Supporting Information for:

Orientation of interfacial water molecules governs the electrochemical nitrogen reduction reaction on the Mo-N_4-C surface

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3. Supplementary Tables

1. Additional Computational details

1.1 DFT Calculations

A hybrid solvation model was taken, where implicit solvation was applied through VASPsol using the Poisson-Boltzmann implicit solvation model with the dielectric constant (ε) of 78.4 (water).[1] In addition, the explicit solvation model is applied by taking the atomic water near the adsorbate species to capture the influence of an electric double layer.[2] The MoN_4 surface was modeled using a supercell of $4 \times 3 \times 1$ with optimized box cell lengths of a = 9.824, b= 12.762, and c = 25 Å. A Monkhorst-Pack k-point mesh was $3 \times 3 \times 1$, with ~15 Å vacuum added in the z-axis.[3] Initially, a CHE model[4] was applied to study the PDS of the N_2 reduction on the MoN_4 catalyst surface. According to this model, the free energy change ($\Delta \boldsymbol{G}$) of each electrochemical step was calculated by the given eq 1

$$\Delta \boldsymbol{G} = \Delta \boldsymbol{E} + \Delta \boldsymbol{E_{ZPE}} - \boldsymbol{T}\Delta \boldsymbol{S} + \Delta \boldsymbol{G_U} + \Delta \boldsymbol{G_{pH}} \quad (1)$$

Here, ΔE represents the DFT calculated total energy, ΔE_{ZPE} (zero-point energy) and S (entropy), calculated by employing the frequency calculation at a temperature (T) of 298.15 K. The ΔG_U represents the applied potential, which is further elaborated as $\Delta G_U = -neU$, where U is the applied potential and n is the number of electrons transferred. The ΔG_{pH} denotes the pH correction applied through the eq 2.

$$\Delta G_{pH} = k_B T \times pH \times \ln 10 \quad (2)$$

where k_B is the Boltzmann constant, and pH is set to 1. The limiting potential of reaction (U_L) is termed as the minimum applied potential to the system at which each reaction step shows thermodynamic feasibility, determined by eq 3.

$$U_L = \frac{-\Delta G_{PDS}}{e} \quad (3)$$

Here, $\Delta \boldsymbol{G_{PDS}}$ is the free energy change of the PDS step, and it is the maximum $\Delta \boldsymbol{G}$ throughout the reaction step.

1.2 Representation of Electrolyte model

In our simulations, we used one H_3O^+ molecule with 40 water molecules to represent an acidic environment. This setup is intended to capture proton availability and proton transfer behaviour at the electrified interface, rather than reproduce the exact bulk pH quantitatively. However, the counterion was not explicitly included due to considerations of the electric double-layer (EDL) effect. According to classical electrochemical theory, under an applied potential, ionic species become spatially separated, where ions of one specific charge preferentially accumulate near the electrode surface, while their counterions are redistributed away from the Helmholtz plane due to electrostatic repulsion.[5] Consequently, neglecting the counterion allows the simulations to focus on the chemically relevant interfacial region. This approximation has been commonly adopted in previous studies.[6–8] Similarly, we clarify that the Debye length of 3.04 Å was employed within the VASPsol framework to provide continuum electrostatic screening of the surrounding electrolyte. This parameter does not correspond to an exact

bulk concentration in our finite simulation cell (1.3 M), but approximates long-range screening beyond the explicitly modelled solvent layer.

1.3 Reaction pulling speed and potential control

In addition, the pulling speed (the incremental change of the collective variable per MD step) employed in the SG-AIMD plays a critical role in determining the smoothness and quality of the slow growth barrier. A large pulling speed can lead to nonequilibrium effects and an uneven free-energy curve, whereas a sufficiently slow pulling speed ensures better convergence and a smoother barrier. Therefore, we employed a pulling speed of 0.0004 Å/time step, which is sufficiently slow to minimize nonequilibrium artifacts and yield a well-converged, smooth free-energy profile. In addition, a test of different pulling speeds is provided in Figure S13, demonstrate the barrier is relatively smooth and lower as compared to 0.0006 and 0.0008 Å/time step.

In our constant-potential simulations, the number of electrons is adjusted periodically to maintain the desired electrode potential through NEADJUST = 5, meaning the potential is updated every five MD steps. Therefore, the x-axis represents the update index, which corresponds to the number of potential adjustment events during the simulation, as shown in Figures S17, S20, and S24.

1.4 Selection of CV for Calcuation of *H and *NH_2 barrier

The selection of the CV for *H and *NH_2 based on the two aspects: (I) the water spontaneously adsorbs on the MoN_4 site during equilibration. This reflects the intrinsic oxyphilic nature of the Mo center under aqueous conditions and represents the thermodynamically preferred state. Therefore, pre-adsorbed water taken as CV (initial state) for calculating the *H adsorption reaction barrier, as shown in Figure S11c. But, when the Mo site is pre-occupied by some other species like *NH_2 and *N_2, the site is blocked for the incoming H_2O molecule. In other words, the presence or absence of *H_2O is not imposed manually but emerges naturally from competitive adsorption thermodynamics configuration under adsorbate coverage. Therefore, both HER and NRR pathways were evaluated from their respective thermodynamically stable surface configurations. Introducing a manually fixed *H_2O species during NRR steps would artificially constrain the system and disrupt the spontaneous competitive adsorption behaviour. Another aspect is that (II) This adsorption competition leads to a lower *H barrier than the *NH_2 protonation, indicating that the indicating that HER is kinetically more favorable than NRR on MoN_4. This intrinsic oxophilic nature and the resulting preference toward *H formation may partially account for the limited experimental reports of Mo on N-doped graphene for selective NRR.

