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Mechanistic Insights and Predictive Screening of M@C₂N

Catalysts for Urea Electrosynthesis from N₂ and CO₂

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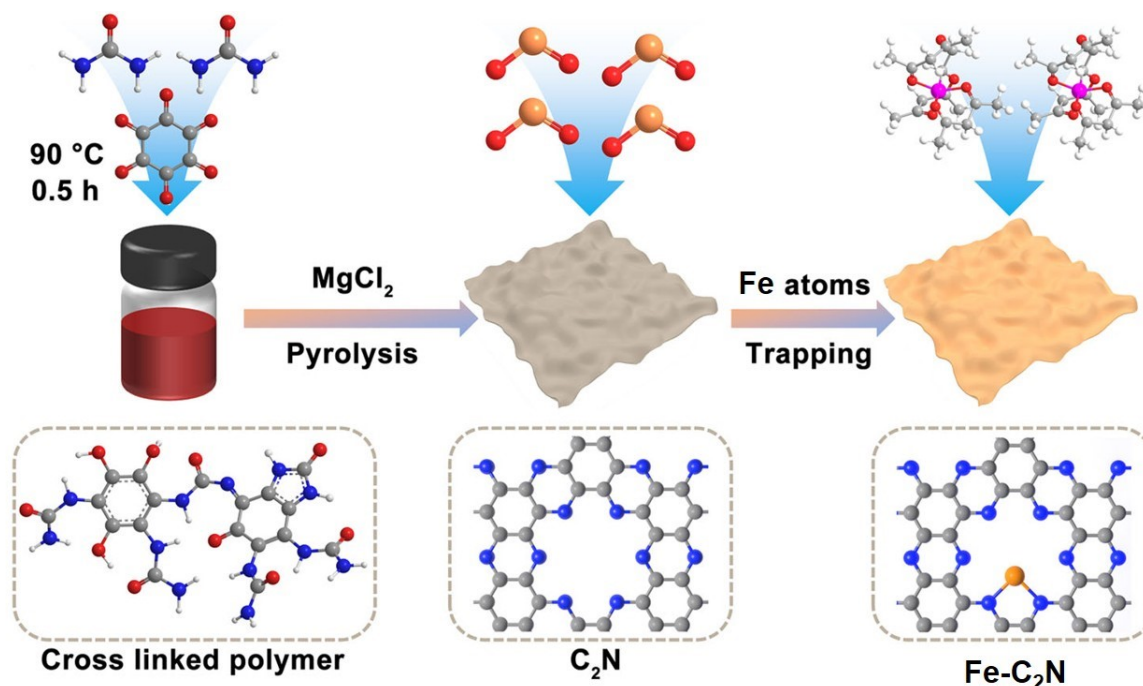
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Scheme S1. Proposed synthesis route for Fe-C₂N (Nb@C₂N, Mo@C₂N, and Re@C₂N)

The synthesis routes have been developed by Wang and co-workers¹ such as the thermal treatment of a mixture of cyclohexanehexone and urea, followed by calcination at various temperatures (500-1000 °C) in the presence of MgCl₂ under nitrogen atmosphere. The carbonized products are then purified and dried to yield C₂N materials with different crystallinities and surface properties. Details are below.

Preparation of C₂N

1. A well-ground mixture of cyclohexanehexone and urea was prepared in a molar ratio of 1:4.5.
2. This mixture was gently heated at 90 °C for 30 minutes.
3. The resulting cross-linked product was then mixed with anhydrous MgCl₂ in a mass ratio of 1:3.75 and ground thoroughly.
4. The mixture was calcined at 500, 800, 900, and 1000 °C for 2 hours, with a heating rate of 3 °C/min under a nitrogen atmosphere.
5. After cooling to room temperature, the carbonized samples were washed sequentially with 0.5 M sulfuric acid, deionized water, and ethanol.
6. Finally, the washed samples were dried overnight in a vacuum oven at 60 °C to yield C₂N-500, C₂N-800, C₂N-900, and C₂N-1000, respectively.

Preparation of Fe-C₂N

1. 90 mg of the prepared C₂N was mixed with 6 mg of iron (III) acetylacetonate (Fe(acac)₃) using a simple grinding method.
2. The resulting powder was then placed in a tube furnace and heated to 900 °C at a rate of 3 °C per minute under a flowing nitrogen atmosphere.
3. Once the target temperature was reached, the material was annealed for 2 hours.
4. After naturally cooling to room temperature, the final product, Fe-C₂N, was obtained and used directly without any further treatment.

Although the direct synthesis of Nb@C₂N, Mo@C₂N, and Re@C₂N has not yet been documented in the literature, we propose that it is achievable by substituting the commonly used iron precursor, such as iron (III) acetylacetonate, with suitable alternatives. These include niobium oxalate (C₁₀H₅NbO₂₀)² or niobium pentachloride (NbCl₅)³ for Nb, molybdenum(V) chloride (MoCl₅)⁴ for Mo, and ammonium perrhenate (NH₄ReO₄)⁵ for Re, enabling the synthesis of single-atom catalysts based on each metal.

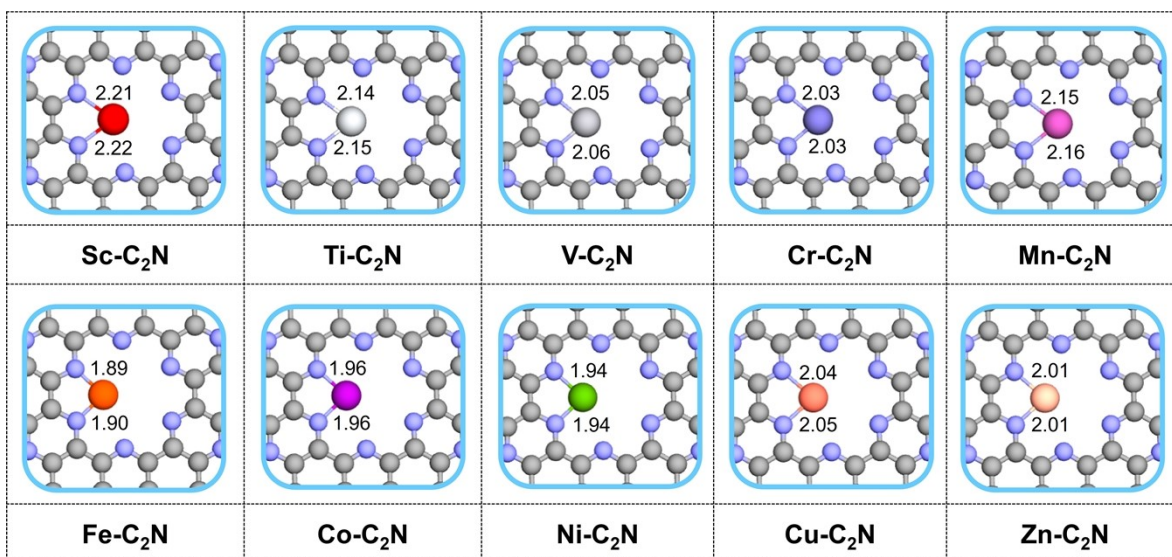


Figure S1 – Stable optimized configurations of 3*d*-M@C₂N

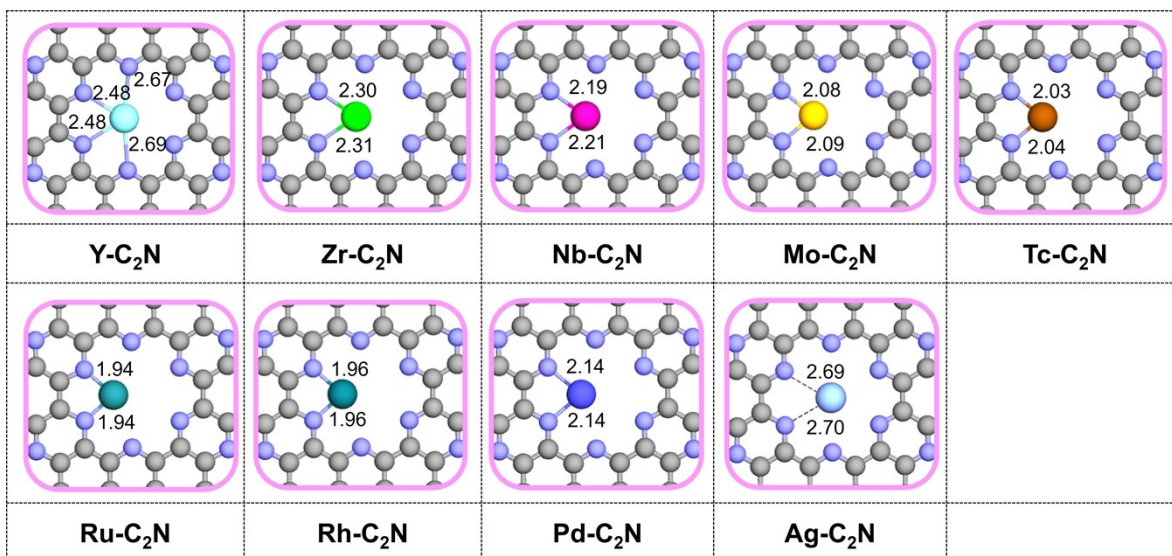


Figure S2 – Stable optimized configurations of 4*d*-M@C₂N

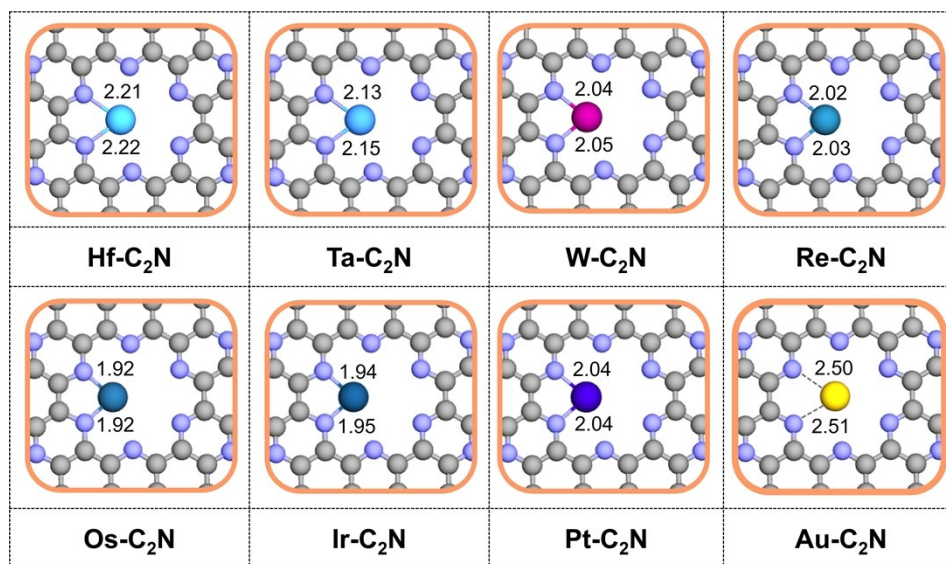


Figure S3 – Stable optimized configurations of 5d-M@C₂N

Table S1. Computed formation energy (E_f) and dissolution potential (U_{diss}) of metals, and number of transferred electrons (N_e) during the dissolution. The standard dissolution potentials (U°_{diss}) of metal atoms are also listed for comparison.

Metal	N_e	U°_{diss} (V)	E_f (eV)	U_{diss} (V)
Sc	3	-2.08	-7.56	0.44
Ti	2	-1.63	-6.98	1.86
V	2	-1.18	-6.02	1.83
Cr	2	-0.91	-4.46	1.32
Mn	2	-1.19	-4.36	0.26
Fe	2	-0.45	-4.27	1.69
Co	2	-0.28	-5.07	2.26
Ni	2	-0.26	-4.87	2.17
Cu	2	0.34	-3.31	2.00
Zn	2	-0.76	-1.39	-0.06
Y	3	-2.37	-8.60	0.50
Zr	4	-1.45	-8.57	0.69

Nb	3	-1.10	-7.27	1.32
Mo	3	-0.20	-5.32	1.57
Ru	2	0.46	-6.65	3.78
Rh	2	0.60	-5.34	3.27
Pd	2	0.95	-3.30	4.25
Ag	1	0.80	-2.92	3.72
Hf	4	-1.55	-8.30	0.52
Ta	3	-0.60	-7.80	2.00
W	3	0.10	-6.57	2.29
Re	3	0.30	-4.98	1.96
Os	8	0.84	-5.87	1.57
Ir	3	1.16	-5.75	3.08
Pt	2	1.18	-4.19	3.27
Au	3	1.50	-2.22	2.24

