0.95794	0.49973	T	T	T
0.66597	0.95782	0.49969	T	T	T
0.83297	0.95807	0.49997	T	T	T
0.40977	0.41882	0.50735	T	T	T
0.59023	0.41882	0.50735	T	T	T
0.40977	0.58118	0.50735	T	T	T
0.59023	0.58118	0.50735	T	T	T
0.50000	0.50000	0.53068	T	T	T

Pt (100)					
1.00000					
13.87310	0.00000	0.00000			
0.00000	13.87310	0.00000			
0.00000	0.00000	30.00000			
Pt					
125					
Selective	dynamics				
Direct					
0.00000	0.06667	0.00000	F	F	F
0.20000	0.06667	0.00000	F	F	F
0.40000	0.06667	0.00000	F	F	F
0.60000	0.06667	0.00000	F	F	F
0.80000	0.06667	0.00000	F	F	F
0.00000	0.26667	0.00000	F	F	F
0.20000	0.26667	0.00000	F	F	F
0.40000	0.26667	0.00000	F	F	F
0.60000	0.26667	0.00000	F	F	F
0.80000	0.26667	0.00000	F	F	F
0.00000	0.46667	0.00000	F	F	F
0.20000	0.46667	0.00000	F	F	F
0.40000	0.46667	0.00000	F	F	F
0.60000	0.46667	0.00000	F	F	F
0.80000	0.46667	0.00000	F	F	F
0.00000	0.66667	0.00000	F	F	F
0.20000	0.66667	0.00000	F	F	F
0.40000	0.66667	0.00000	F	F	F
0.60000	0.66667	0.00000	F	F	F
0.80000	0.66667	0.00000	F	F	F
0.00000	0.86667	0.00000	F	F	F
0.20000	0.86667	0.00000	F	F	F
0.40000	0.86667	0.00000	F	F	F
0.60000	0.86667	0.00000	F	F	F
0.80000	0.86667	0.00000	F	F	F
0.10000	0.16667	0.06540	F	F	F
0.30000	0.16667	0.06540	F	F	F
0.50000	0.16667	0.06540	F	F	F
0.70000	0.16667	0.06540	F	F	F
0.90000	0.16667	0.06540	F	F	F
0.10000	0.36667	0.06540	F	F	F
0.30000	0.36667	0.06540	F	F	F
0.50000	0.36667	0.06540	F	F	F
0.70000	0.36667	0.06540	F	F	F
0.90000	0.36667	0.06540	F	F	F

0.10000	0.56667	0.06540	F	F	F
0.30000	0.56667	0.06540	F	F	F
0.50000	0.56667	0.06540	F	F	F
0.70000	0.56667	0.06540	F	F	F
0.90000	0.56667	0.06540	F	F	F
0.10000	0.76667	0.06540	F	F	F
0.30000	0.76667	0.06540	F	F	F
0.50000	0.76667	0.06540	F	F	F
0.70000	0.76667	0.06540	F	F	F
0.90000	0.76667	0.06540	F	F	F
0.10000	0.96667	0.06540	F	F	F
0.30000	0.96667	0.06540	F	F	F
0.50000	0.96667	0.06540	F	F	F
0.70000	0.96667	0.06540	F	F	F
0.90000	0.96667	0.06540	F	F	F
0.00000	0.06667	0.13080	F	F	F
0.20000	0.06667	0.13080	F	F	F
0.40000	0.06667	0.13080	F	F	F
0.60000	0.06667	0.13080	F	F	F
0.80000	0.06667	0.13080	F	F	F
0.00000	0.26667	0.13080	F	F	F
0.20000	0.26667	0.13080	F	F	F
0.40000	0.26667	0.13080	F	F	F
0.60000	0.26667	0.13080	F	F	F
0.80000	0.26667	0.13080	F	F	F
0.00000	0.46667	0.13080	F	F	F
0.20000	0.46667	0.13080	F	F	F
0.40000	0.46667	0.13080	F	F	F
0.60000	0.46667	0.13080	F	F	F
0.80000	0.46667	0.13080	F	F	F
0.00000	0.66667	0.13080	F	F	F
0.20000	0.66667	0.13080	F	F	F
0.40000	0.66667	0.13080	F	F	F
0.60000	0.66667	0.13080	F	F	F
0.80000	0.66667	0.13080	F	F	F
0.00000	0.86667	0.13080	F	F	F
0.20000	0.86667	0.13080	F	F	F
0.40000	0.86667	0.13080	F	F	F
0.60000	0.86667	0.13080	F	F	F
0.80000	0.86667	0.13080	F	F	F
0.10000	0.16667	0.19639	T	T	T
0.30000	0.16667	0.19639	T	T	T
0.50000	0.16667	0.19639	T	T	T
0.70000	0.16667	0.19639	T	T	T

0.90000	0.16667	0.19639	T	T	T
0.10000	0.36667	0.19639	T	T	T
0.30000	0.36667	0.19639	T	T	T
0.50000	0.36667	0.19639	T	T	T
0.70000	0.36667	0.19639	T	T	T
0.90000	0.36667	0.19639	T	T	T
0.10000	0.56667	0.19639	T	T	T
0.30000	0.56667	0.19639	T	T	T
0.50000	0.56667	0.19639	T	T	T
0.70000	0.56667	0.19639	T	T	T
0.90000	0.56667	0.19639	T	T	T
0.10000	0.76667	0.19639	T	T	T
0.30000	0.76667	0.19639	T	T	T
0.50000	0.76667	0.19639	T	T	T
0.70000	0.76667	0.19639	T	T	T
0.90000	0.76667	0.19639	T	T	T
0.10000	0.96667	0.19639	T	T	T
0.30000	0.96667	0.19639	T	T	T
0.50000	0.96667	0.19639	T	T	T
0.70000	0.96667	0.19639	T	T	T
0.90000	0.96667	0.19639	T	T	T
0.00000	0.06667	0.26151	T	T	T
0.20000	0.06667	0.26151	T	T	T
0.40000	0.06667	0.26151	T	T	T
0.60000	0.06667	0.26151	T	T	T
0.80000	0.06667	0.26151	T	T	T
0.00000	0.26667	0.26151	T	T	T
0.20000	0.26667	0.26151	T	T	T
0.40000	0.26667	0.26151	T	T	T
0.60000	0.26667	0.26151	T	T	T
0.80000	0.26667	0.26151	T	T	T
0.00000	0.46667	0.26151	T	T	T
0.20000	0.46667	0.26151	T	T	T
0.40000	0.46667	0.26151	T	T	T
0.60000	0.46667	0.26151	T	T	T
0.80000	0.46667	0.26151	T	T	T
0.00000	0.66667	0.26151	T	T	T
0.20000	0.66667	0.26151	T	T	T
0.40000	0.66667	0.26151	T	T	T
0.60000	0.66667	0.26151	T	T	T
0.80000	0.66667	0.26151	T	T	T
0.00000	0.86667	0.26151	T	T	T
0.20000	0.86667	0.26151	T	T	T
0.40000	0.86667	0.26151	T	T	T

0.60000	0.86667	0.26151	T	T	T
0.80000	0.86667	0.26151	T	T	T