2. Supplementary Figures

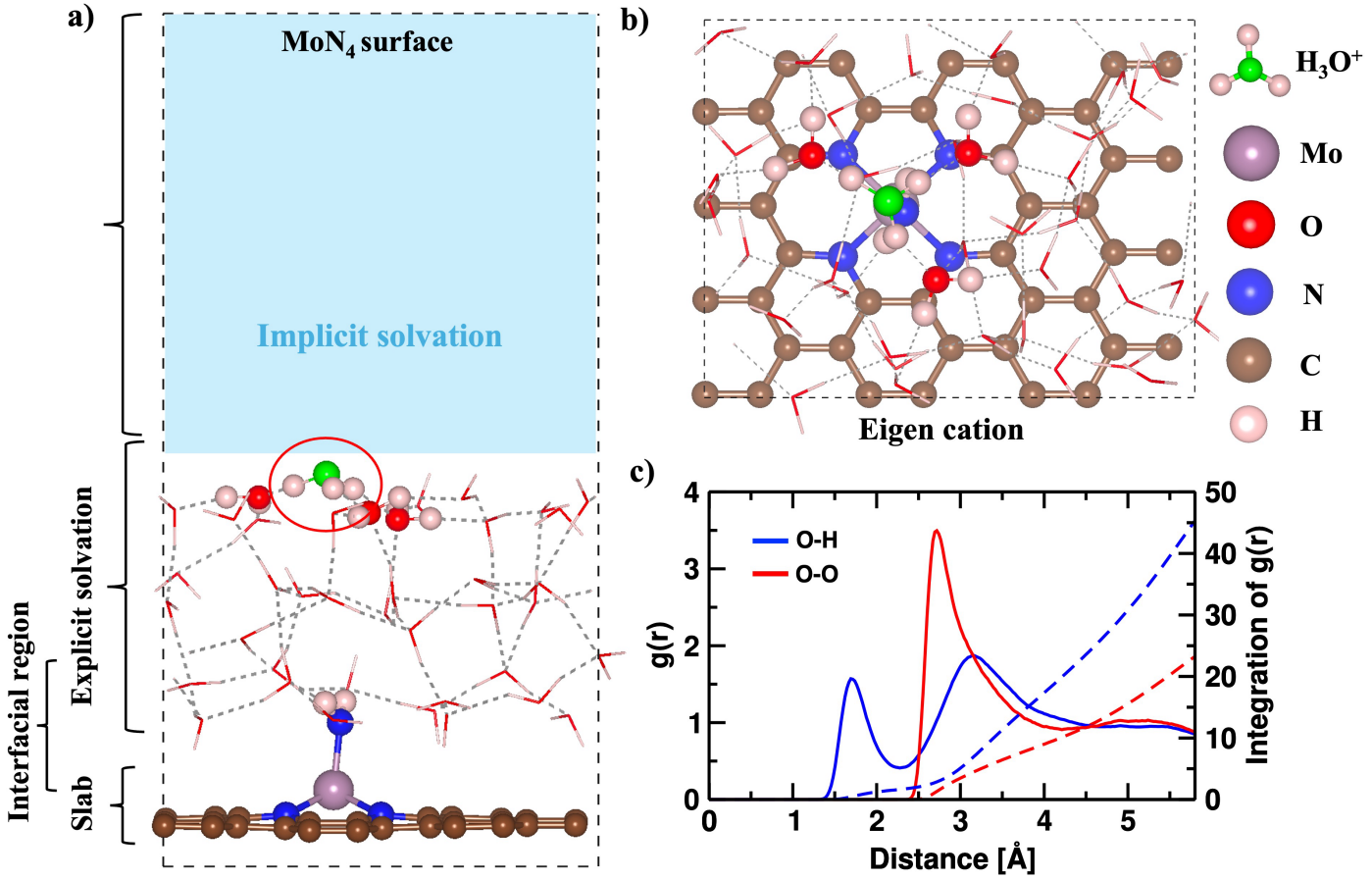

Figure S1. (a) The representative structure of the MoN_4/H_2O electrode-electrolyte interface, where H_3O^+ represents the acidic medium (green color). (b) The present H_3O^+ makes a solvation shell with 3 H_2O, termed the Eigen cation ($H_9O_4^+$). (c) The radial distribution function (RDF) of equilibrated water with integration of g(r)of the O-H and O-O.

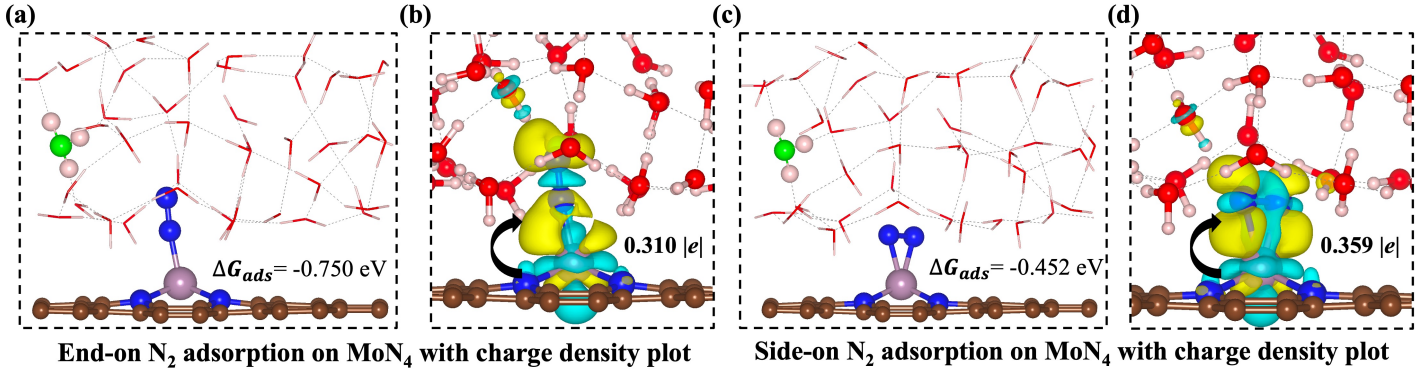

Figure S2. (a-b) The end-on N_2 adsorption at the MoN_4/H_2O interface, along with its charge density plot. (c-d) The side-on N_2 adsorption at the MoN_4/H_2O interface, along with its charge density plot in acidic medium with an isosurface value of 0.0003 e $Å^{-3}$. The yellow region shows charge accumulation, and the cyan region shows charge depletion.