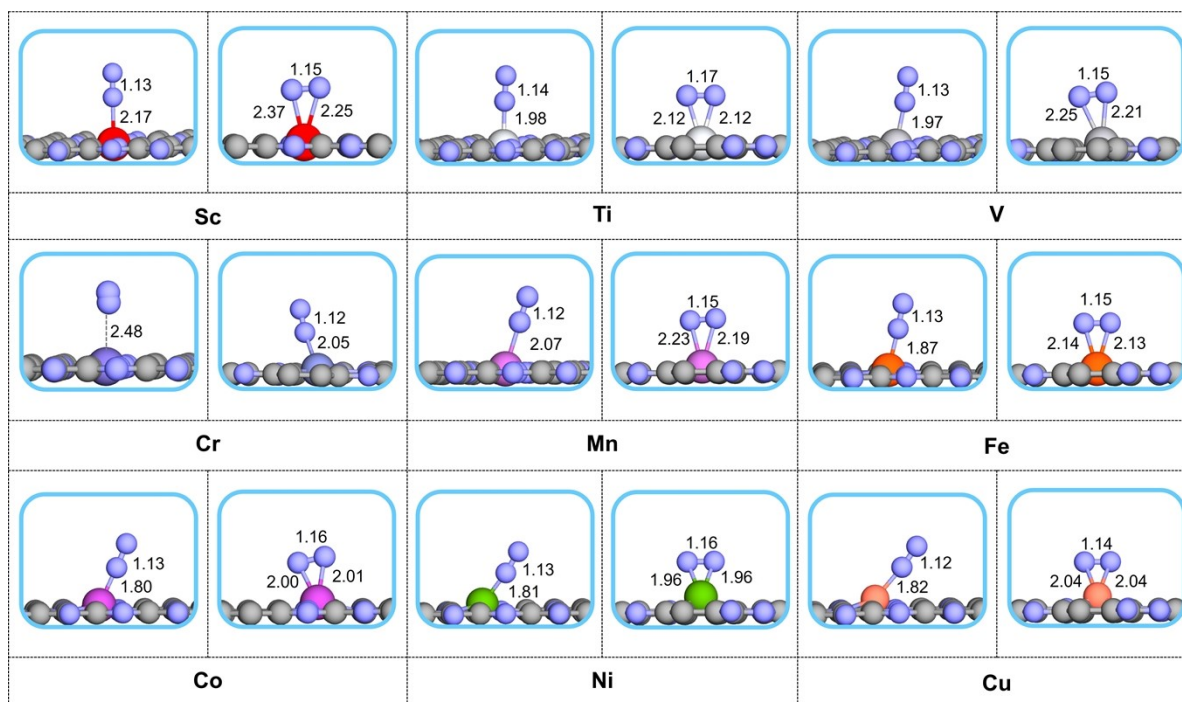


Figure S4 – Stable optimized N₂ adsorption configurations of 3d-M@C₂N

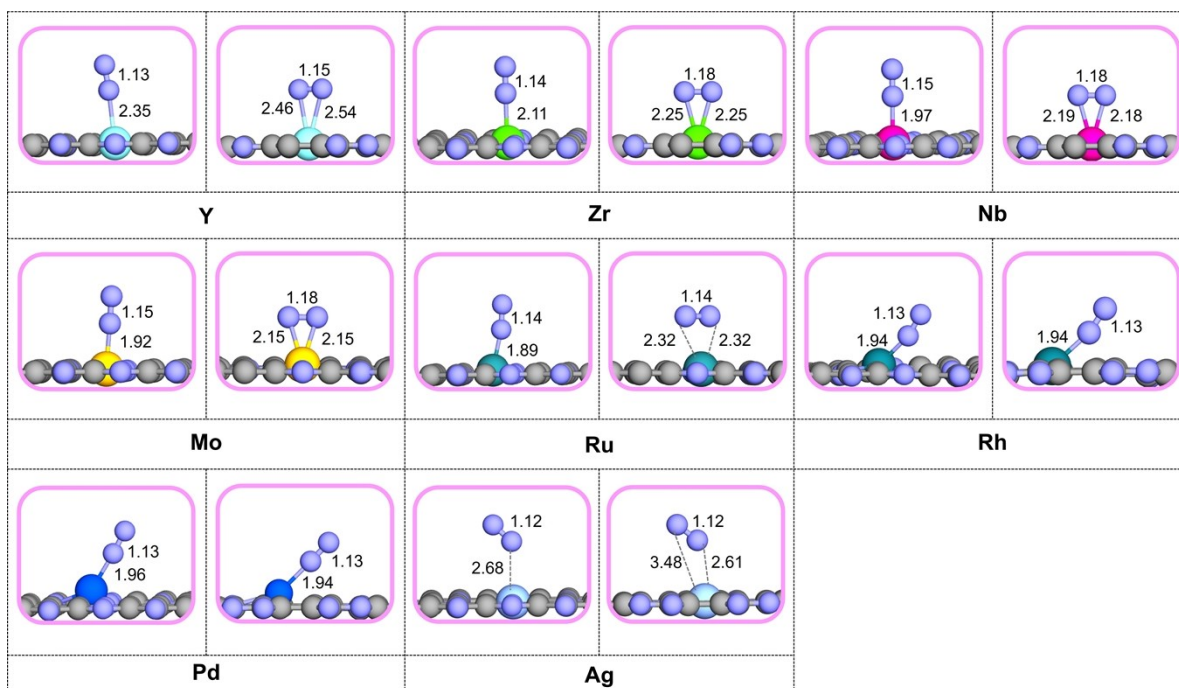


Figure S5 – Stable optimized N₂ adsorption configurations of 4*d*-M@C₂N

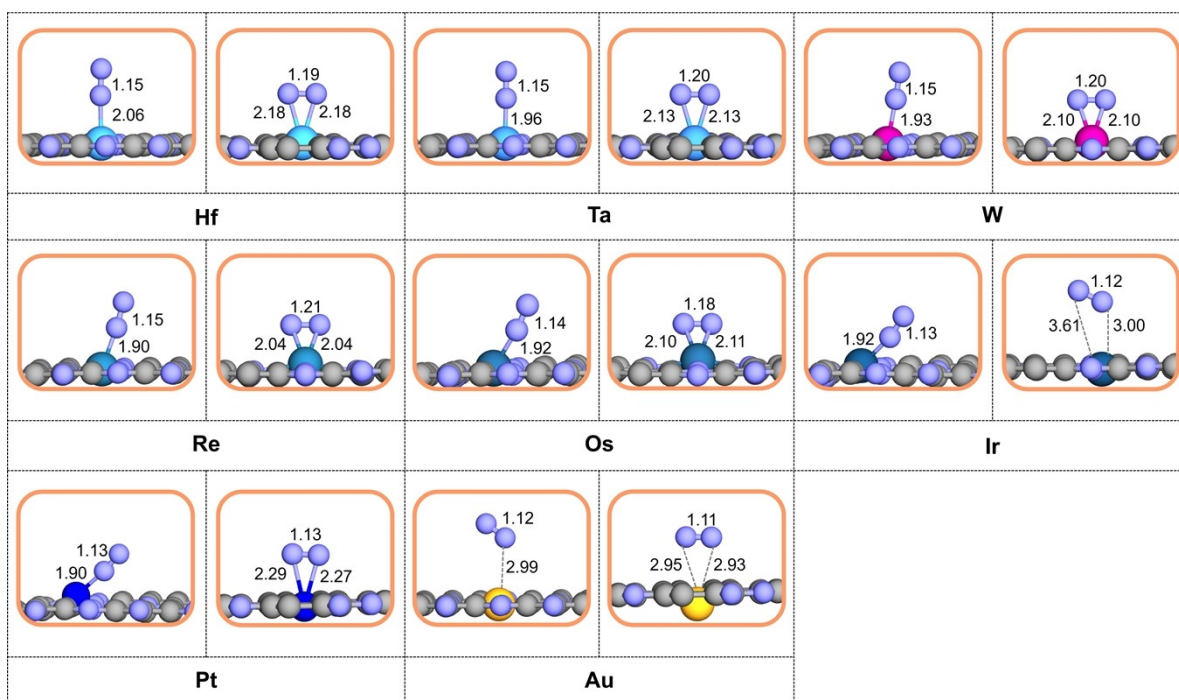


Figure S6 – Stable optimized N₂ adsorption configurations of 5*d*-M@C₂N

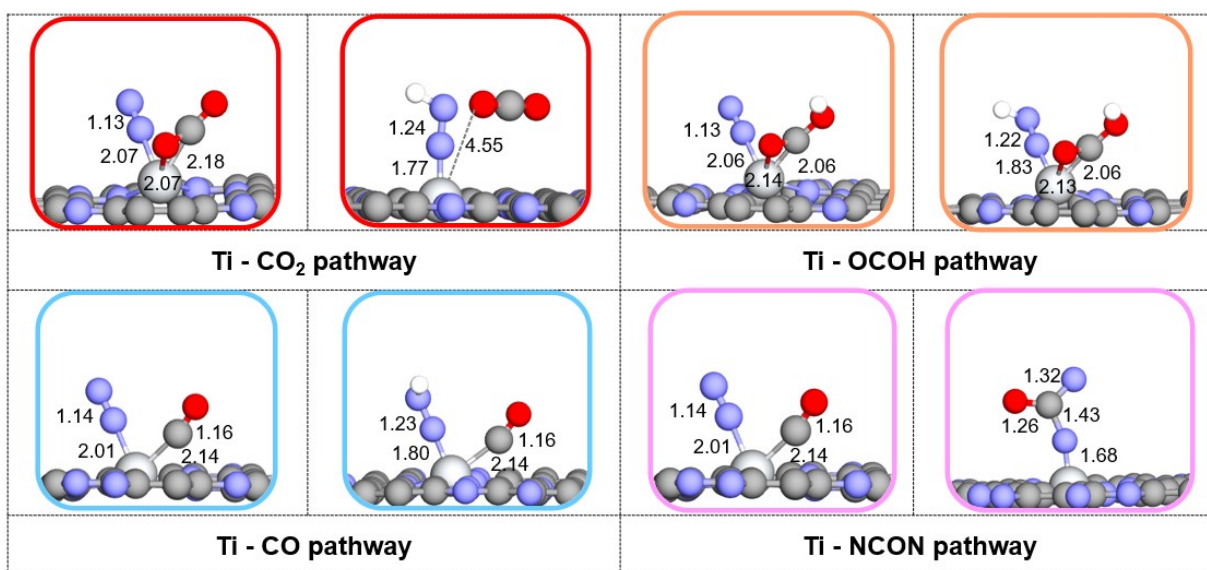


Figure S7 – Atomic structures of critical step through the four possible pathways; the CO₂ pathway ($\Delta G^*_{\text{CO}_2+\text{NNH}}$), OCOH pathway ($\Delta G^*_{\text{OCOH}+\text{NNH}}$), the CO pathway ($\Delta G^*_{\text{CO}+\text{NNH}}$), and the NCON pathway (ΔG^*_{NCON}) on Ti@C₂N.

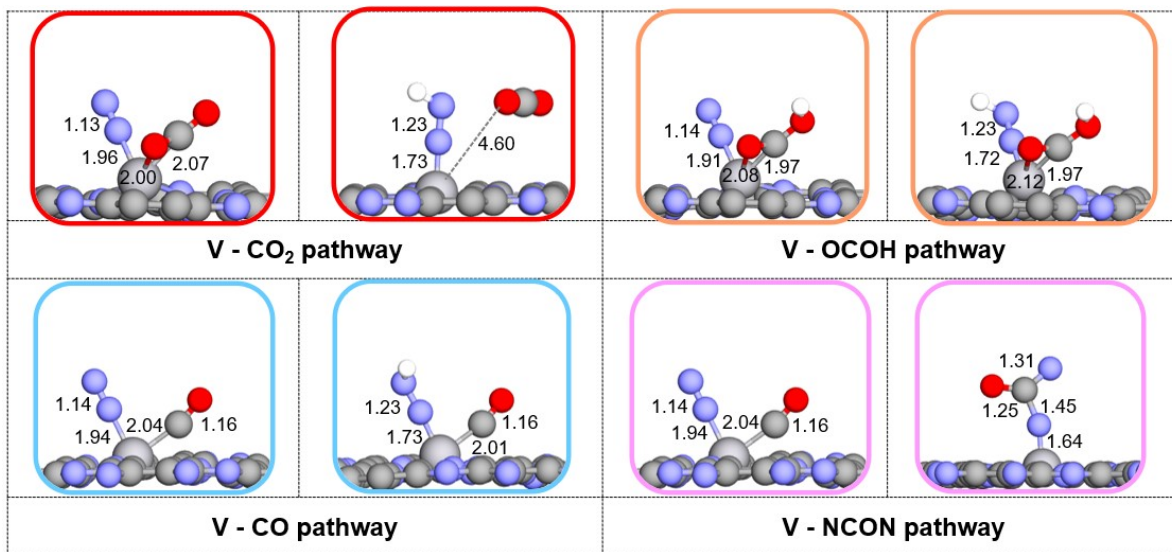


Figure S8 – Atomic structures of critical step through the four possible pathways; the CO₂ pathway ($\Delta G^*_{\text{CO}_2+\text{NNH}}$), OCOH pathway ($\Delta G^*_{\text{OCOH}+\text{NNH}}$), the CO pathway ($\Delta G^*_{\text{CO}+\text{NNH}}$), and the NCON pathway (ΔG^*_{NCON}) on V@C₂N.

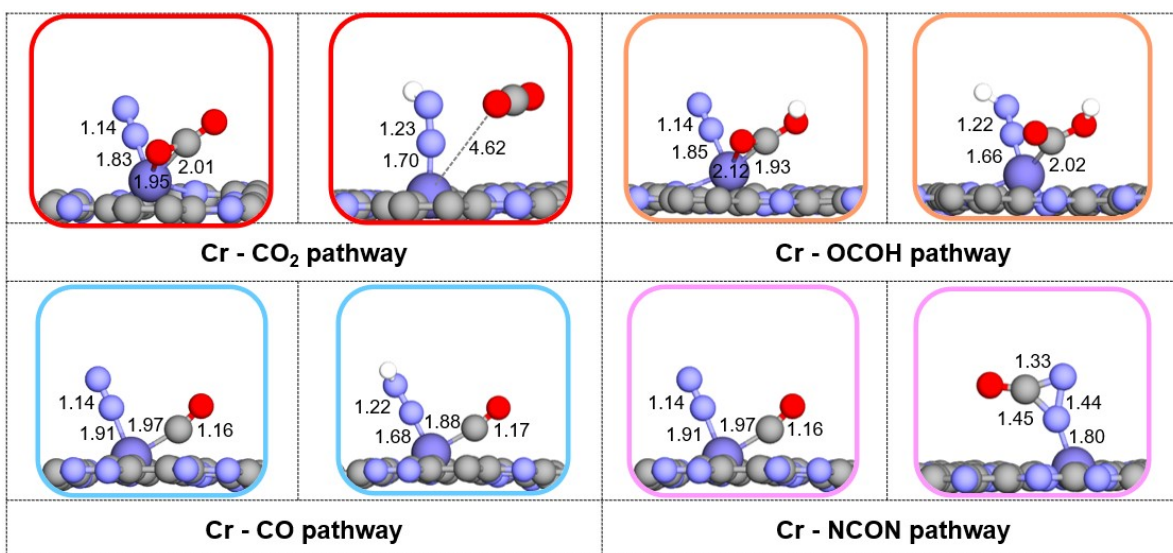


Figure S9 – Atomic structures of critical step through the four possible pathways; the CO₂ pathway ($\Delta G^*_{\text{CO}_2+\text{NNH}}$), OCOH pathway ($\Delta G^*_{\text{OCOH}+\text{NNH}}$), the CO pathway ($\Delta G^*_{\text{CO}+\text{NNH}}$), and the NCON pathway (ΔG^*_{NCON}) on Cr@C₂N.

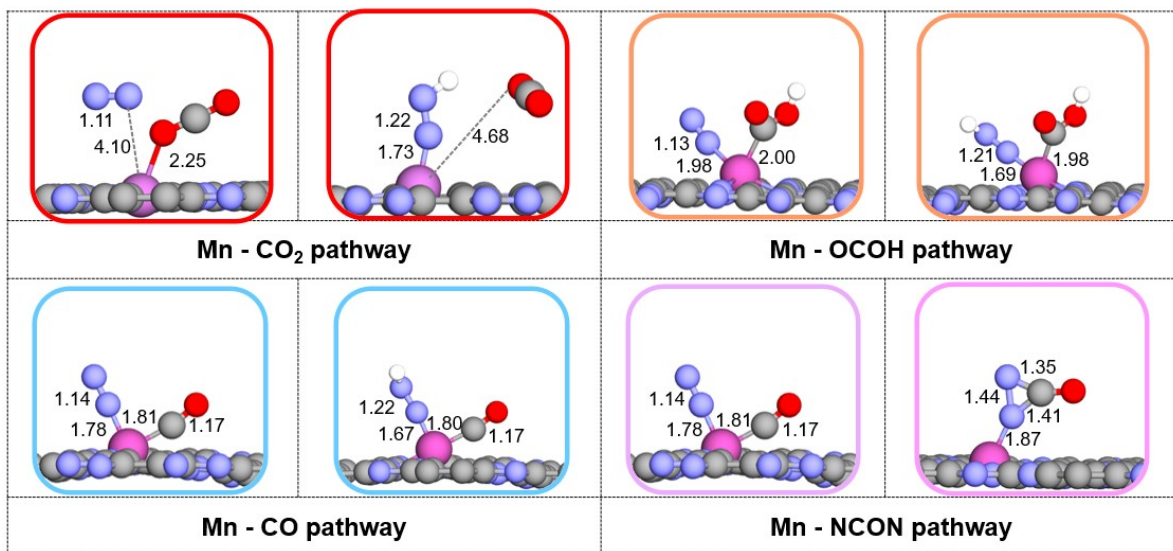


Figure S10 – Atomic structures of critical step through the four possible pathways; the CO₂ pathway ($\Delta G^*_{\text{CO}_2+\text{NNH}}$), OCOH pathway ($\Delta G^*_{\text{OCOH}+\text{NNH}}$), the CO pathway ($\Delta G^*_{\text{CO}+\text{NNH}}$), and the NCON pathway (ΔG^*_{NCON}) on Mn@C₂N.

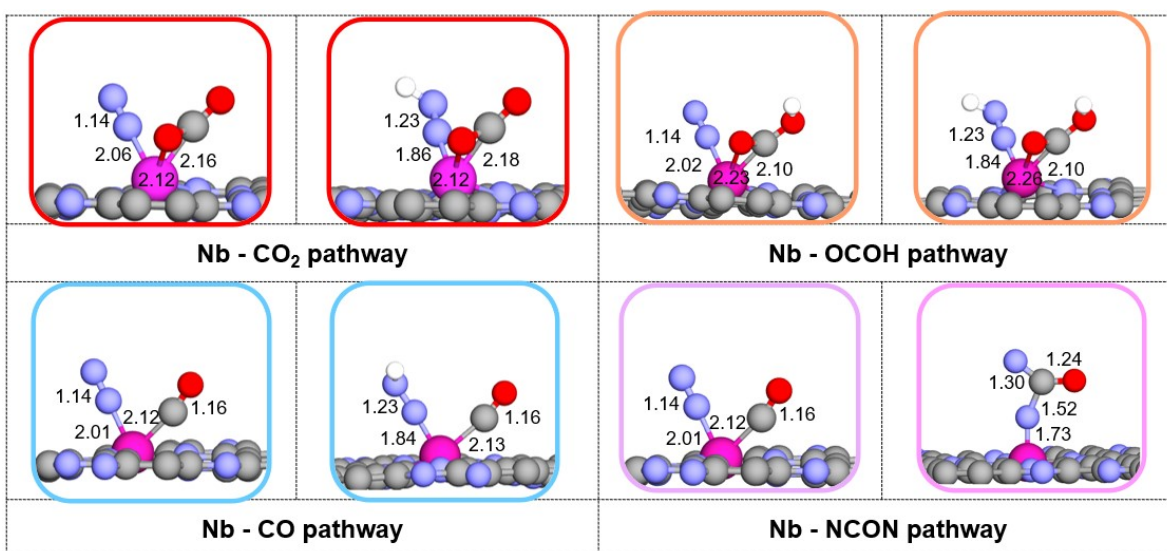


Figure S11 – Atomic structures of critical step through the four possible pathways; the CO₂ pathway ($\Delta G^*_{\text{CO}_2+\text{NNH}}$), OCOH pathway ($\Delta G^*_{\text{OCOH}+\text{NNH}}$), the CO pathway ($\Delta G^*_{\text{CO}+\text{NNH}}$), and the NCON pathway (ΔG^*_{NCON}) on Nb@C₂N.

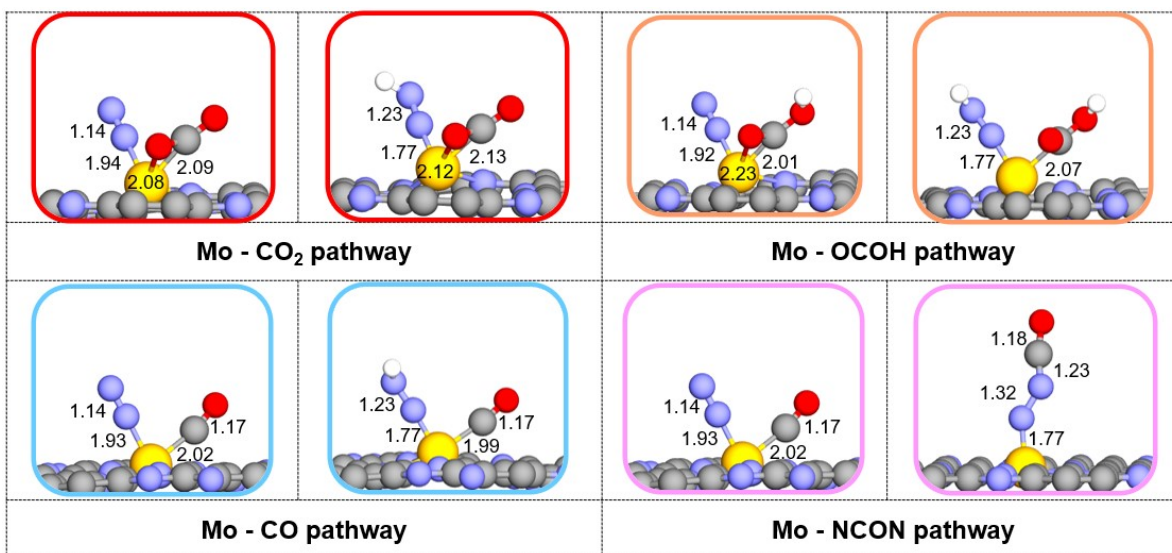


Figure S12 – Atomic structures of critical step through the four possible pathways; the CO₂ pathway ($\Delta G^*_{\text{CO}_2+\text{NNH}}$), OCOH pathway ($\Delta G^*_{\text{OCOH}+\text{NNH}}$), the CO pathway ($\Delta G^*_{\text{CO}+\text{NNH}}$), and the NCON pathway (ΔG^*_{NCON}) on Mo@C₂N.

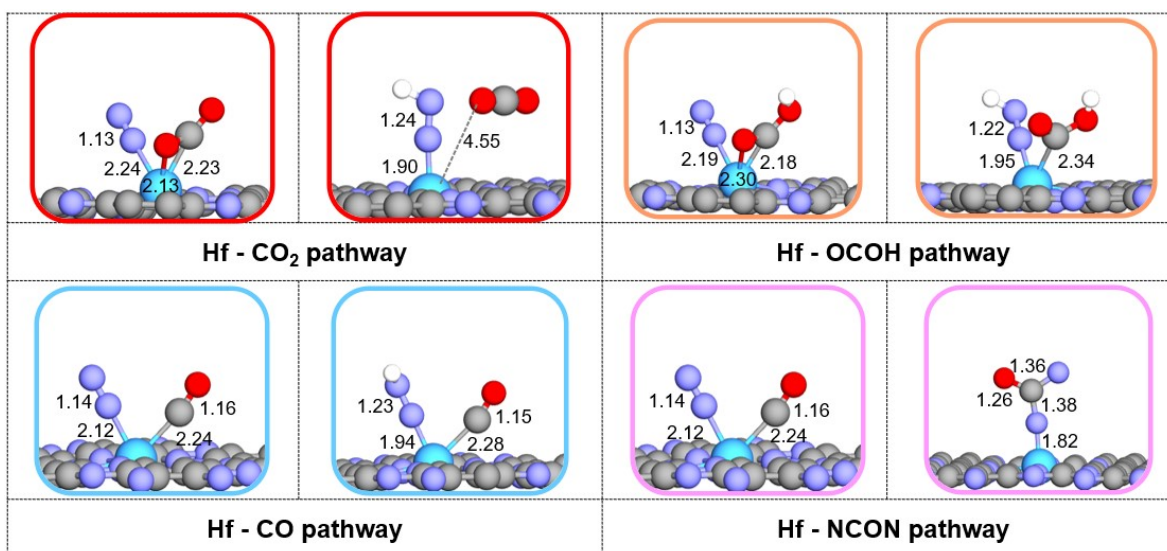


Figure S13 – Atomic structures of critical step through the four possible pathways; the CO₂ pathway ($\Delta G^*_{\text{CO}_2+\text{NNH}}$), OCOH pathway ($\Delta G^*_{\text{OCOH}+\text{NNH}}$), the CO pathway ($\Delta G^*_{\text{CO}+\text{NNH}}$), and the NCON pathway (ΔG^*_{NCON}) on Hf@C₂N.