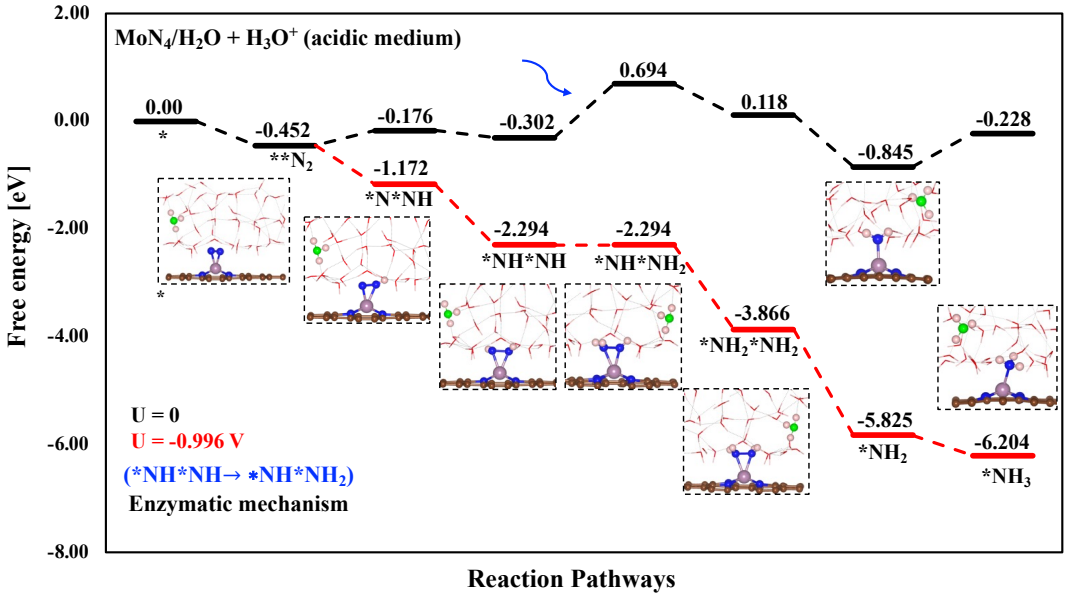

Figure S3. The free energy profile of Enzymatic mechansim at the MoN_4/H_2O interface in acidic medium, with optimized NRR intermediates.

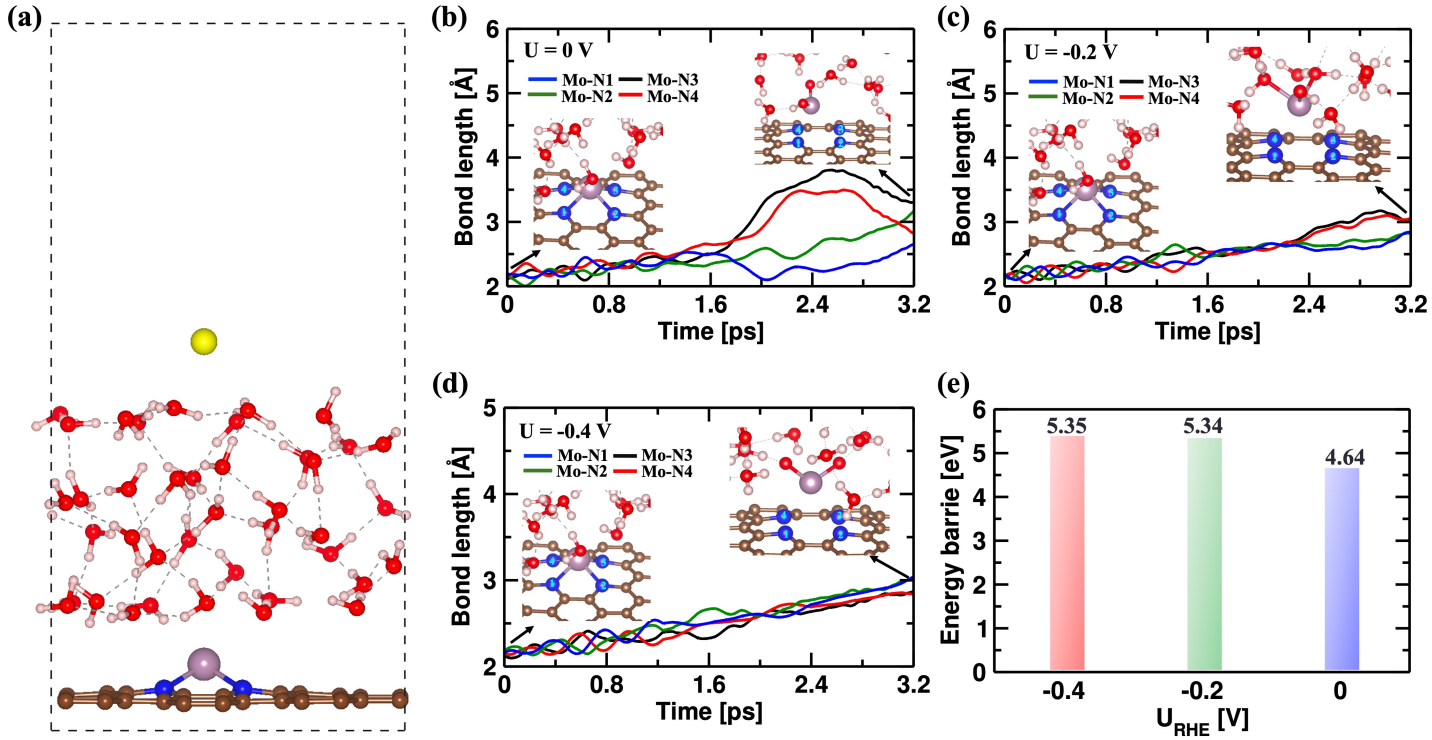

Figure S4. (a) The simulation box of the MoN_4/H_2O interface with 40 water molecules, where Helium is represented in the yellow colour, (b-d) The change in the Mo-N bond length at potential of 0, -0.2, and -0.4 V vs RHE, during the leaching of the Mo, extracted from SG-AIMD simulation (e) The reaction of the Mo leaching from the N-doped graphene surface (N_4G).

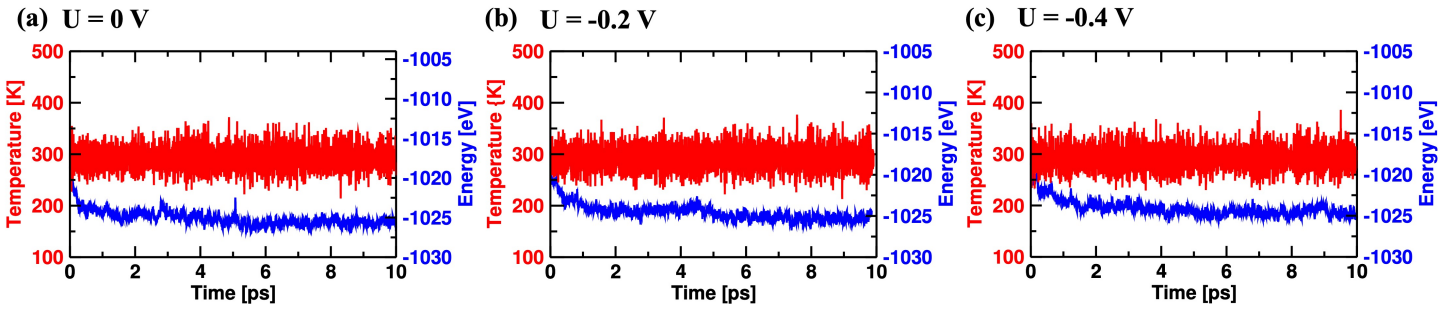

Figure S5. The equilibrated temperature and energy plot of the MoN_4/H_2O interface, during the CP-AIMD at (a) 0 V, (b) -0.2 V, and (c) -0.4 V vs RHE.

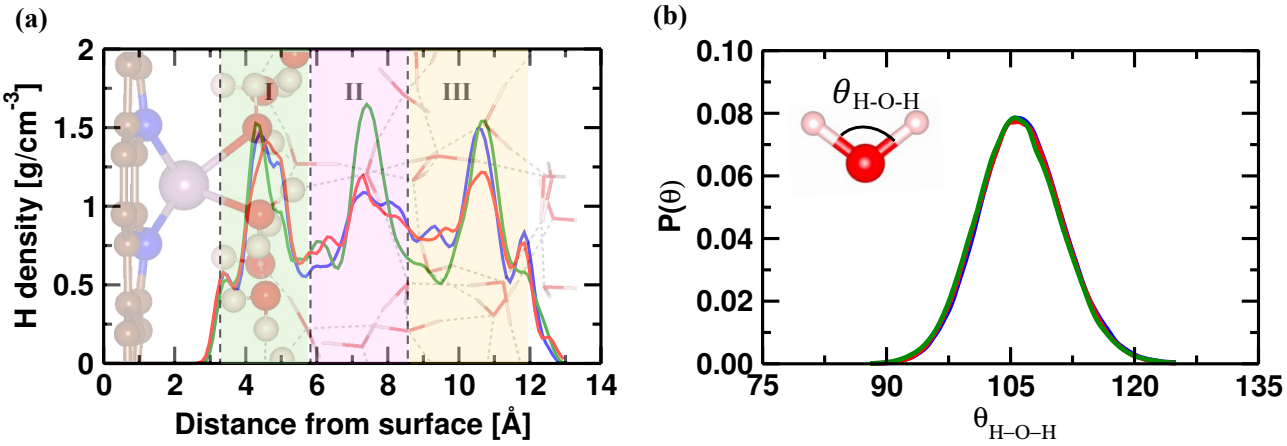

Figure S6. (a) The H density along the surface (z-axis), (b) Probability distribution of the H-O-H angle of water at 0, -0.2, and -0.4 V vs RHE.

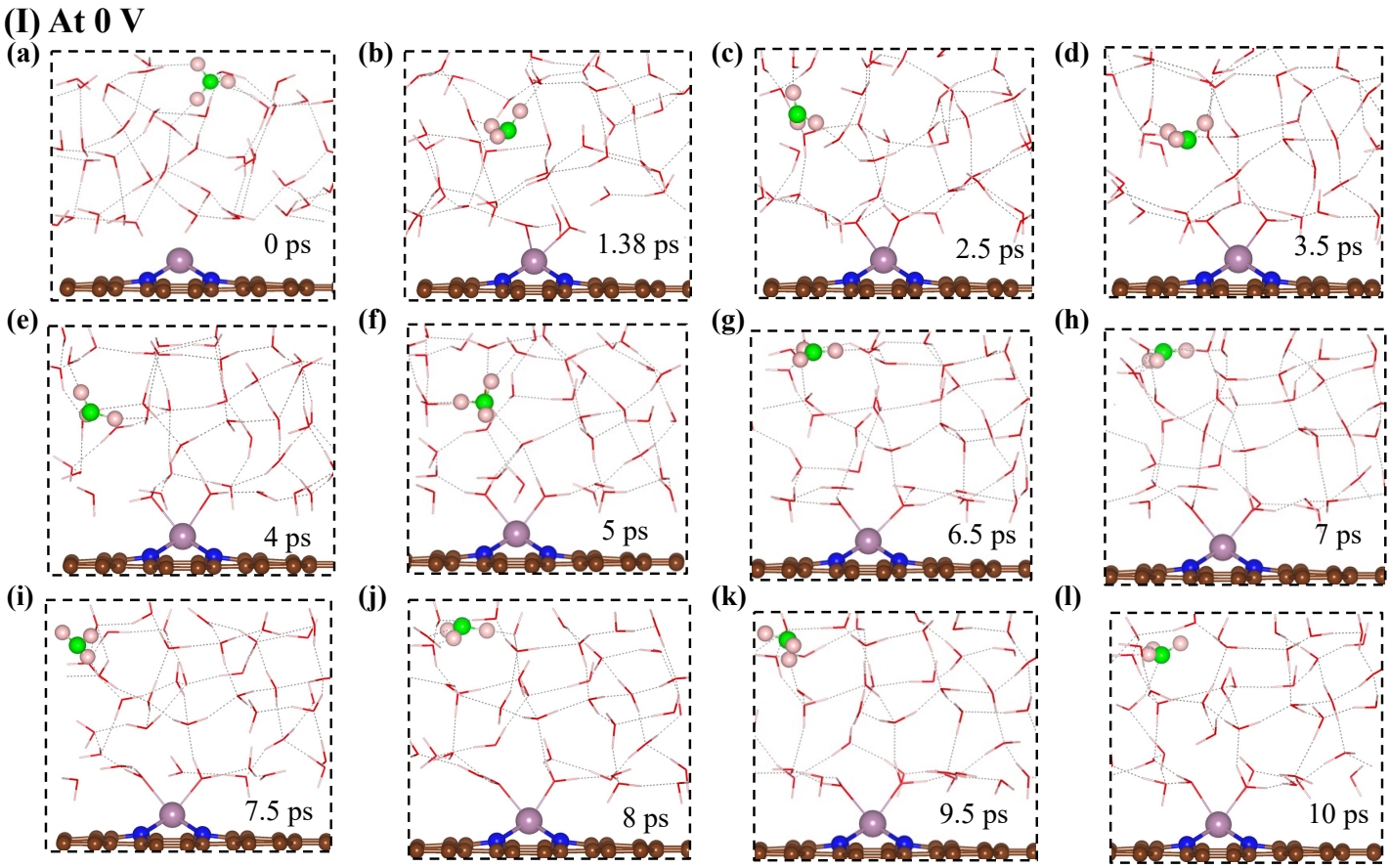

Figure S7. (a-l) The selective snapshot of the H_3O^+ diffusion at 0 V vs RHE in acidic medium at the MoN_4/H_2O electrochemical interface.