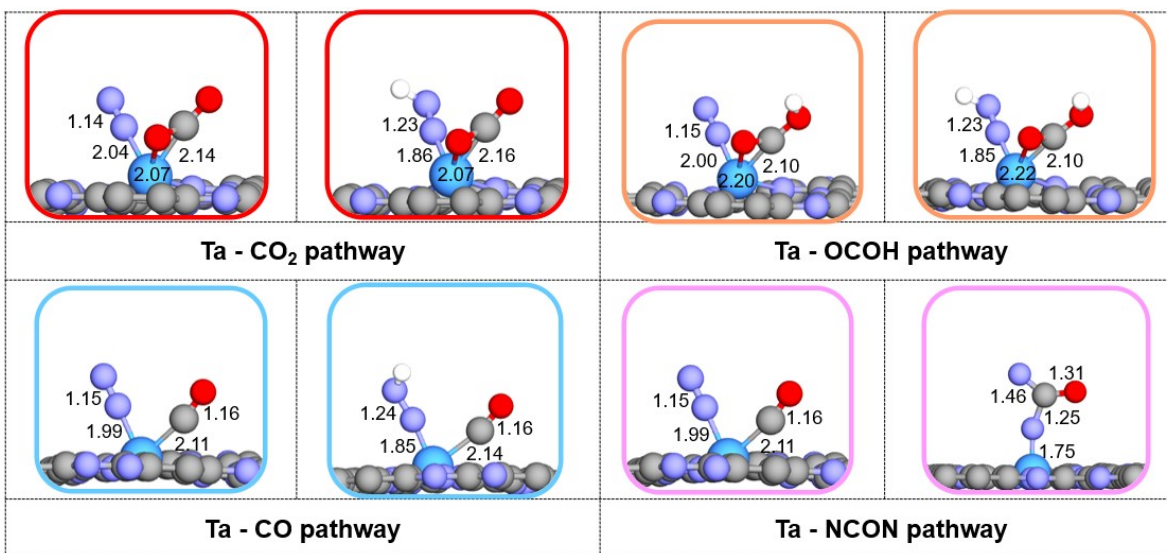


Figure S14 – Atomic structures of critical step through the four possible pathways; the CO₂ pathway ($\Delta G^*_{\text{CO}_2+\text{NNH}}$), OCOH pathway ($\Delta G^*_{\text{OCOH}+\text{NNH}}$), the CO pathway ($\Delta G^*_{\text{CO}+\text{NNH}}$), and the NCON pathway (ΔG^*_{NCON}) on Ta@C₂N.

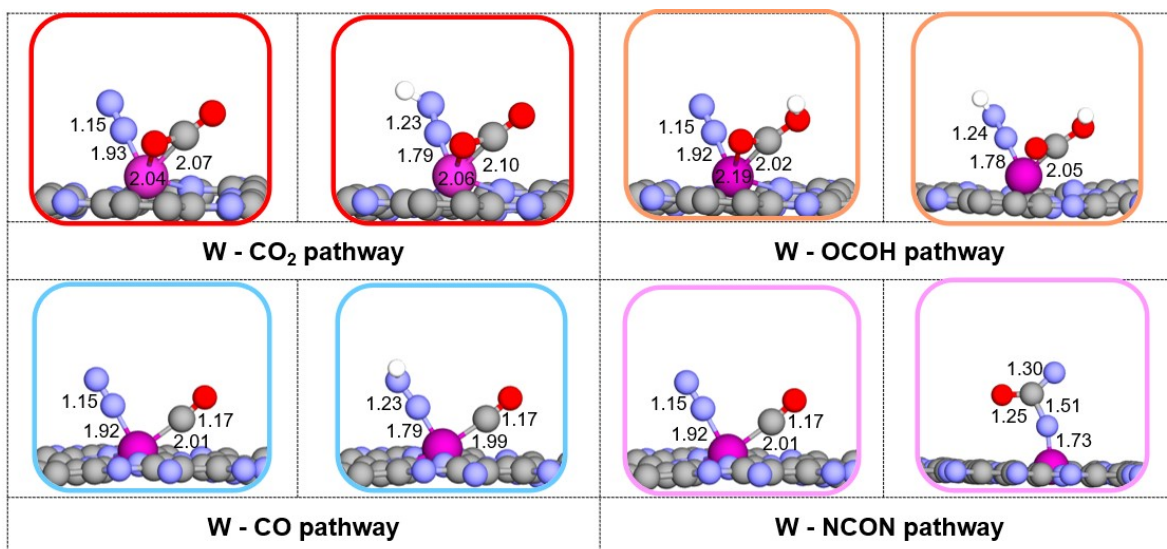


Figure S15 – Atomic structures of critical step through the four possible pathways; the CO₂ pathway ($\Delta G^*_{\text{CO}_2+\text{NNH}}$), OCOH pathway ($\Delta G^*_{\text{OCOH}+\text{NNH}}$), the CO pathway ($\Delta G^*_{\text{CO}+\text{NNH}}$), and the NCON pathway (ΔG^*_{NCON}) on W@C₂N.

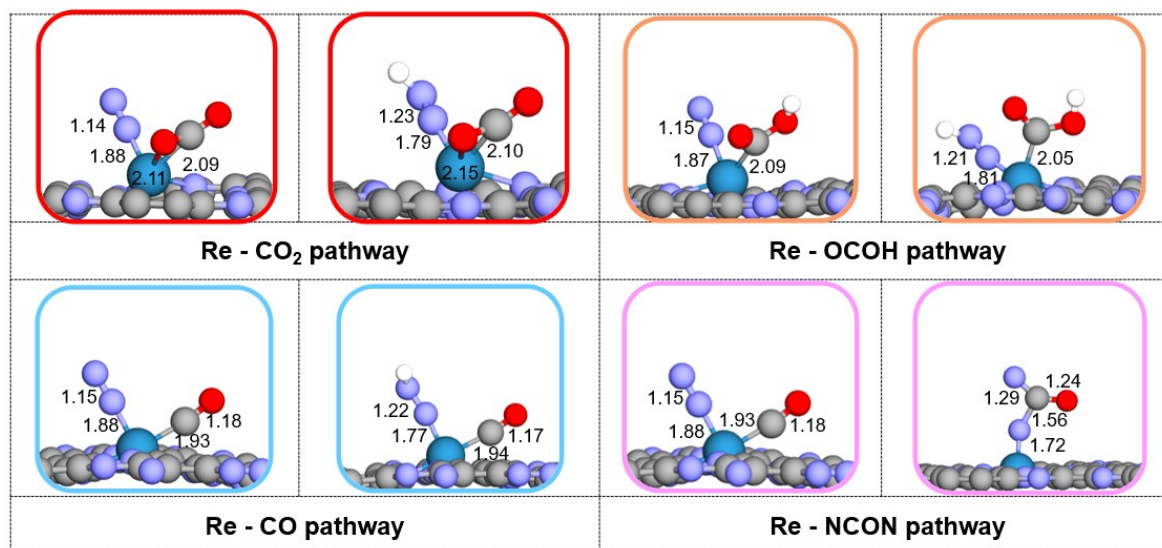


Figure S16 – Atomic structures of critical step through the four possible pathways; the CO₂ pathway ($\Delta G^*_{\text{CO}_2+\text{NNH}}$), OCOH pathway ($\Delta G^*_{\text{OCOH}+\text{NNH}}$), the CO pathway ($\Delta G^*_{\text{CO}+\text{NNH}}$), and the NCON pathway (ΔG^*_{NCON}) on Re@C₂N.

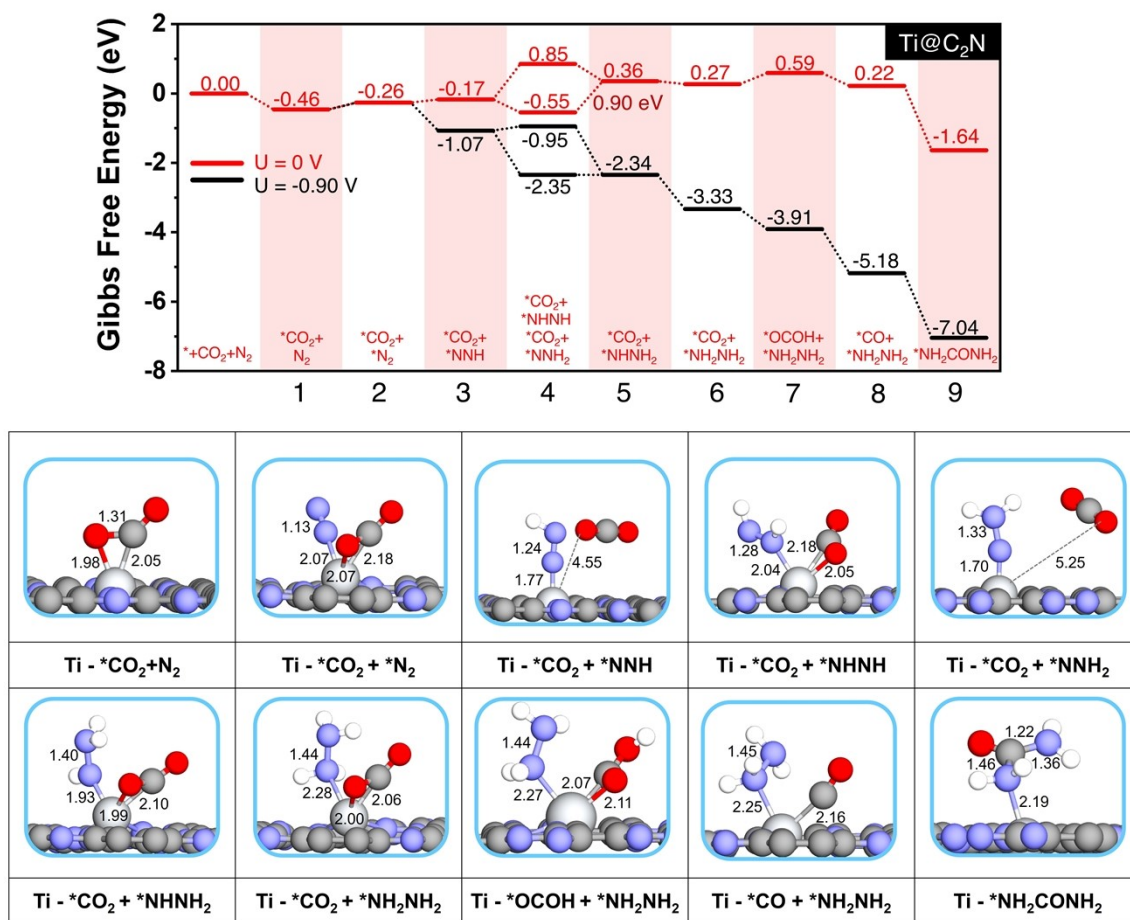


Figure S17 – Gibbs free energy diagrams and atomic structures of critical step through the CO₂ pathways for urea formation on Ti@C₂N.

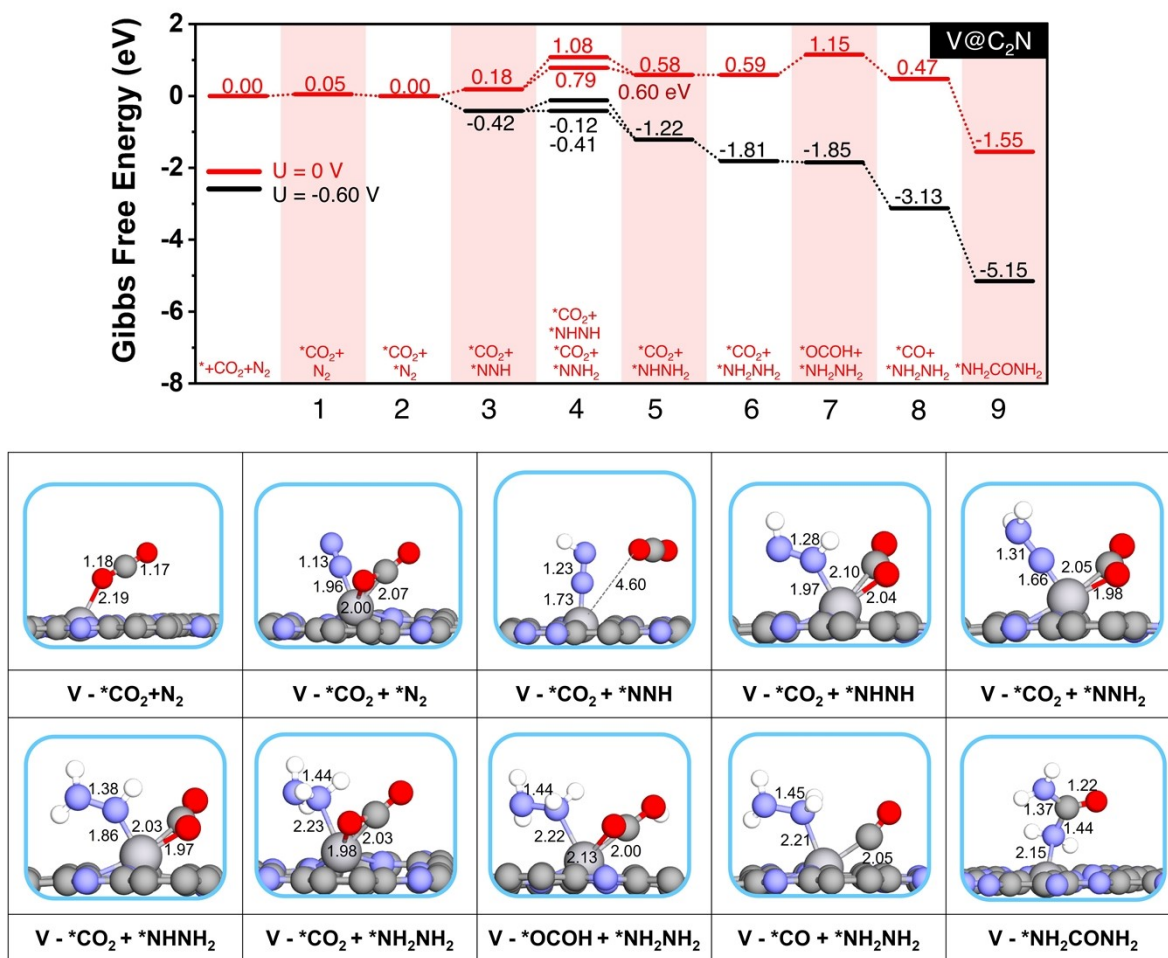


Figure S18 – Gibbs free energy diagrams and atomic structures of critical step through the CO_2 pathways for urea formation on $\text{V@C}_2\text{N}$.

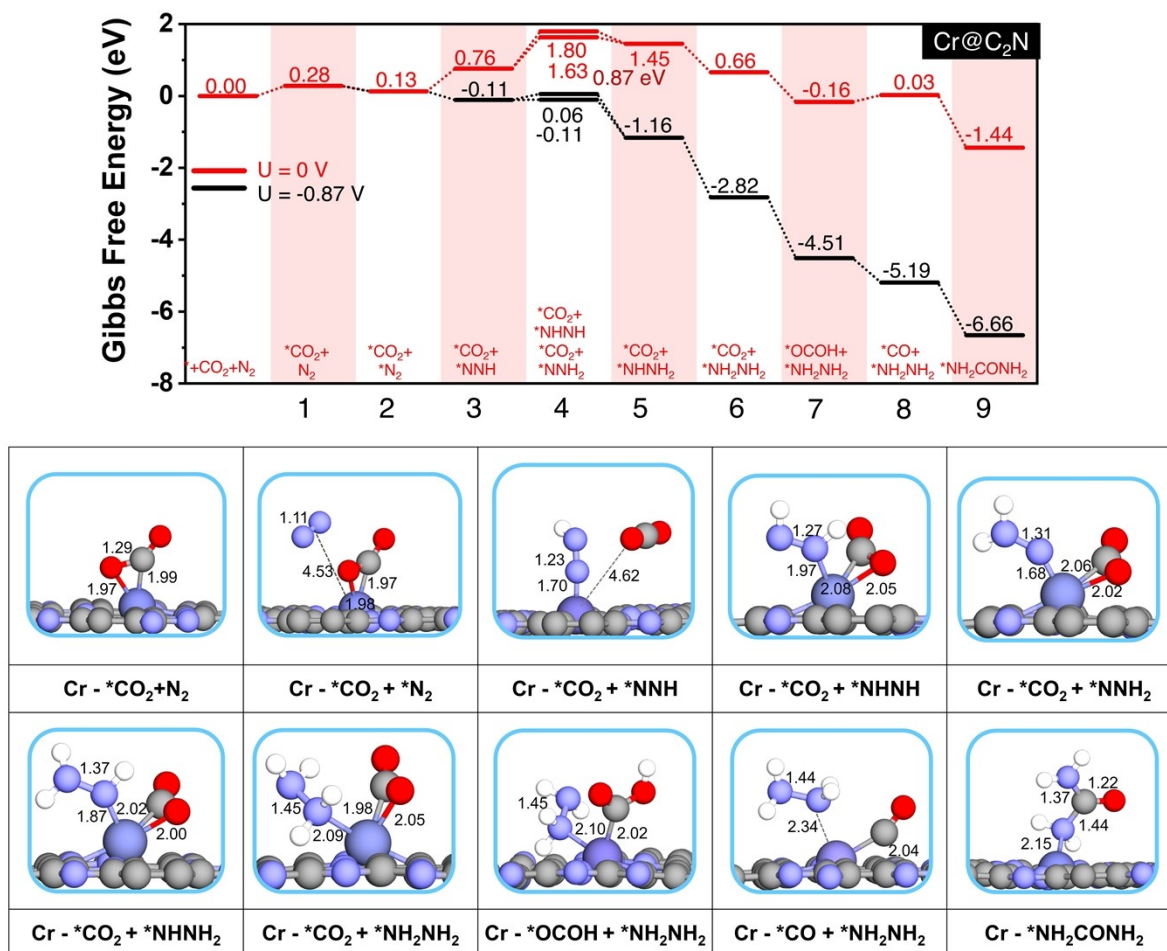


Figure S19 – Gibbs free energy diagrams and atomic structures of critical step through the CO₂ pathways for urea formation on Cr@C₂N.