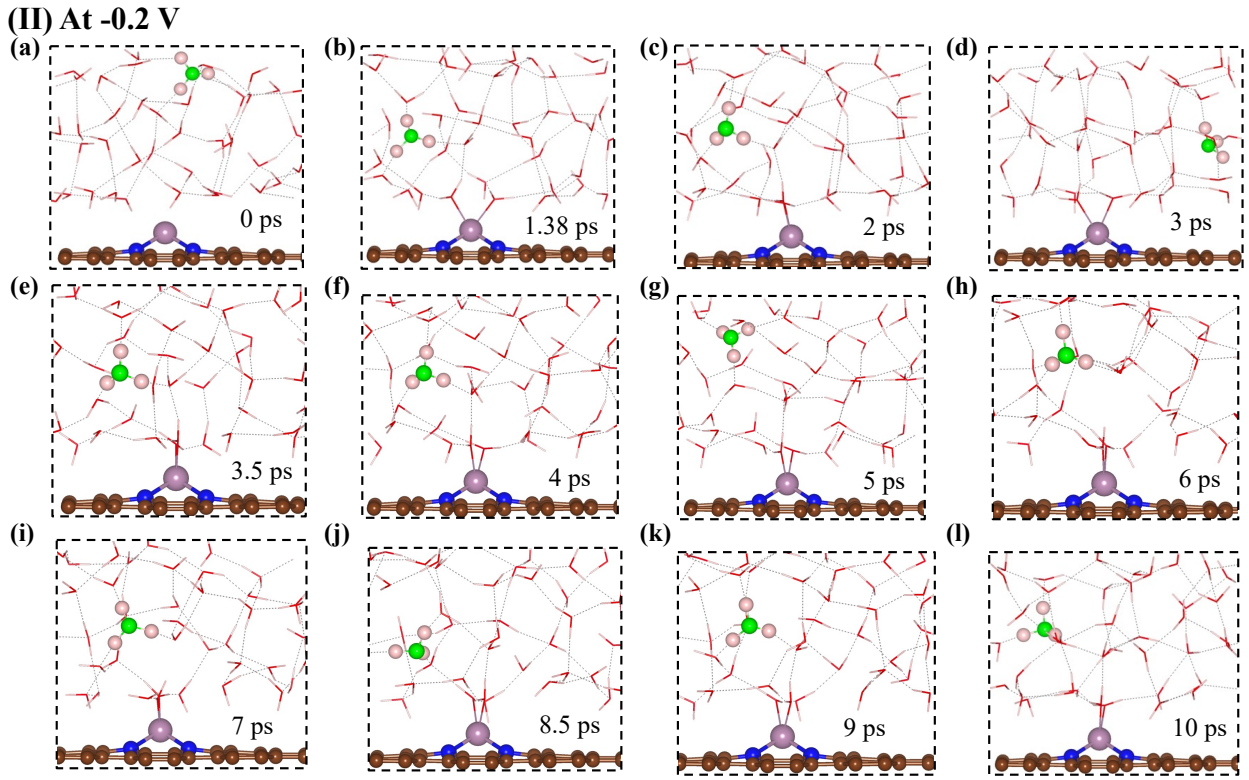

Figure S8. (a-l) The selective snapshot of the H_3O^+ diffusion at -0.2 V vs RHE in acidic medium at the MoN_4/H_2O electrochemical interface.