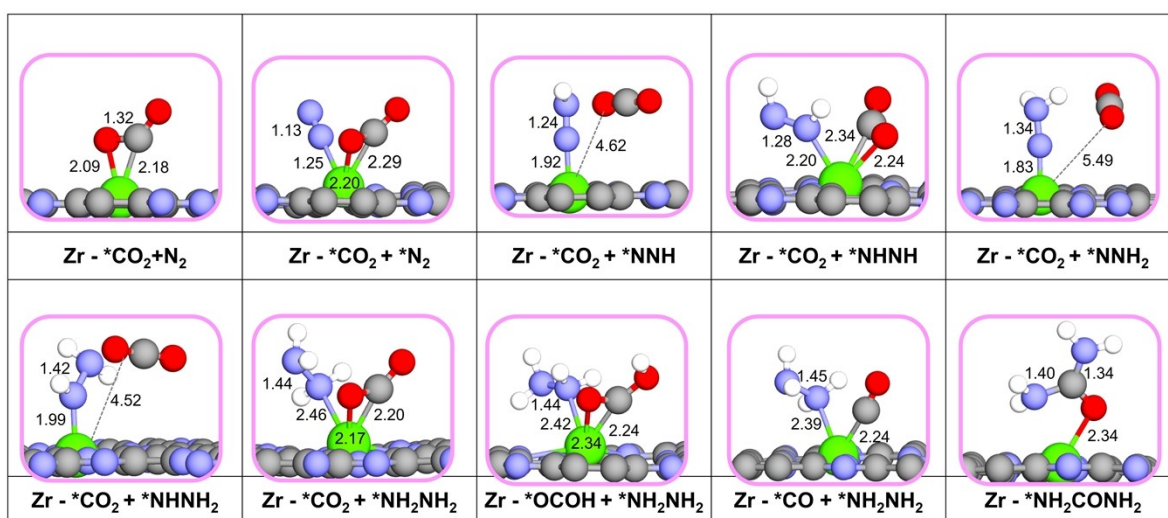
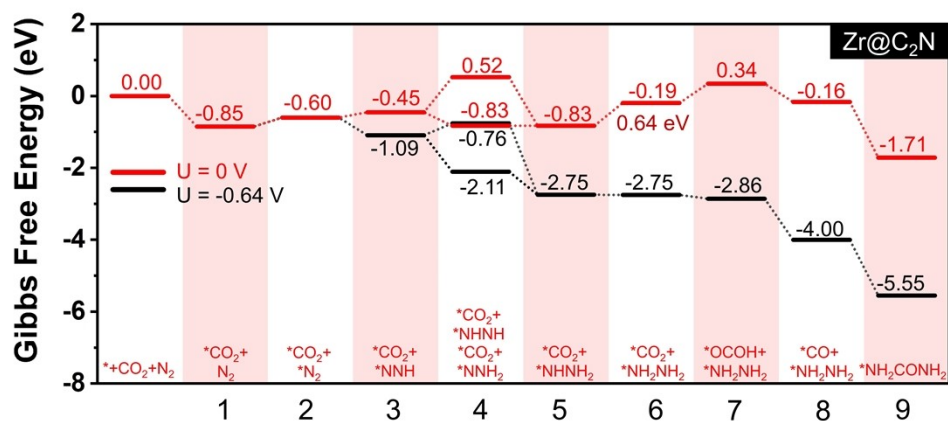


Figure S20 – Gibbs free energy diagrams and atomic structures of critical step through the CO₂ pathways for urea formation on Zr@C₂N.

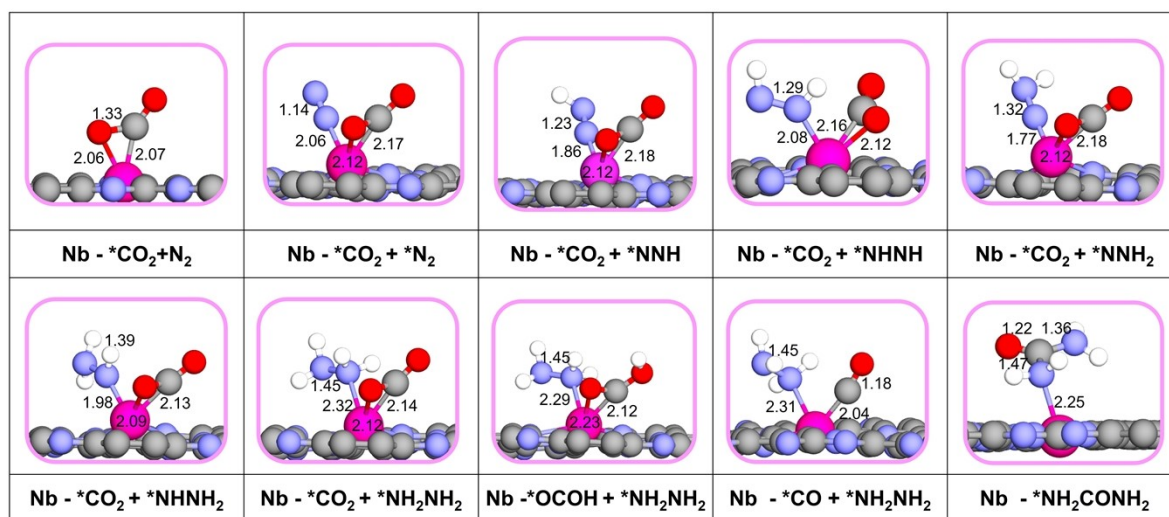
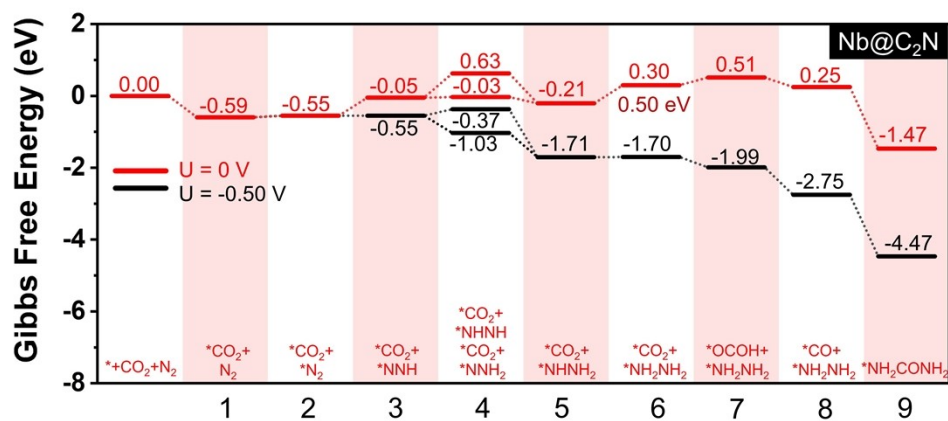


Figure S21 – Gibbs free energy diagrams and atomic structures of critical step through the CO₂ pathways for urea formation on Nb@C₂N.

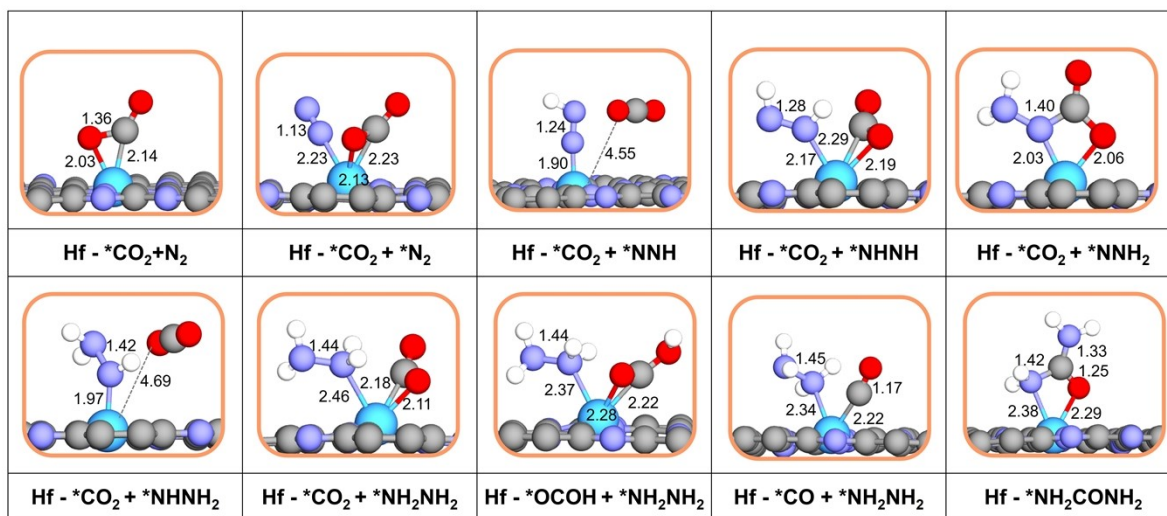
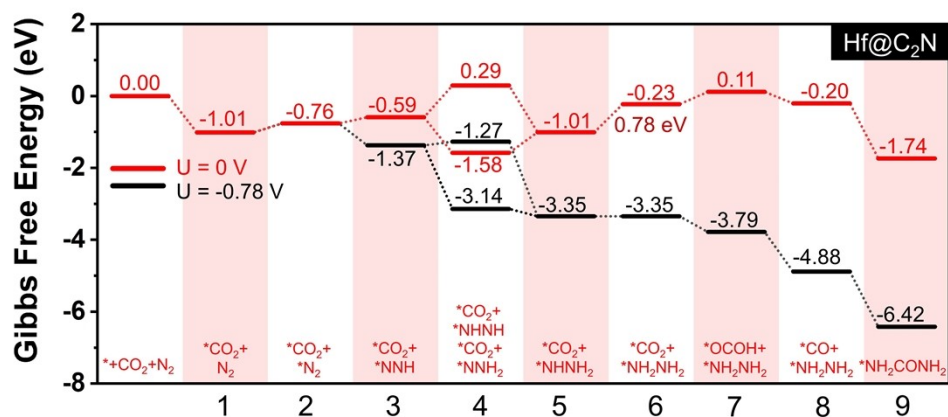


Figure S22 – Gibbs free energy diagrams and atomic structures of critical step through the CO₂ pathways for urea formation on Hf@C₂N.

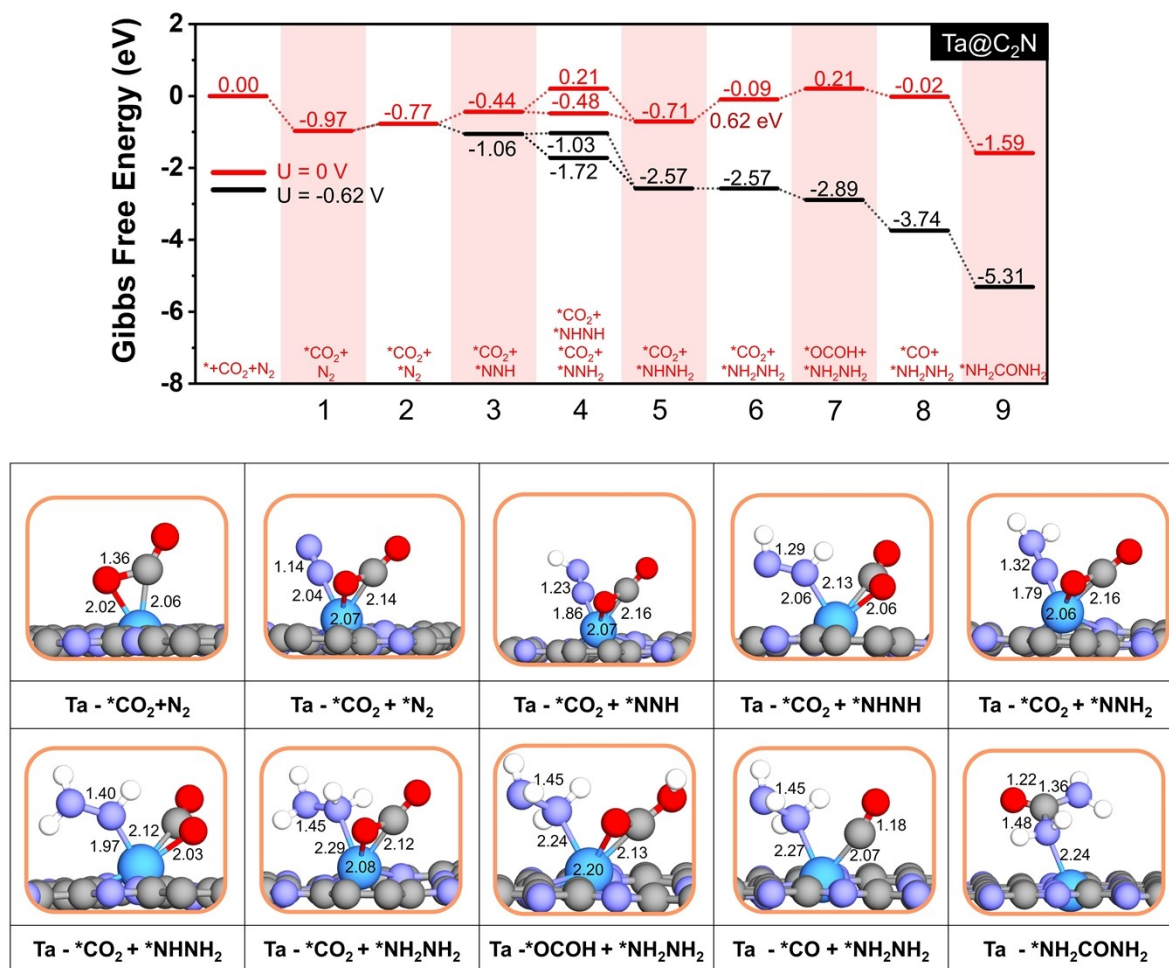


Figure S23 – Gibbs free energy diagrams and atomic structures of critical step through the CO₂ pathways for urea formation on Ta@C₂N.

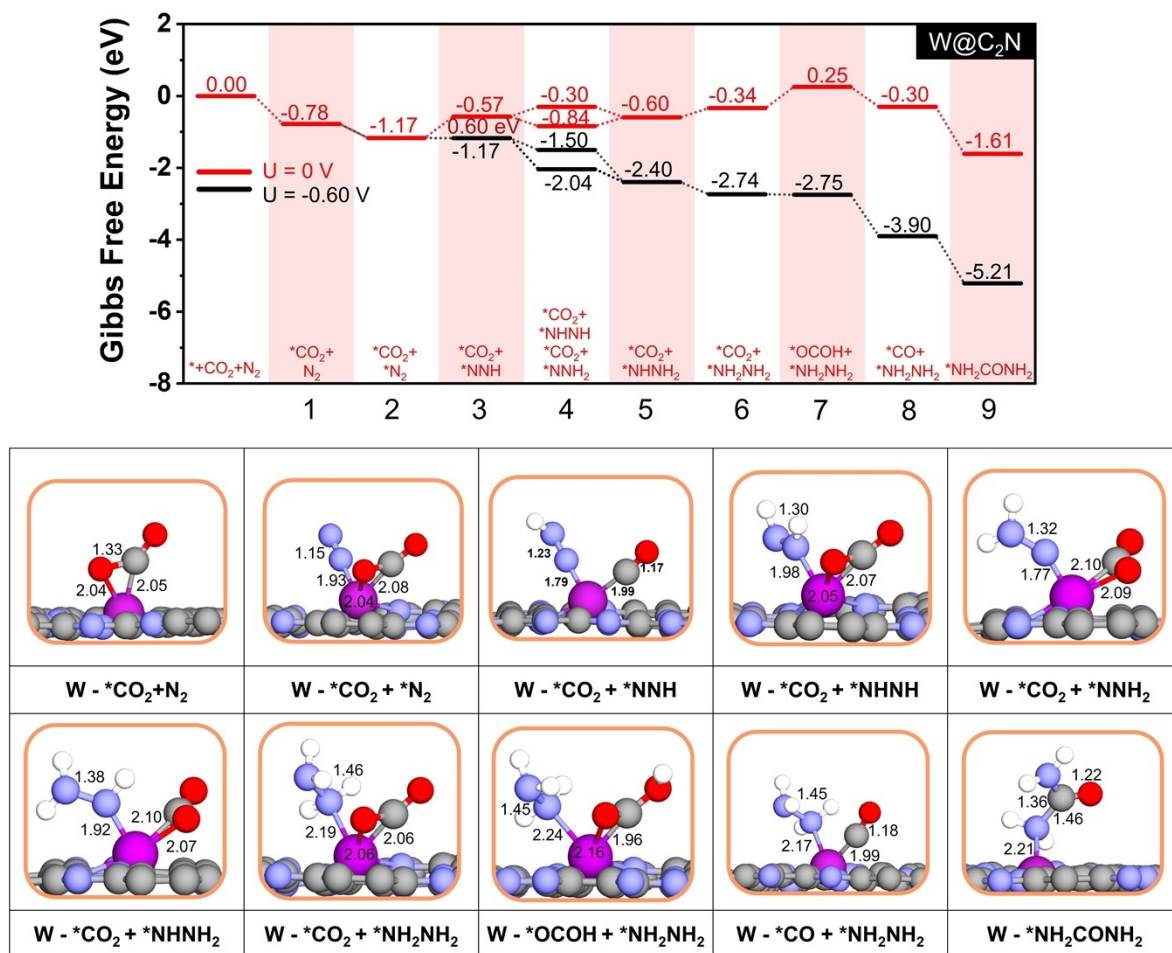


Figure S24 – Gibbs free energy diagrams and atomic structures of critical step through the CO_2 pathways for urea formation on $\text{W@C}_2\text{N}$.

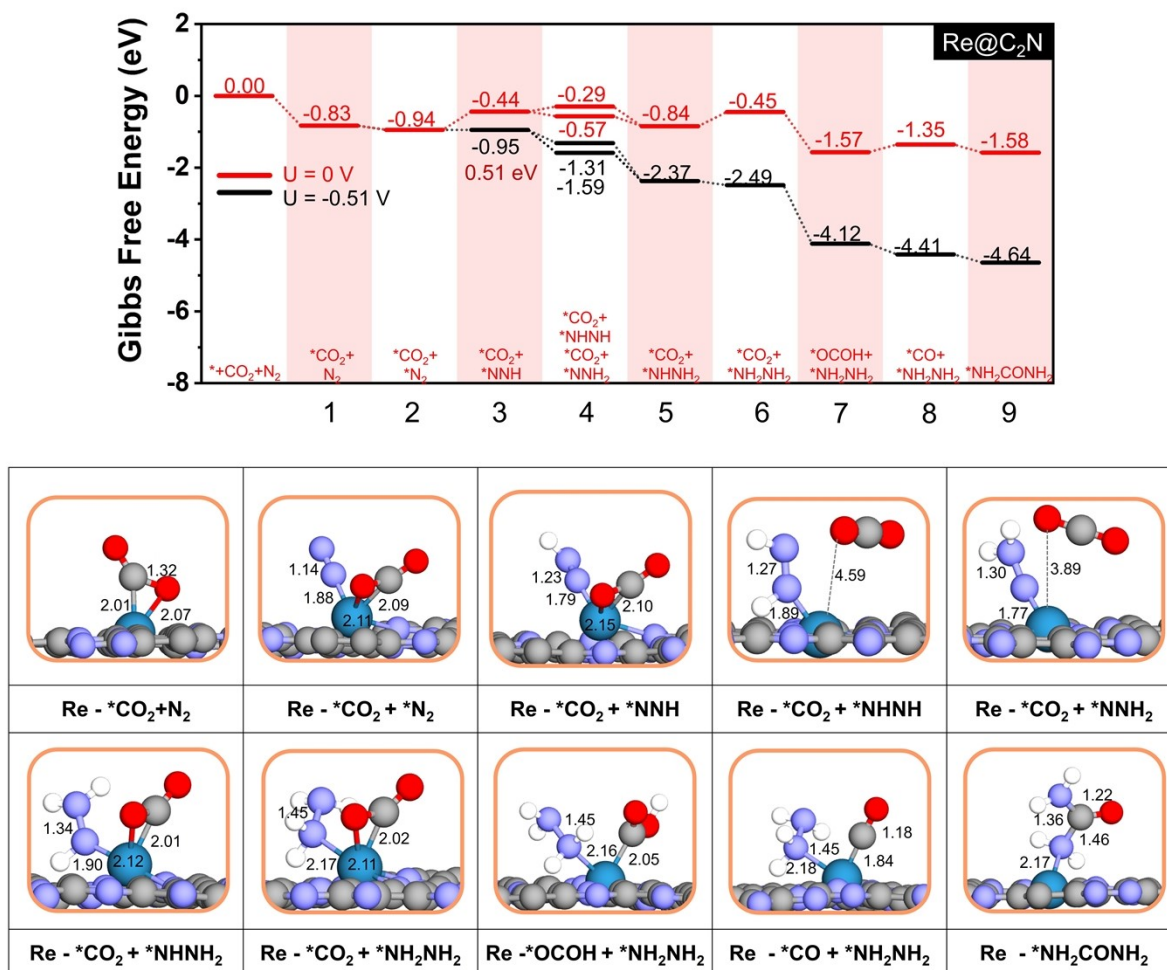


Figure S25 – Gibbs free energy diagrams and atomic structures of critical step through the CO₂ pathways for urea formation on Re@C₂N.

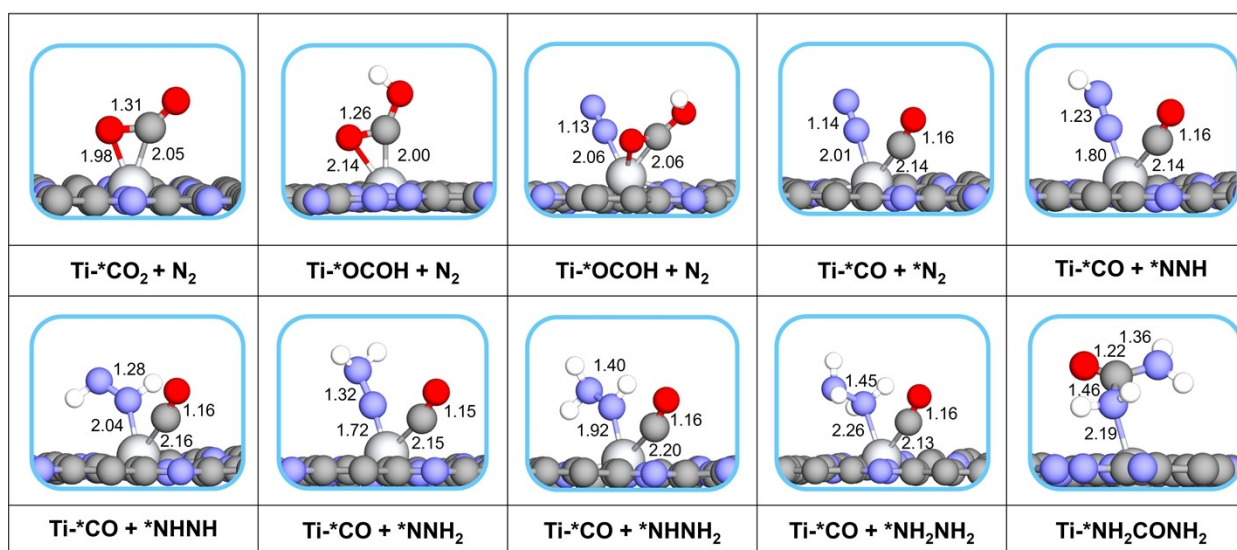
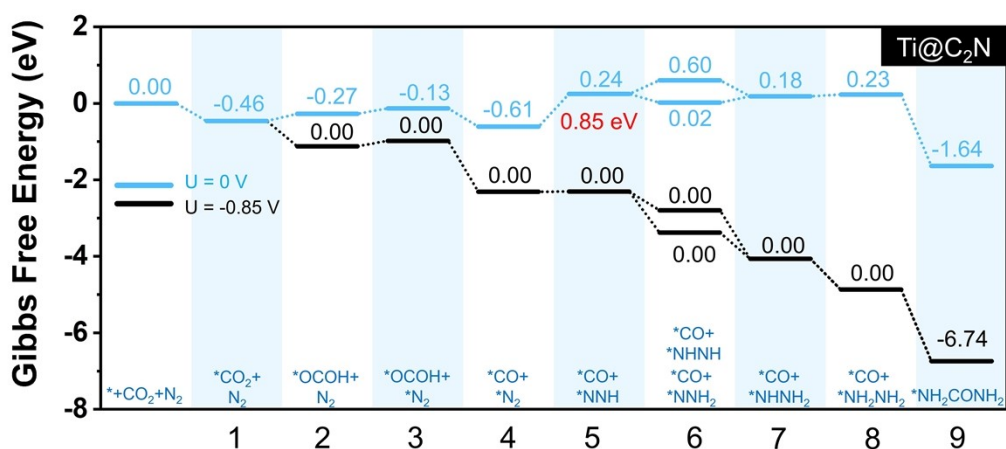


Figure S26 – Gibbs free energy diagrams and atomic structures of critical step through the CO pathways for urea formation on Ti@C₂N.

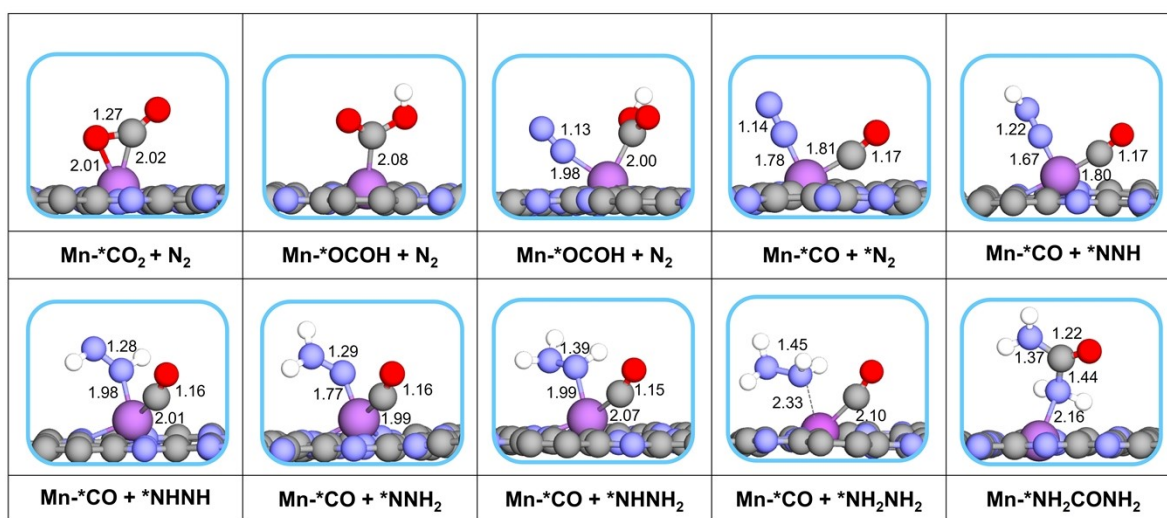
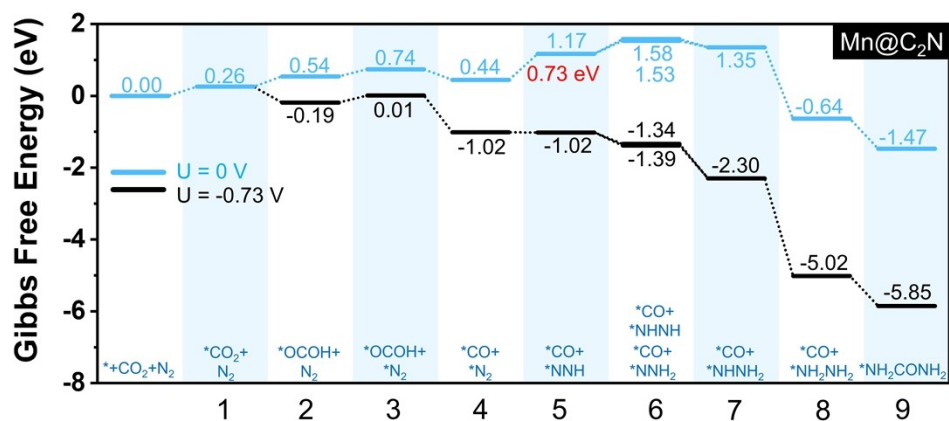


Figure S27 – Gibbs free energy diagrams and atomic structures of critical step through the CO pathways for urea formation on Mn@C₂N.

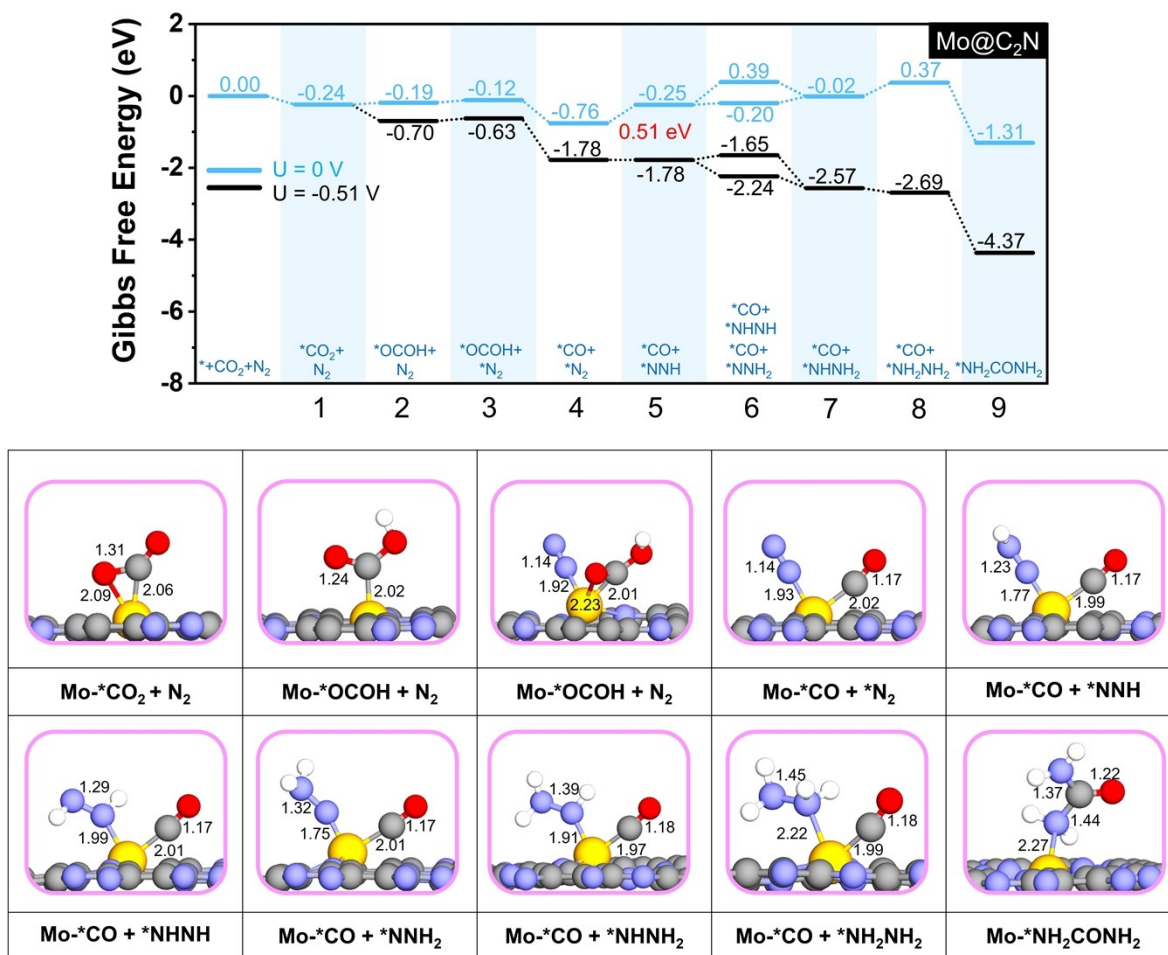


Figure28 – Gibbs free energy diagrams and atomic structures of critical step through the CO pathways for urea formation on Mo@C₂N.

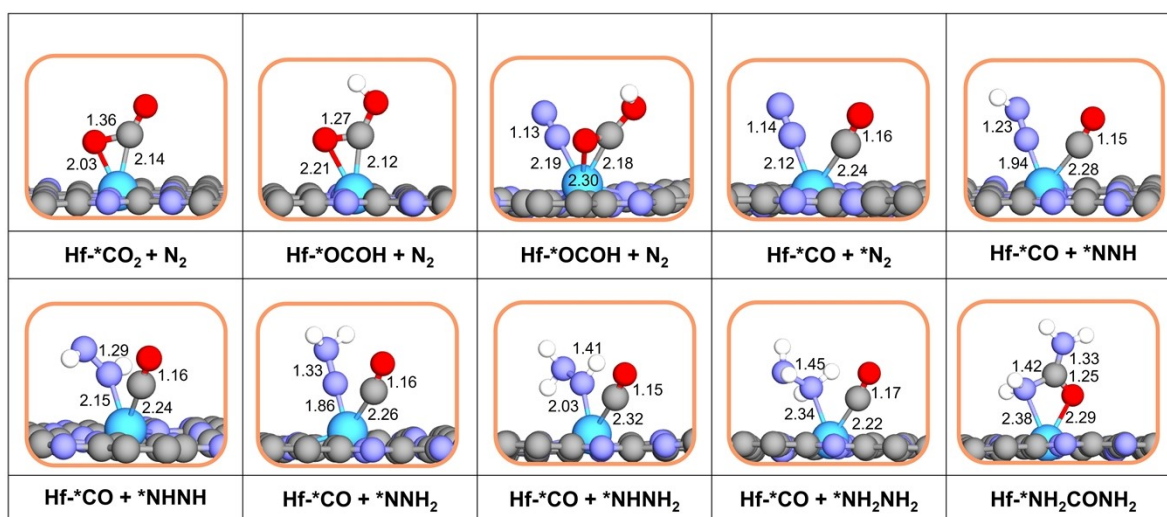
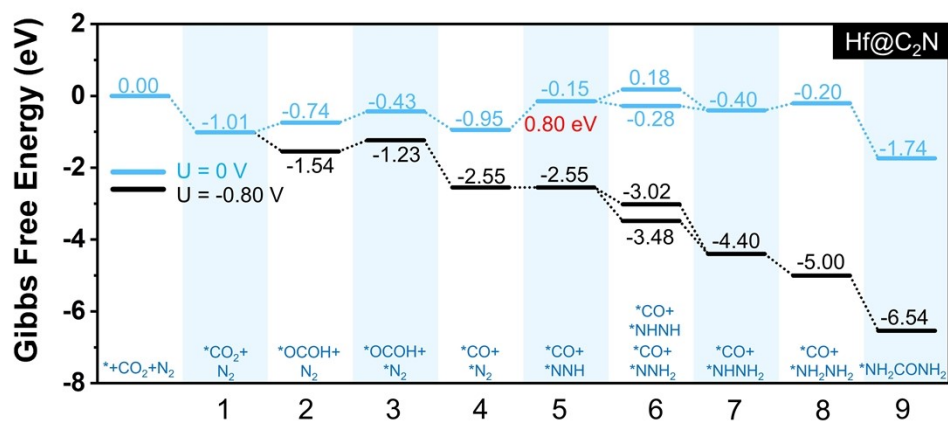
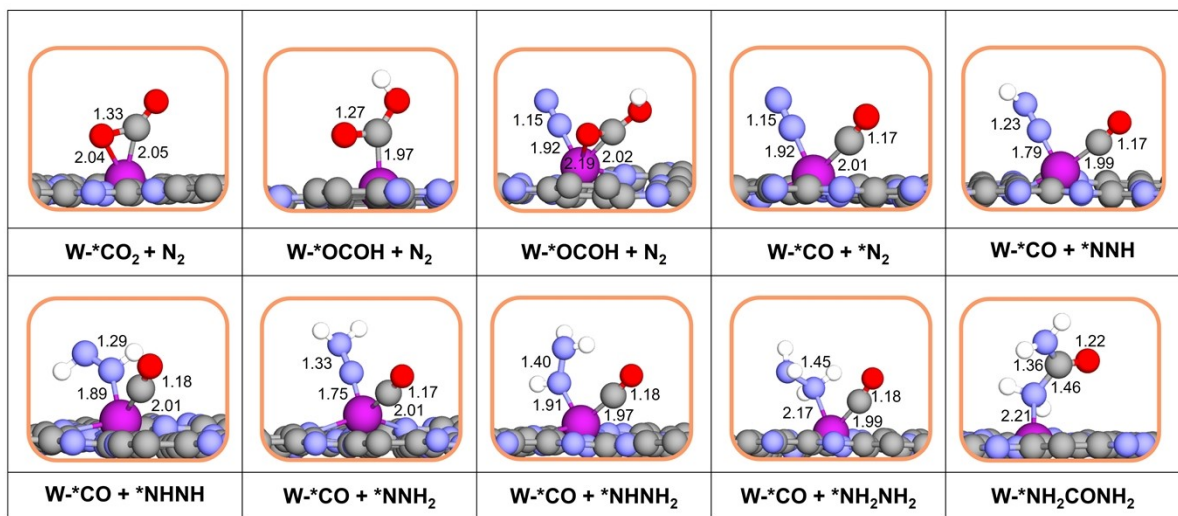


Figure29 – Gibbs free energy diagrams and atomic structures of critical step through the CO pathways for urea formation on Hf@C₂N.

pathways for urea formation on W@C₂N.