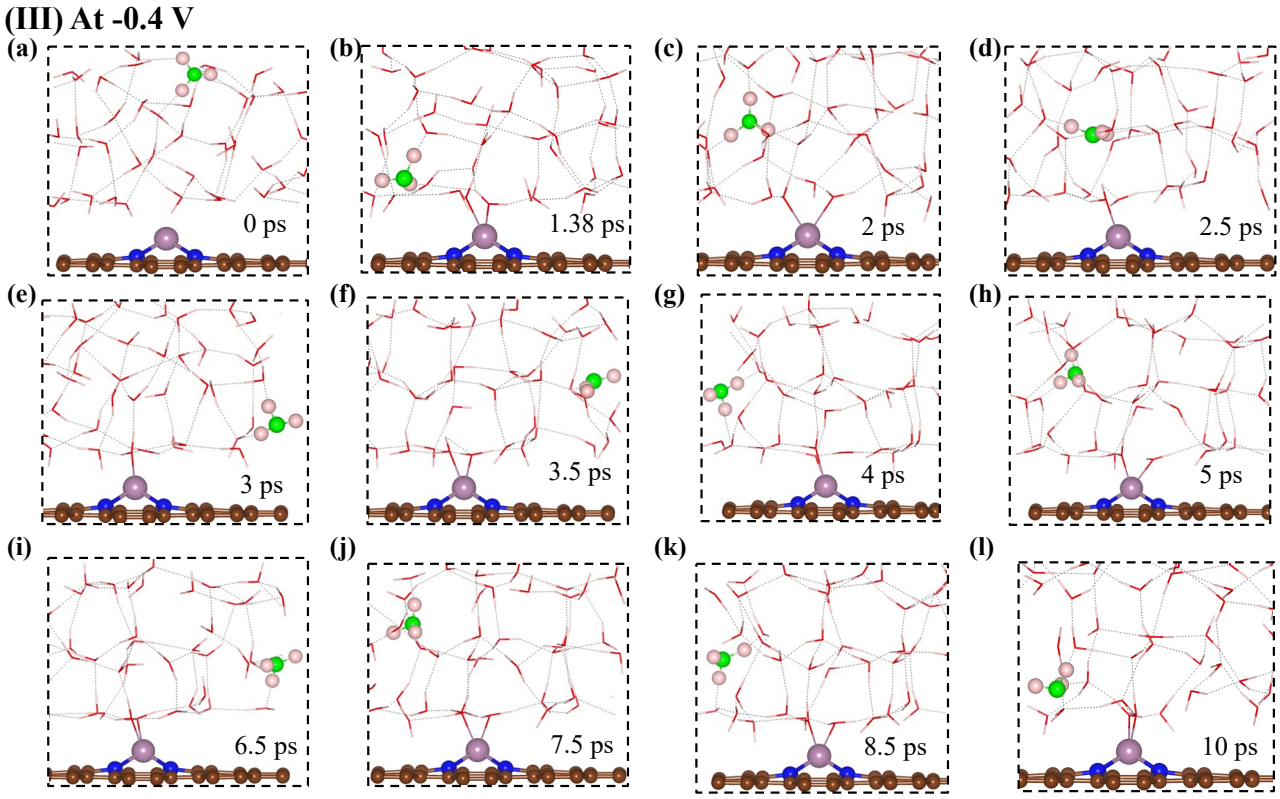

Figure S9. (a-l) The selective snapshot of the H_3O^+ diffusion at -0.4 V vs RHE in acidic medium at the MoN_4/H_2O electrochemical interface.

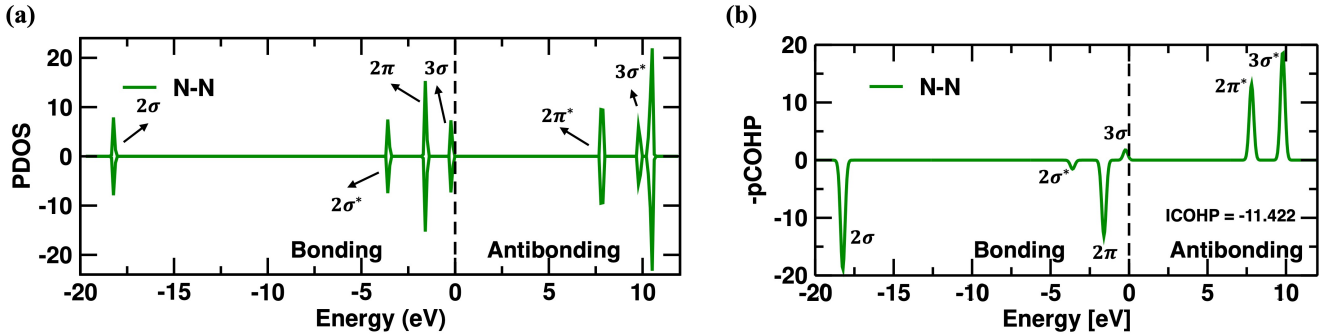

Figure S10. (a) The projected density of states (PDOS) and (b) ICOHP plot of the free N_2 molecule.

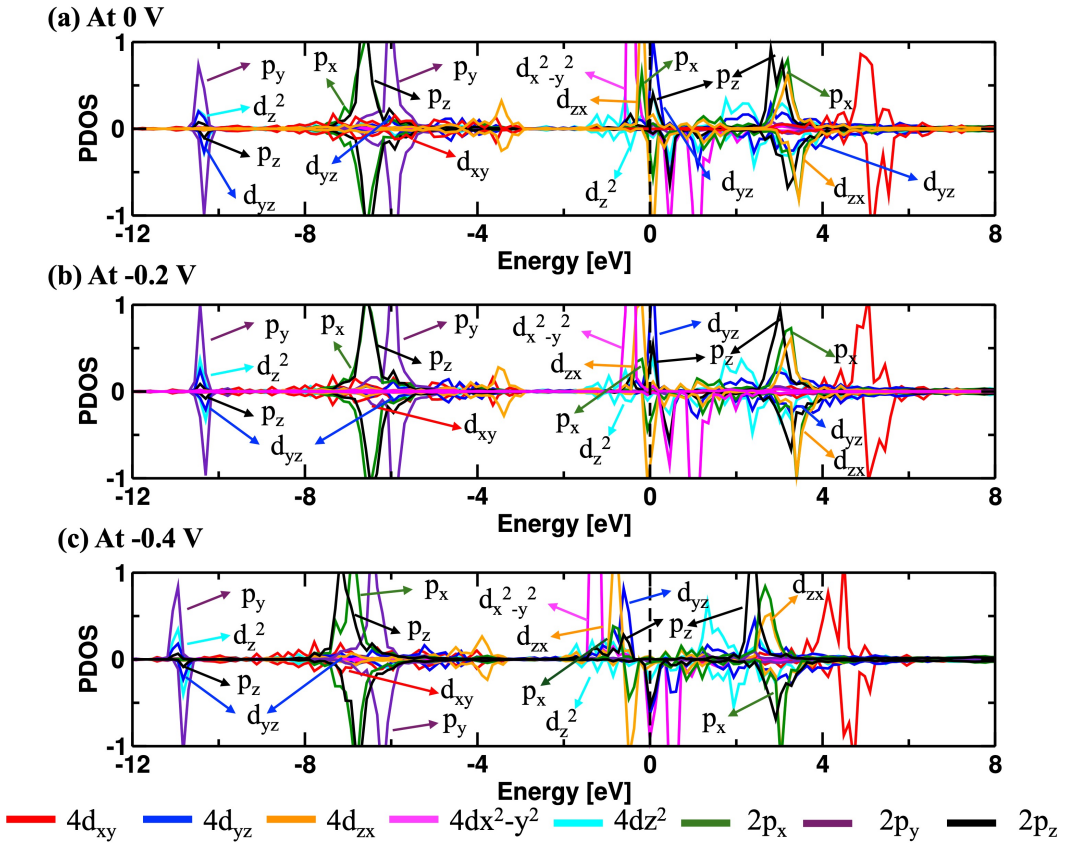

Figure S11. The Orbital-wise PDOS analysis of the $*N_2$ with Metal (Mo) in end-on configuration at (a) 0 V, (b) -0.2 V, and (c) -0.4 V vs RHE.