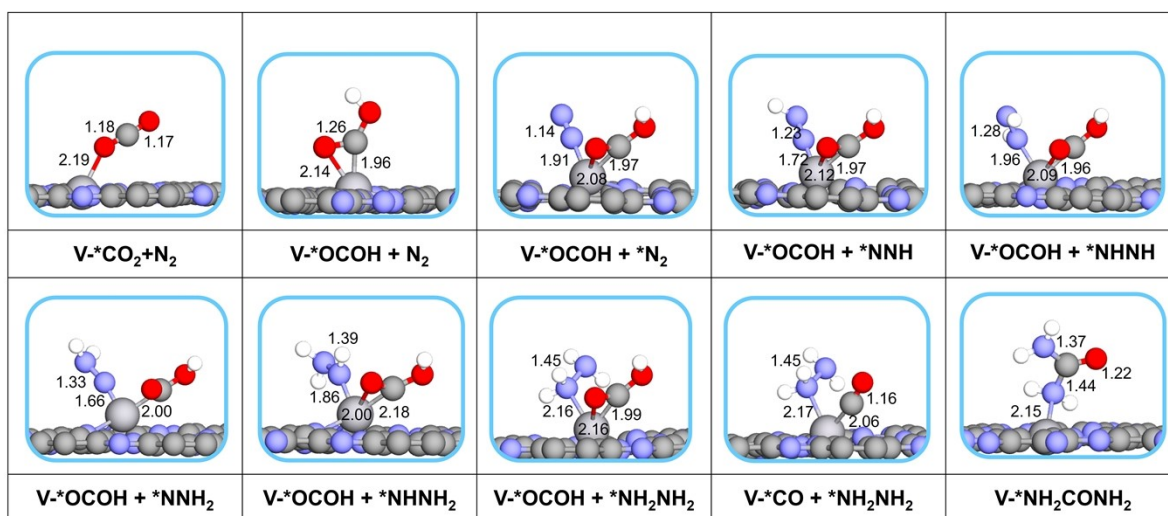
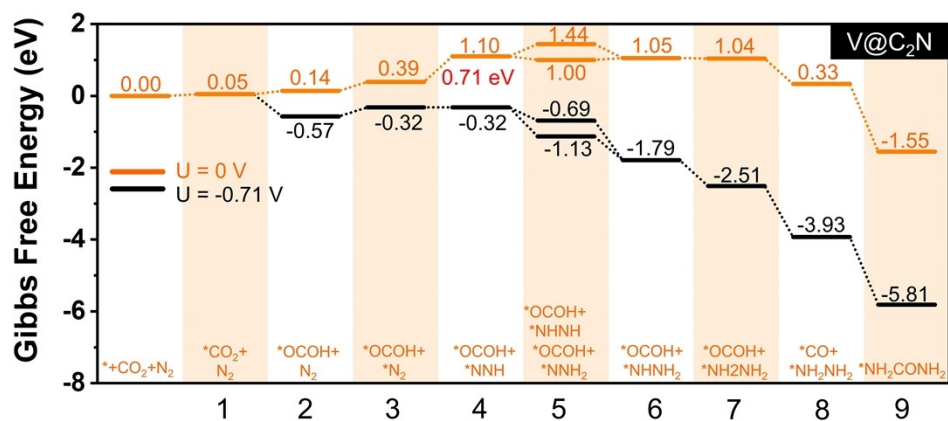
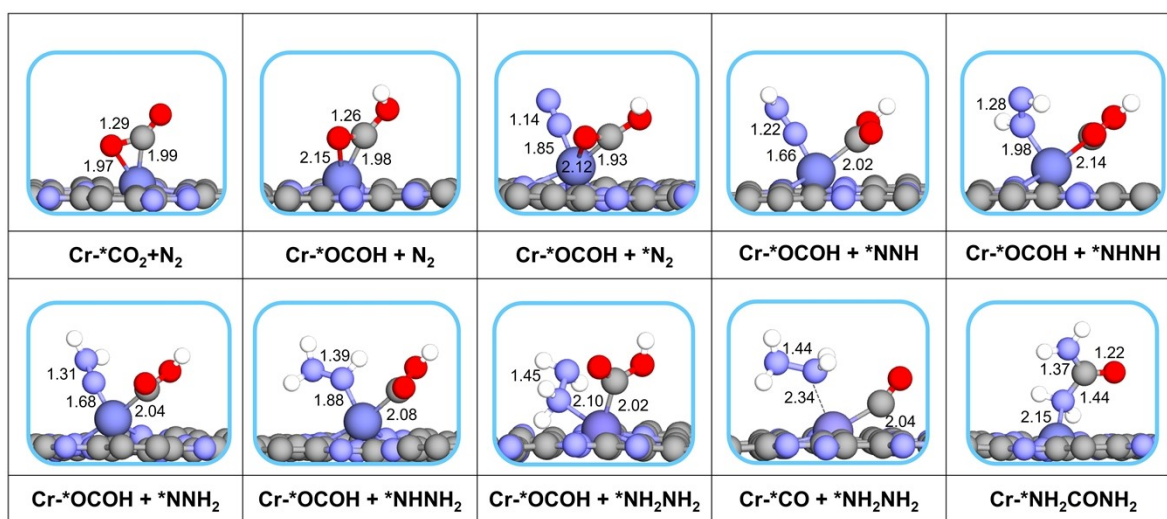


Figure31 – Gibbs free energy diagrams and atomic structures of critical step through the OCOH pathways for urea formation on V@C₂N.



OCOH pathways for urea formation on Cr@C₂N.

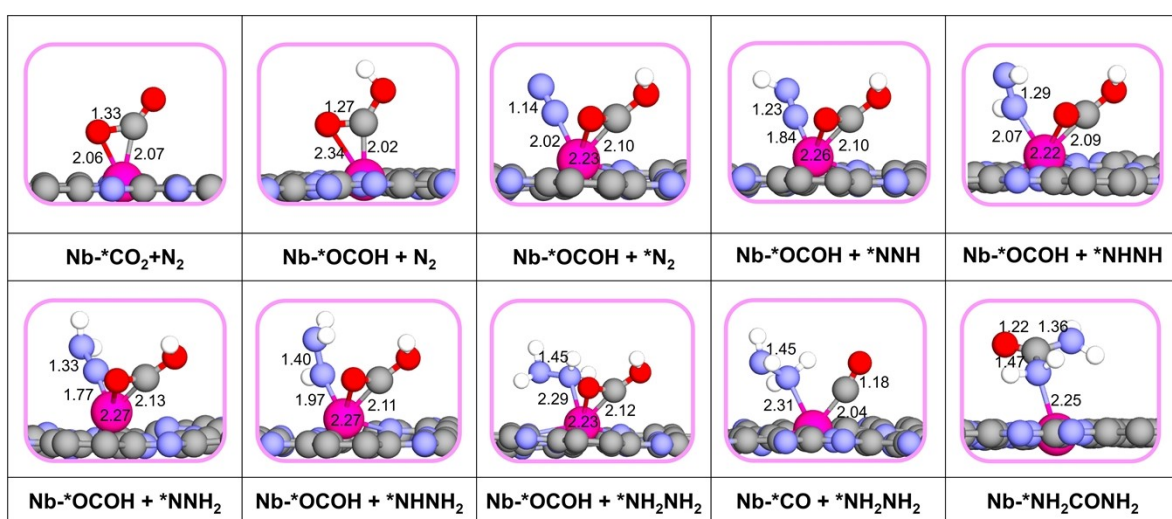
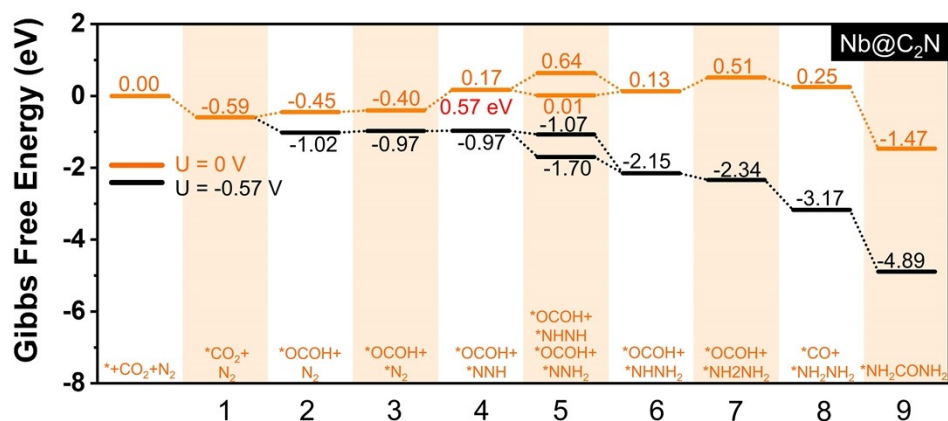


Figure33 – Gibbs free energy diagrams and atomic structures of critical step through the OCOH pathways for urea formation on Nb@C₂N.

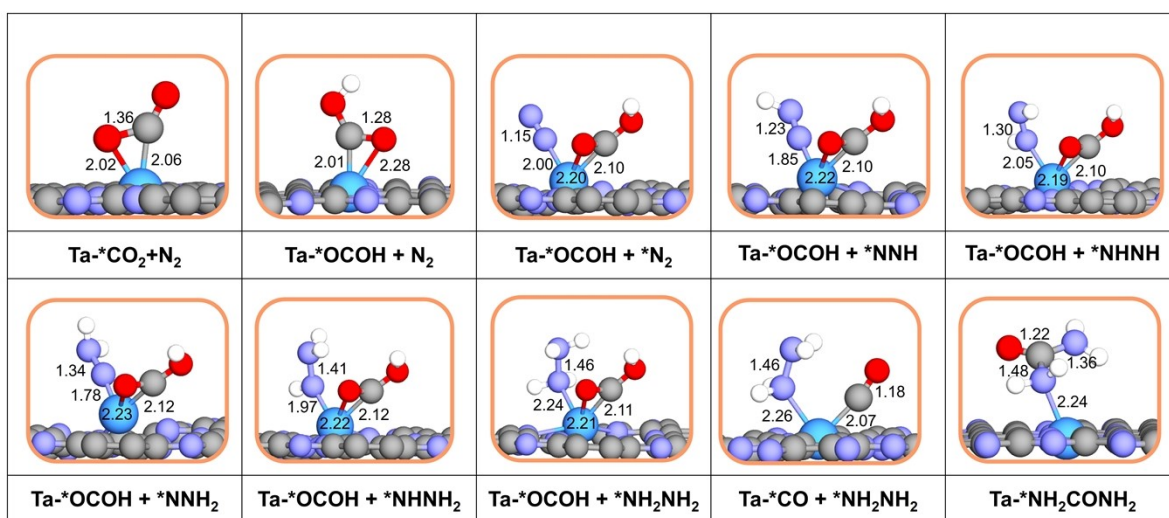
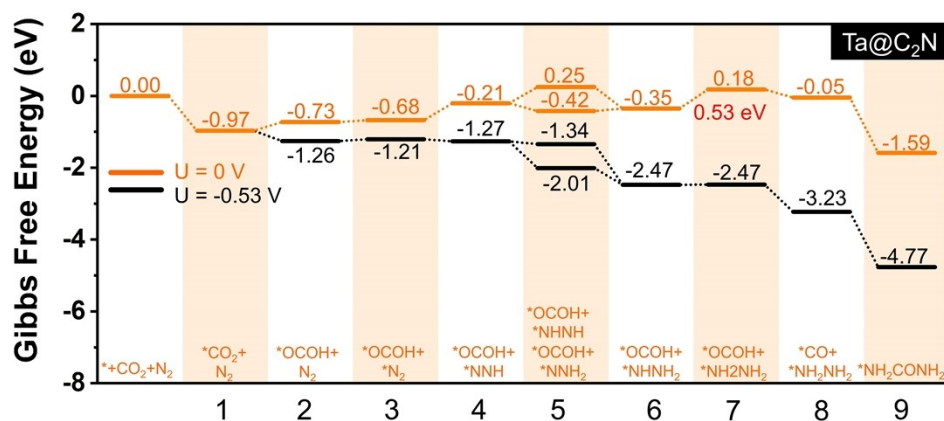


Figure34 – Gibbs free energy diagrams and atomic structures of critical step through the OCOH pathways for urea formation on Ta@C₂N.

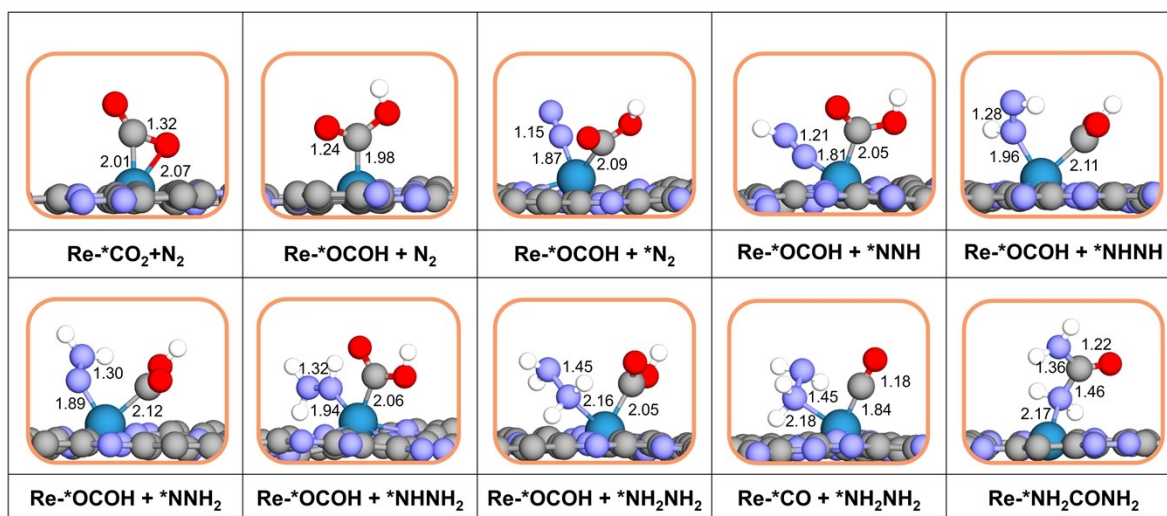
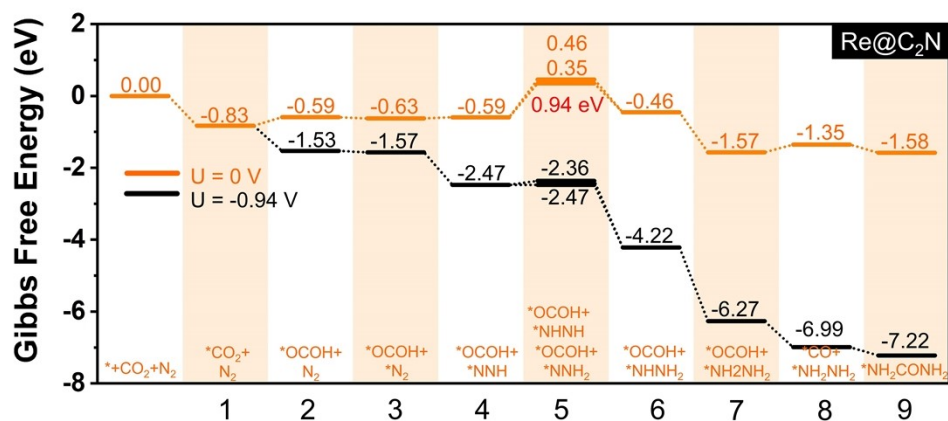


Figure35 – Gibbs free energy diagrams and atomic structures of critical step through the OCOH pathways for urea formation on Re@C₂N.

Table S2 The limiting potential of urea production (U_L) on the screened M@C₂N surface (M; Ti, V, Cr, Mn, Nb, Mo, Ru, Hf, Ta, W, and Re).

Catalysts	Urea production		
	Pathway	Limiting step	U_L
Ti@C ₂ N	CO	$*CO + *N_2 \rightarrow *CO + *NNH$	-0.85
Mn@C ₂ N	CO	$*CO + *N_2 \rightarrow *CO + *NNH$	-0.73
Mo@C ₂ N	CO	$*CO + *N_2 \rightarrow *CO + *NNH$	-0.51
Hf@C ₂ N	CO	$*CO + *N_2 \rightarrow *CO + *NNH$	-0.80
W@C ₂ N	CO	$*CO + *NHNH_2 \rightarrow *CO + *NH_2NH_2$	-0.56
V@C ₂ N	OCOH	$*OCOH + *N_2 \rightarrow *OCOH + *NNH$	-0.71
Cr@C ₂ N	OCOH	$*OCOH + *N_2 \rightarrow *OCOH + *NNH$	-0.73
Nb@C ₂ N	OCOH	$*OCOH + *N_2 \rightarrow *OCOH + *NNH$	-0.57
Ta@C ₂ N	OCOH	$*OCOH + *NHNH_2 \rightarrow *OCOH + *NH_2NH_2$	-0.53
Re@C ₂ N	OCOH	$*OCOH + *NHNH_2 \rightarrow *OCOH + *NH_2NH_2$	-0.94
Ti@C ₂ N	CO ₂	$*CO_2 + *NHNH_2 \rightarrow *CO + *NH_2NH_2$	-0.90
V@C ₂ N	CO ₂	$*CO_2 + *NHNH_2 \rightarrow *CO + *NH_2NH_2$	-0.60
Cr@C ₂ N	CO ₂	$*CO_2 + *NHNH_2 \rightarrow *CO + *NH_2NH_2$	-0.87
Zr@C ₂ N	CO ₂	$*CO_2 + *NHNH_2 \rightarrow *CO + *NH_2NH_2$	-0.64
Nb@C ₂ N	CO ₂	$*CO_2 + *N_2 \rightarrow *CO_2 + *NNH$	-0.50
Hf@C ₂ N	CO ₂	$*CO_2 + *NHNH_2 \rightarrow *CO + *NH_2NH_2$	-0.78
Ta@C ₂ N	CO ₂	$*CO_2 + *NHNH_2 \rightarrow *CO + *NH_2NH_2$	-0.62
W@C ₂ N	CO ₂	$*CO_2 + *N_2 \rightarrow *CO_2 + *NNH$	-0.60
Re@C ₂ N	CO ₂	$*CO_2 + *N_2 \rightarrow *CO_2 + *NNH$	-0.51