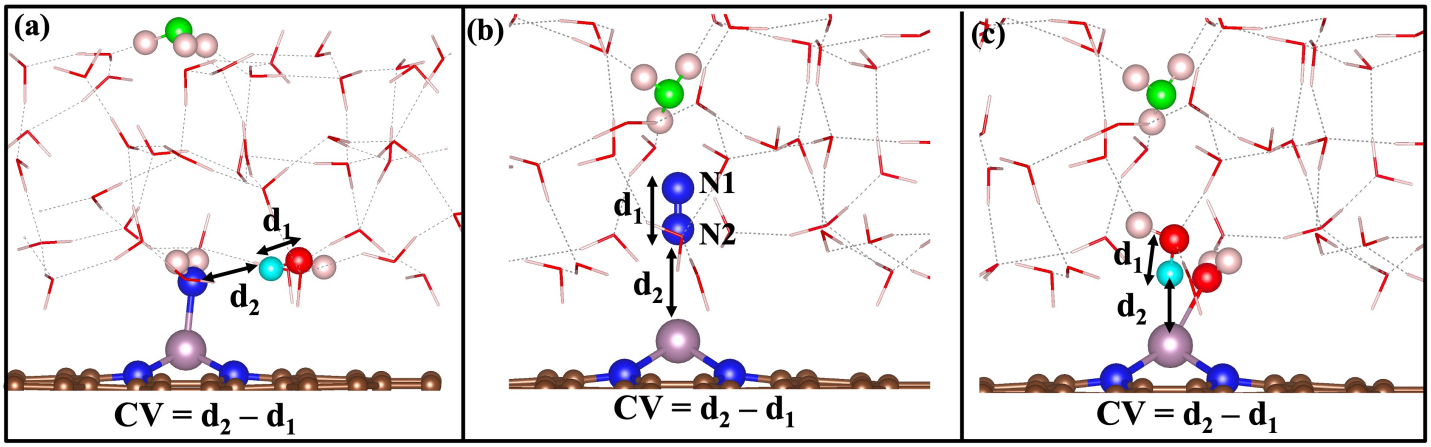

Figure S12. (a) The snapshots of the collective variable (CV) for the slow growth for (a) *NH_2 protonation (b) *N_2 adsorption, and (c) *H adsorption at 0, -0.2, and -0.4 V vs RHE in acidic medium with pH=1 on MoN_4/H_2O interface. The H_3O^+ represents the acidic medium shown by green colour, and the transferred proton is represented by cyan colour.

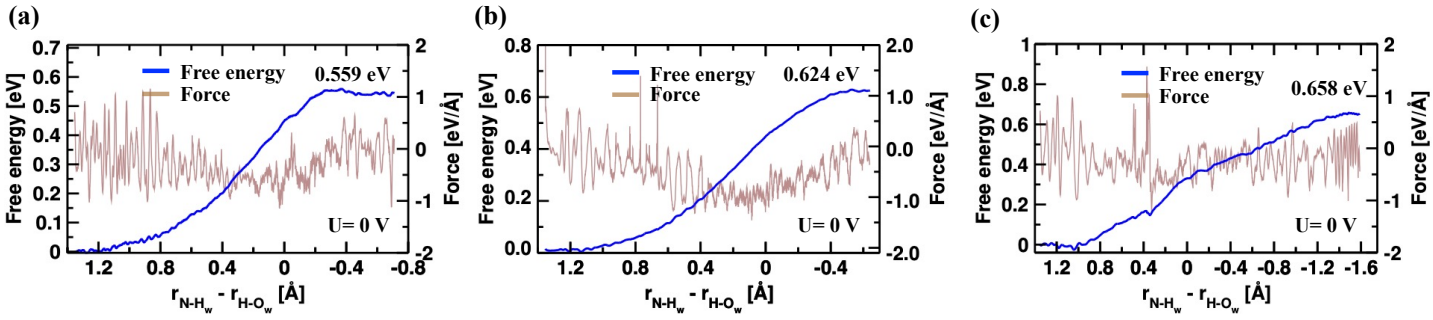

Figure S13. The reaction barrier for (a) *NH_2 protonation at 0 V with (a) pulling speed of 0.0004 Å/time step (given in main manuscript), (b) with pulling speed of 0.0006 Å/time step, and (c) with pulling speed of 0.0008 Å/time step with pH=1 on the MoN_4/H_2O interface. The resulting barrier shows only minor variations within ±0.05 eV.

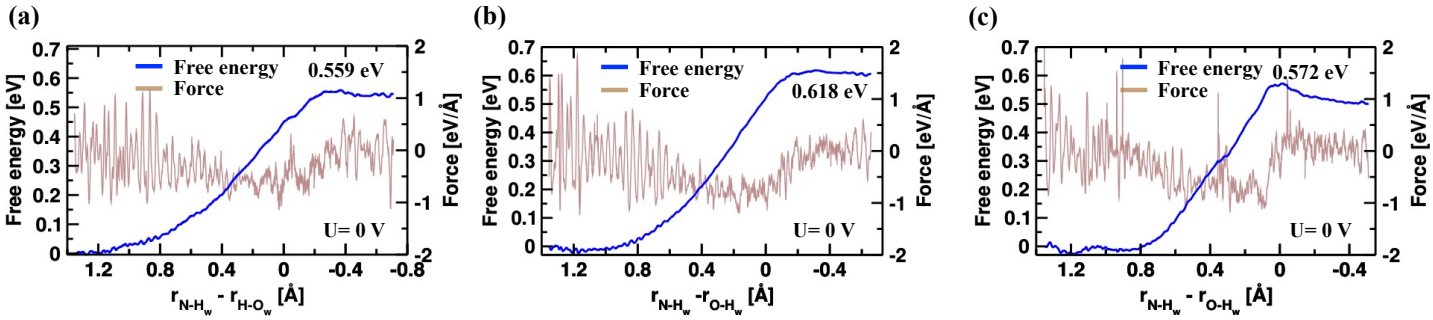

Figure S14. The three independent simulations of the* NH_2 to *NH_3 formation at 0 V, (a) first simulation (provided in main manuscript), (b) second simulation, (c) third simulation at pulling speed of 0.0004 Å/time step. The resulting barrier shows only minor variations within ± 0.03 eV.