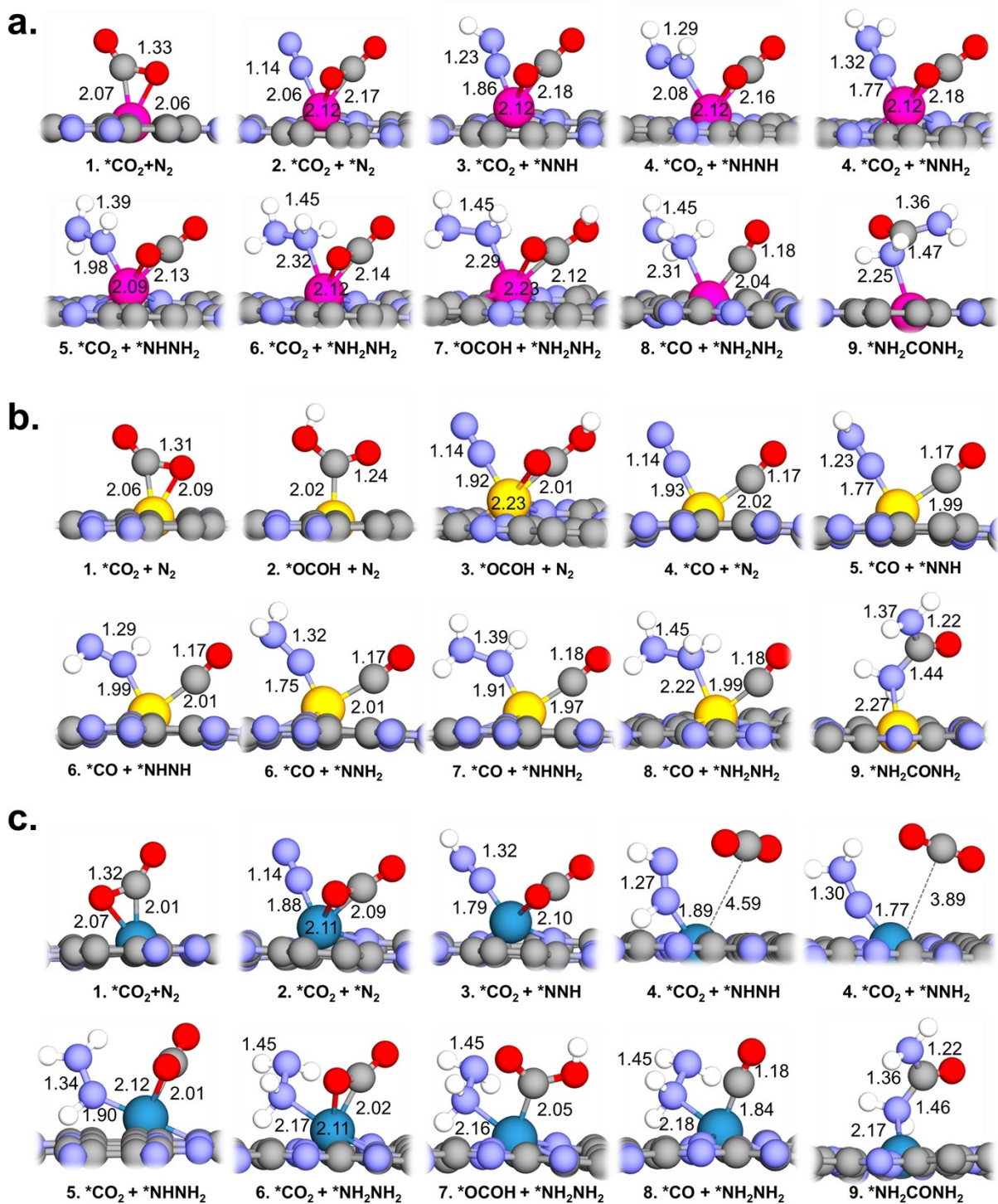


Figure36 – The geometrical structures of (a.) Nb@C₂N, (b.) Mo@C₂N and (c.) Re@C₂N catalysts

Table R3 Gibbs free energy (G, eV) and Nb magnetization values (μ_B) of the intermediates in the $*CO_2 + *N_2 \rightarrow *CO_2 + *NNH$ step on Nb@C₂N at different U values.

	U		PBE0
	U = 0.00	U = 4.0 ^{6, 7}	
$G_{*CO_2 + *N_2}$	-0.55	0.14	-0.56
$G_{*CO_2 + *NNH}$	-0.05	1.08	-0.06
ΔG_{PDS}	0.50	0.95	0.50
Nb magnetization			
*	1.3373	2.0468	1.3368
*CO ₂ +*N ₂	0.9952	1.0032	0.9952
*CO ₂ +*NNH	0.0000	0.0000	0.0000

Table R4 Gibbs free energy (G, eV) and Mo magnetization values (μ_B) of the intermediates in the $*CO + *N_2 \rightarrow *CO + *NNH$ step on Mo@C₂N at different U values.

	U				PBE0
	U = 0.00	U = 2.30 ⁸	U = 4.38 ⁹	U = 8.60 ¹⁰	
$G_{*CO_2 + *N_2}$	-0.76	0.05	0.88	2.17	-0.76
$G_{*CO_2 + *NNH}$	-0.25	0.89	2.12	3.56	-0.26
ΔG_{PDS}	0.51	0.84	1.24	1.39	0.50
Mo magnetization					
*	2.2399	2.2396	3.1396	3.3772	2.2399
*CO+*N ₂	1.2689	1.5954	1.7286	1.7285	1.2695
*CO+*NNH	0.0000	0.0000	0.0000	1.4992	0.0001

Table R5 Gibbs free energy (G, eV) and Re magnetization values (μ_B) of the intermediates in the $*CO_2 + *N_2 \rightarrow *CO_2 + *NNH$ step on Re@C₂N at different U values.

	U		PBE0
	U = 0.00	U = 2.3 ^{11, 12}	
$G_{*CO_2 + *N_2}$	-0.87	0.01	-1.11
$G_{*CO_2 + *NNH}$	-0.44	0.75	-0.70
ΔG_{PDS}	0.43	0.74	0.41
Re magnetization			
*	2.7685	2.0122	2.7680
*CO ₂ +*N ₂	0.0000	0.0005	0.0008
*CO ₂ +*NNH	0.0000	0.0001	0.0001

Table R6 Gibbs free energy (G, eV) of the intermediates in the $^*\text{CO}_2/\text{CO} + ^*\text{N}_2 \rightarrow ^*\text{CO}_2/\text{CO} + ^*\text{NNH}$ step on Nb@C₂N with and without VASPsol calculation.

	Nb		Mo		Re	
	VASP	VASPsol	VASP	VASPsol	VASP	VASPsol 1
$G_{^*\text{CO}_2/\text{CO} + ^*\text{N}_2}$	-0.55	-0.48	-0.76	-0.80	-0.87	-0.95
$G_{^*\text{CO}_2/\text{CO} + ^*\text{NNH}}$	-0.05	0.00	-0.25	-0.28	-0.44	-0.39
ΔG_{PDS}	0.50	0.48	0.51	0.52	0.43	0.57

Table S7. Specific values of different features are included in the descriptor Φ .

Elements	N_d	χ	Φ	Elements	N_d	χ	Φ
Sc	1	1.36	3.66	Rh	8	2.18	23.14
Ti	2	1.54	6.88	Pd	10	2.2	28.79
V	3	1.63	10.04	Ag	10	1.93	30.74
Cr	5	1.66	16.57	Hf	2	1.32	7.43
Mn	5	1.55	17.15	Ta	3	1.51	10.43
Fe	6	1.83	18.94	W	4	2.36	11.12
Co	7	1.88	21.80	Re	5	1.93	15.37
Ni	8	1.92	24.66	Os	6	2.18	17.36
Cu	10	1.9	30.98	Ir	7	2.2	20.16
Y	1	1.22	3.87	Pt	9	2.28	25.46
Zr	2	1.33	7.41	Au	10	2.54	26.80
Nb	4	1.59	13.55	N	N/A	3.04	N/A
Mo	5	2.16	14.53	Substrate [#]	N/A	18.24	N/A
Ru	7	2.2	20.16				

[#] $c_{sub} = nc_N$, where n are 6 in the $M@C_2N$. Therefore, Φ can be simplified as

$$\Phi = \frac{N_d}{\sqrt{c_M / (6 \times 3.04)}} = \frac{N_d}{\sqrt{c_M / 18.24}}$$

Table S8. Specific values of different features are included in the descriptor ϕ .

Elements	N_d	χ	χ_{avg}	ϕ	Elements	N_d	χ	χ_{avg}	ϕ
Sc	1	1.36	4.27	1.40	Rh	8	2.18	4.40	11.59
Ti	2	1.54	4.30	2.83	Pd	10	2.2	4.41	14.50
V	3	1.63	4.31	4.25	Ag	10	1.93	4.36	14.35
Cr	5	1.66	4.32	7.10	Hf	2	1.32	4.26	2.80
Mn	5	1.55	4.30	7.07	Ta	3	1.51	4.29	4.24
Fe	6	1.83	4.35	8.58	W	4	2.36	4.43	5.83
Co	7	1.88	4.35	10.02	Re	5	1.93	4.36	7.17
Ni	8	1.92	4.36	11.47	Os	6	2.18	4.40	8.69
Cu	10	1.9	4.36	14.33	Ir	7	2.2	4.41	10.15
Y	1	1.22	4.24	1.40	Pt	9	2.28	4.42	13.09
Zr	2	1.33	4.26	2.80	Au	10	2.54	4.46	14.68
Nb	4	1.59	4.31	5.66	N	N/A	3.04	N/A	N/A
Mo	5	2.16	4.40	7.24	Substrate [#]	N/A	18.24	N/A	N/A
Ru	7	2.2	4.41	10.15					

Table S9. Values of descriptor Φ and U_L of PDS for urea production over reported electrocatalysts.

Electrocatalysts		Φ	U_L (V)
M@C ₂ N	Sc	3.66	-1.02
	Ti	6.88	-0.85
	V	10.04	-0.60
	Cr	16.57	-0.73
	Mn	17.15	-0.73
	Fe	18.94	-1.07
	Co	21.80	-1.32
	Ni	24.66	-1.14
	Cu	30.98	-1.49
	Y	3.87	-1.07
	Zr	7.41	-0.64
	Nb	13.55	-0.50
	Mo	14.53	-0.51
	Ru	20.16	-1.07
	Rh	23.14	-1.20
	Pd	28.79	-1.31
	Hf	7.43	-0.78
	Ta	10.43	-0.62
	W	11.12	-0.56
	Re	15.37	-0.51
	Os	17.36	-0.88
	Ir	20.16	-1.21
	Pt	25.46	-0.98
M ₂ @C ₃ N ₄ ¹³	Sc	3.24	-0.93
	Ti	6.09	-0.74
	V	8.88	-0.74
	Cr	14.67	-1.54
	Mn	15.18	-1.03

	Fe	16.76	-1.80
	Co	19.30	-1.86
	Ni	21.82	-2.67
	Cu	27.42	-3.41
	Zn	29.42	-3.35
	Y	3.42	-1.90
	Zr	6.55	-0.76
	Nb	11.99	-0.75
	Mo	12.86	-1.31
	Tc	13.67	-1.03
	Ru	17.84	-1.54
	Rh	20.48	-1.69
	Pd	25.48	-2.26
	Ag	27.21	-3.97
	Cd	29.07	-3.08
	Hf	6.58	-1.14
	Ta	9.23	-1.19
	W	9.84	-0.75
	Re	13.60	-1.51
	Os	15.36	-1.04
	Ir	17.84	-1.29
	Pt	22.53	-1.33
	Au	23.72	-3.07
M/p-BN ¹⁴	Fe	26.45	-0.63
	Co	30.44	-0.66
M-B@C ₂ N ¹⁵	Sc	3.56	-0.74
	Ti	6.69	-0.76
	V	9.76	-0.81
	Cr	16.11	-0.81
	Mn	16.68	-1.80
	Fe	18.42	-1.15

Co	21.20	-1.07
Ni	23.97	-1.72
Cu	30.12	-1.47
Zr	7.20	-0.62
Nb	13.17	-0.54
Mo	14.13	-0.53
Ru	19.60	-0.88
Rh	22.50	-1.39
Pd	27.99	-1.65
Ag	29.89	-2.06
PdCu ¹⁶	19.76	-0.64
Mo ₂ B ₂ ¹⁷	19.58	-0.49
Ti ₂ B ₂ ¹⁷	8.92	-0.65
Cr ₂ B ₂ ¹⁷	21.65	-0.52
V ₂ N ₆ C ¹⁸	19.25	-0.59
CuB ₁₂ ¹⁹	35.90	-0.23
CuPc ²⁰	48.52	-1.67
MoP(111) ²¹	28.48	-0.27

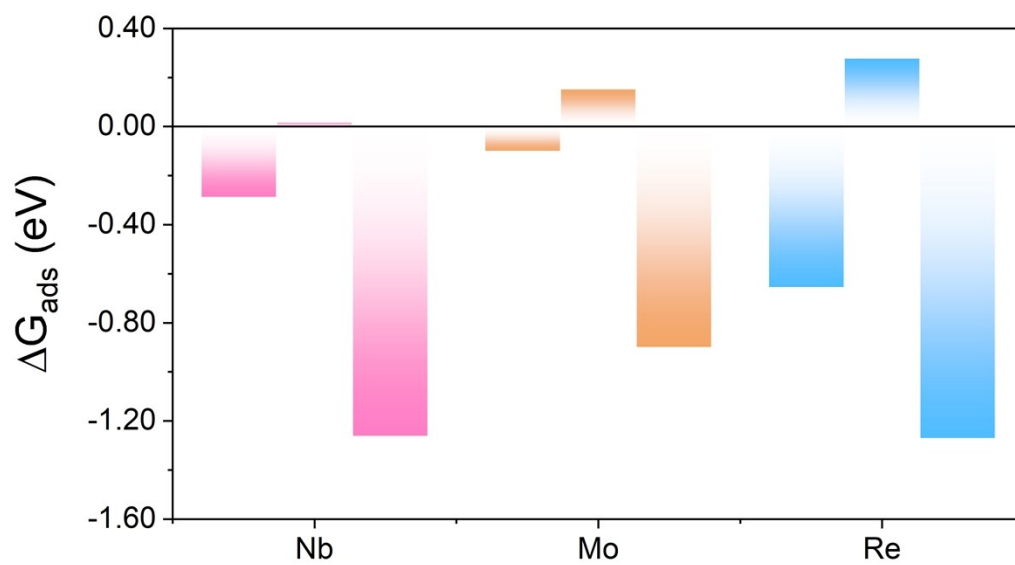


Figure37 – Gibbs free energy adsorption for H^+ , H_2O , and N_2 on $\text{Nb@C}_2\text{N}$, $\text{Mo@C}_2\text{N}$, and $\text{Re@C}_2\text{N}$ catalysts

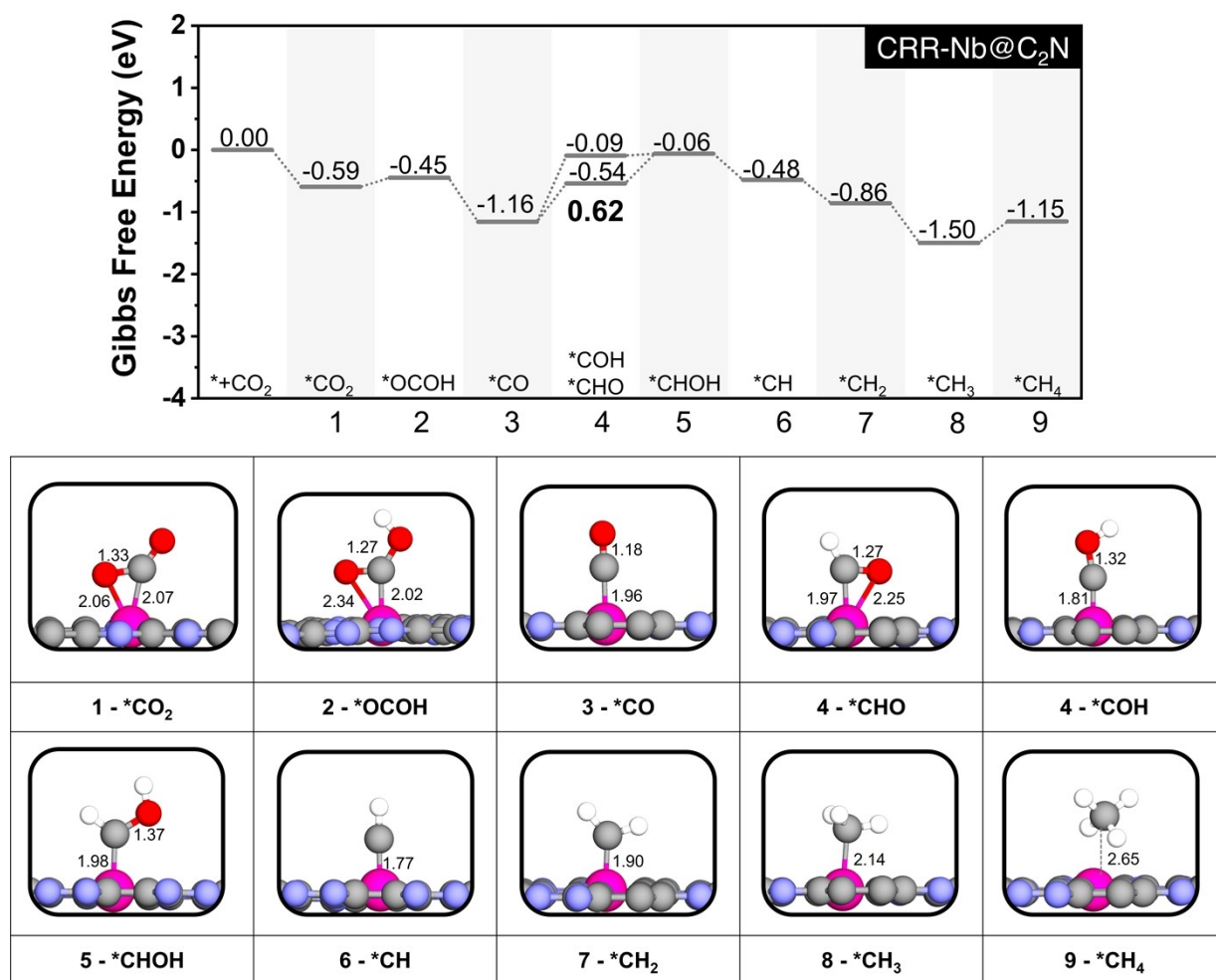


Figure38 – Gibbs free energy diagrams and atomic structures of CRR on Nb@C₂N catalysts

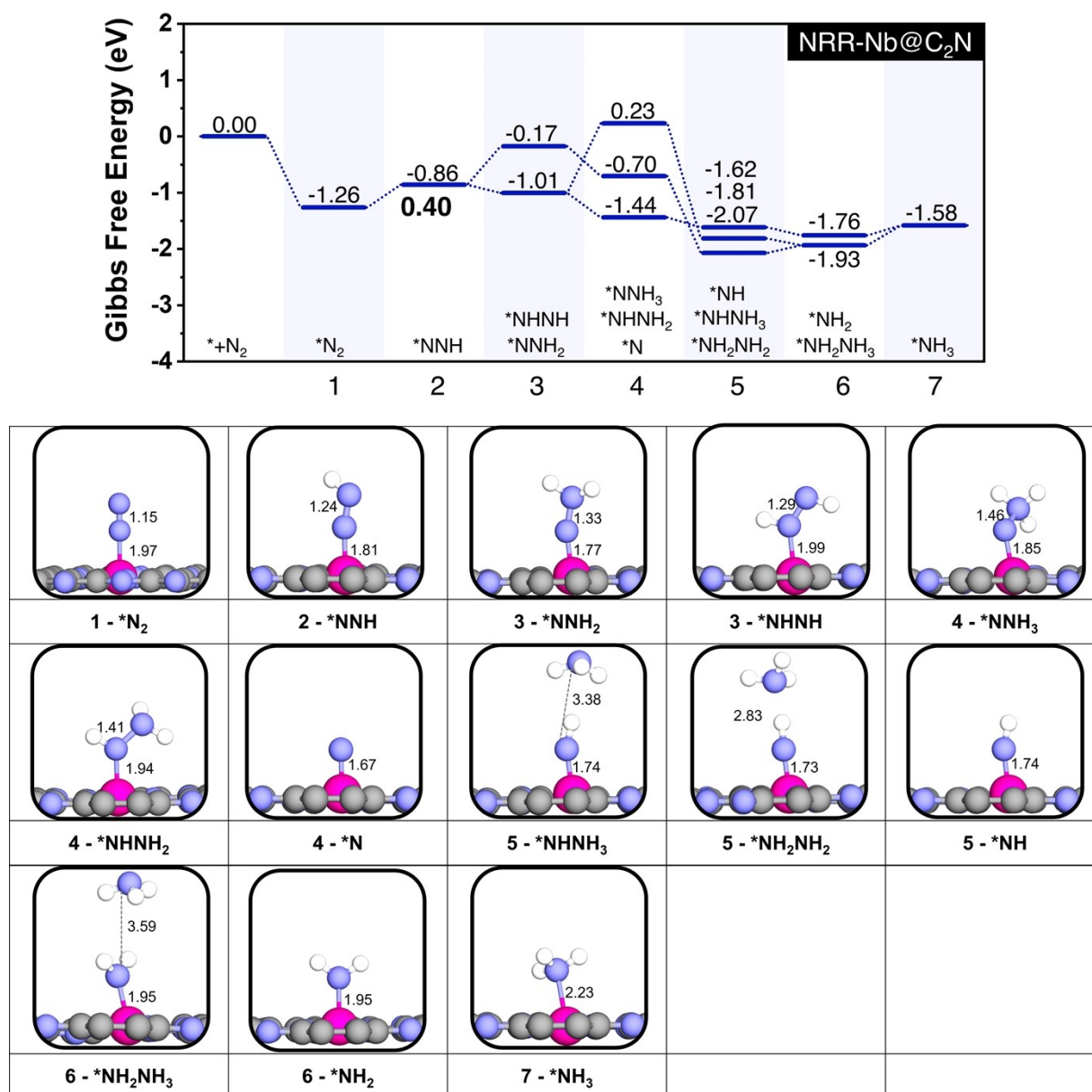


Figure39 – Gibbs free energy diagrams and atomic structures of NRR on Nb@C₂N catalysts

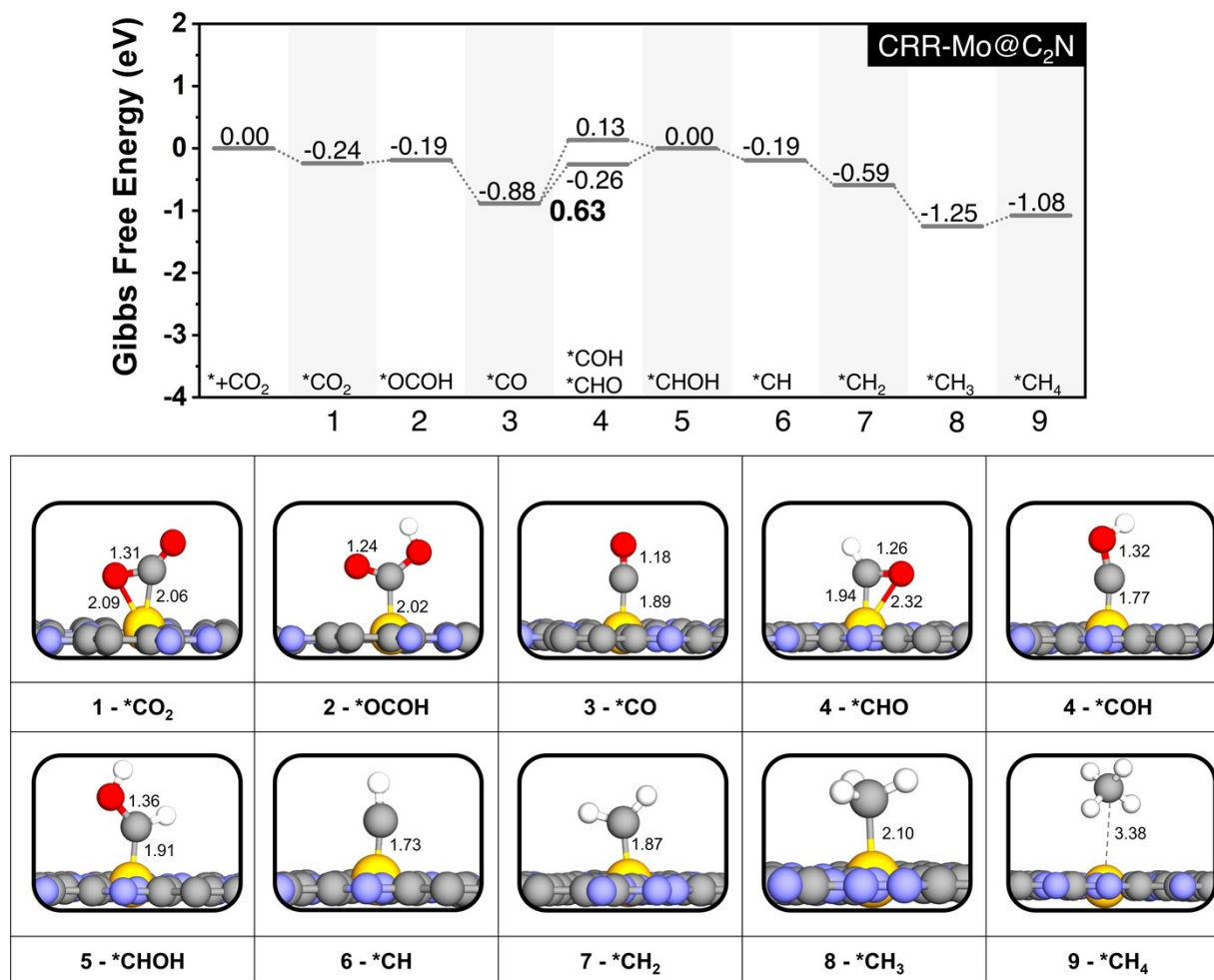


Figure40 – Gibbs free energy diagrams and atomic structures of CRR on Mo@C₂N catalysts

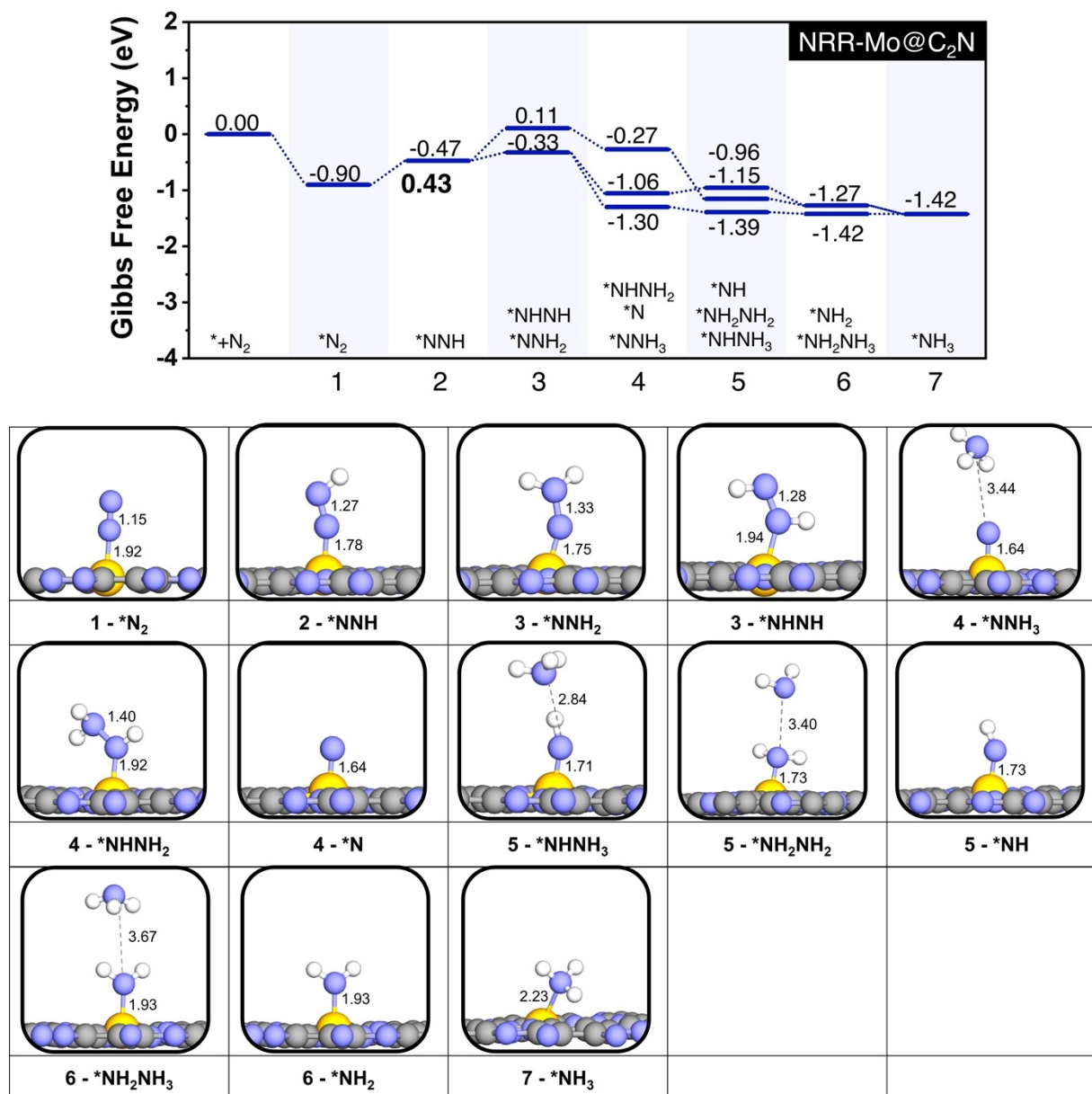


Figure41 – Gibbs free energy diagrams and atomic structures of NRR on Mo@C₂N catalysts

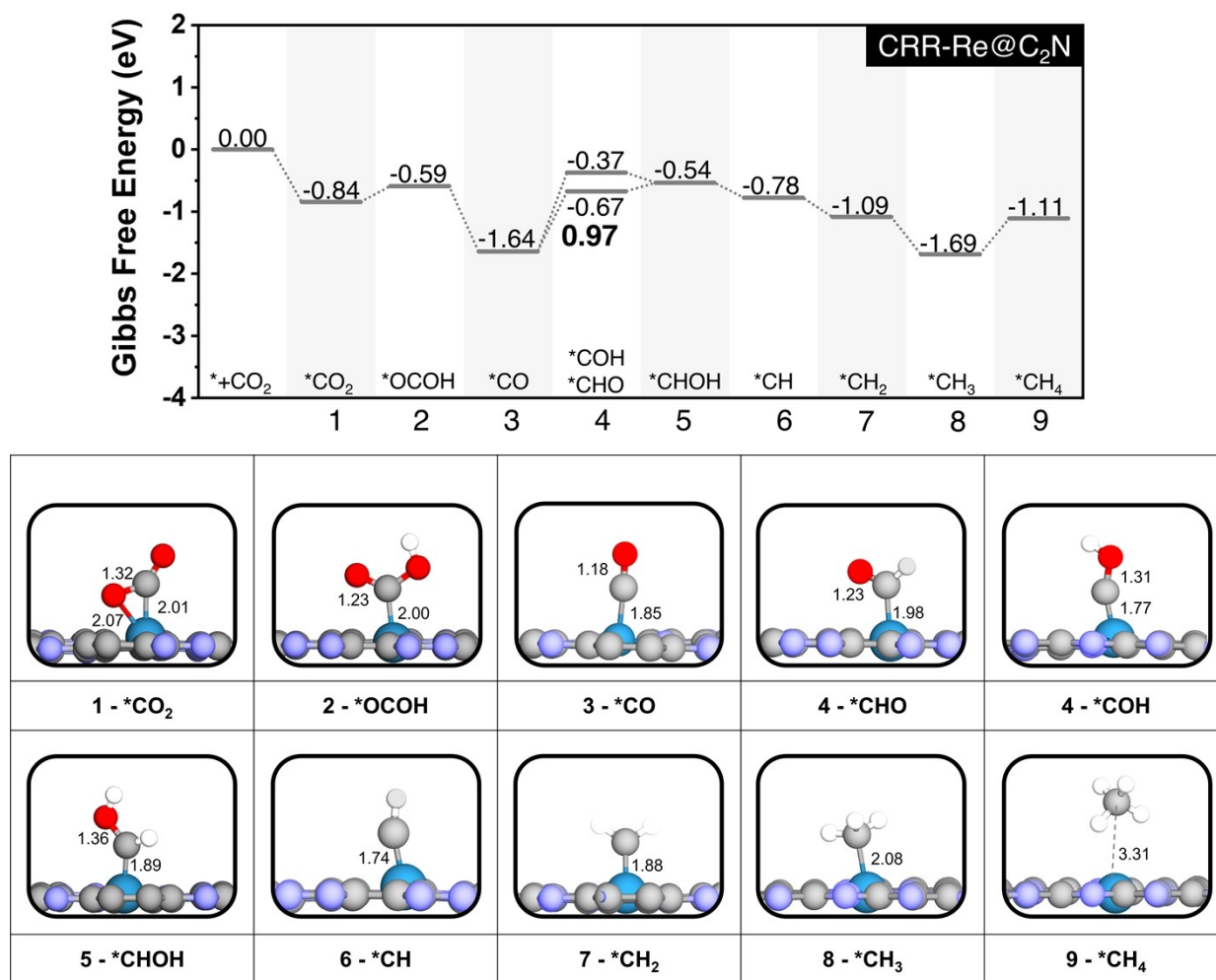


Figure42 – Gibbs free energy diagrams and atomic structures of CRR on Re@C₂N catalysts

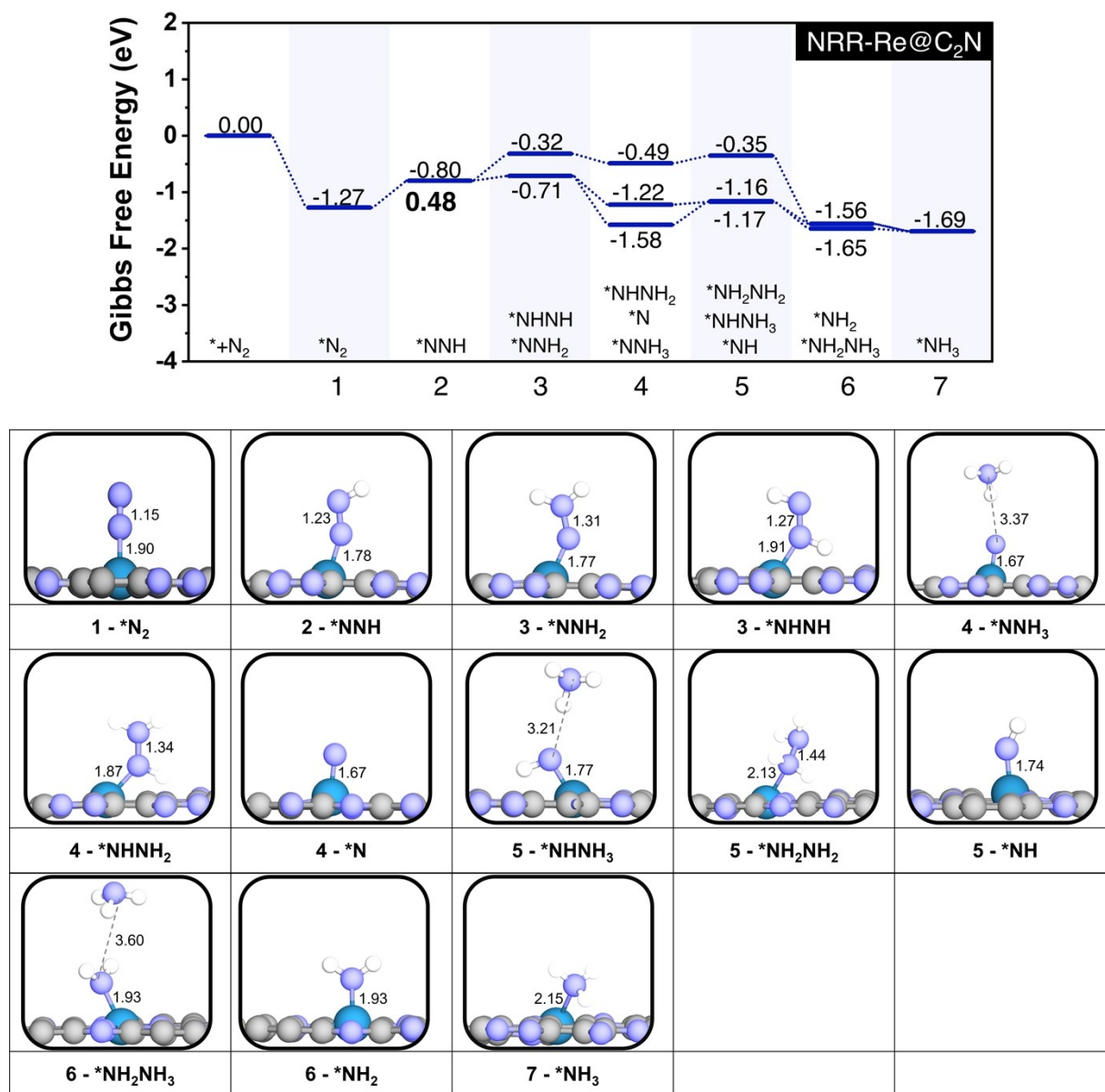


Figure43 – Gibbs free energy diagrams and atomic structures of NRR on Re@C₂N catalysts

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