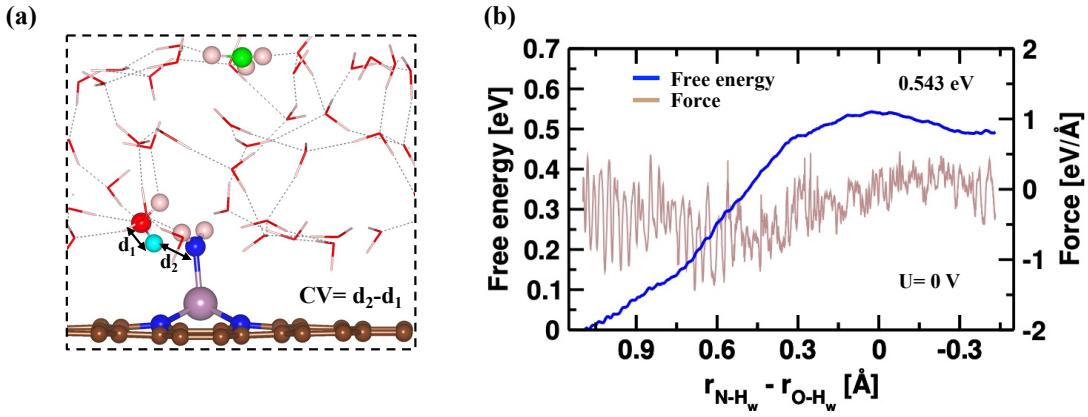

Figure S15. (a) The different initial configurations for the *NH_2 to *NH_3 formation at 0 V, (b) Free energy profiles and the corresponding forces during enhanced sampling along the reaction coordinate of pulling speed of 0.0004 Å/time step.

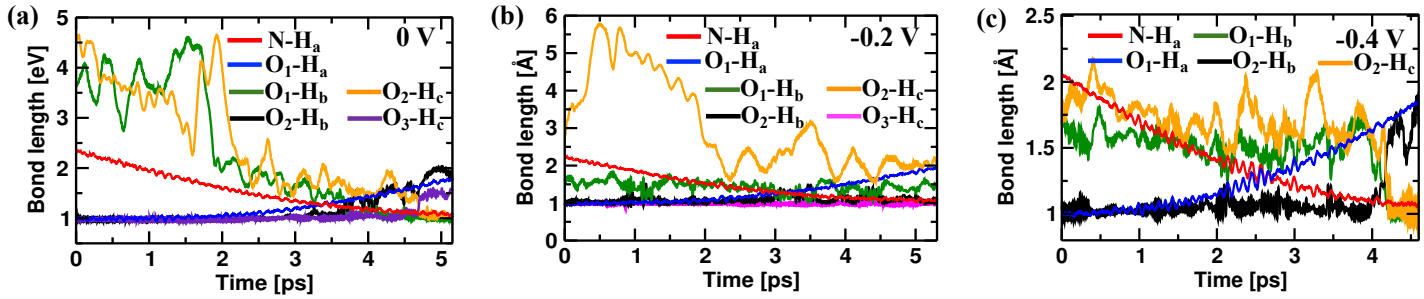

Figure S16. The change in the N-H and O-H bond length with time at applied potential of (a) 0 V, (b) -0.2 V, and (c) -0.4 V vs RHE in acidic medium at MoN_4/H_2O interface.

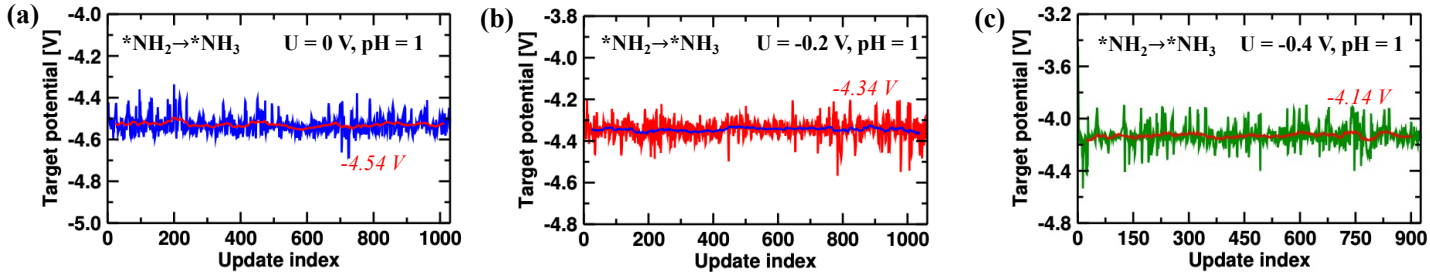

Figure S17. The evolution of the target potential during SG-AIMD simulation of the*NH_2 to *NH_3 formation at (a) 0, (b) -0.2, and (c) -0.4 V vs RHE.

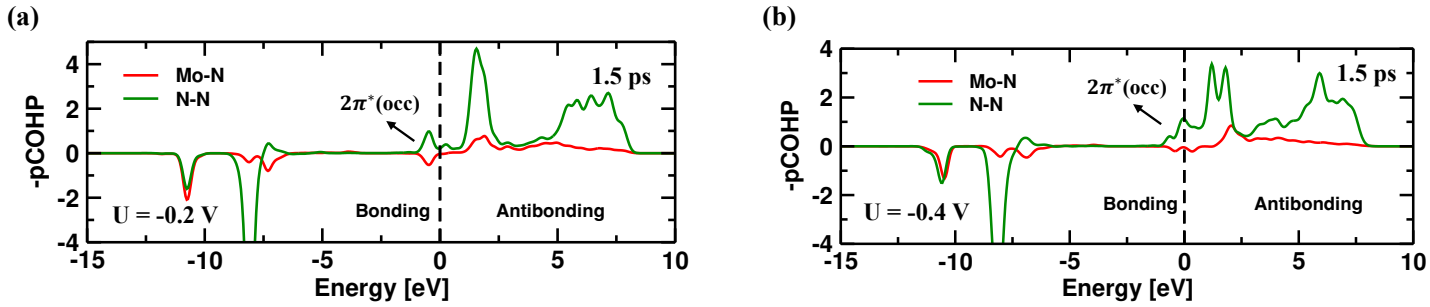

Figure S18. (a) The pCOHP plot of the N_2 adsorption at 1.5 ps with applied potential of -0.2 V vs RHE. (b) The pCOHP plot of the N_2 adsorption at 1.5 ps with applied potential of -0.4 V vs RHE.

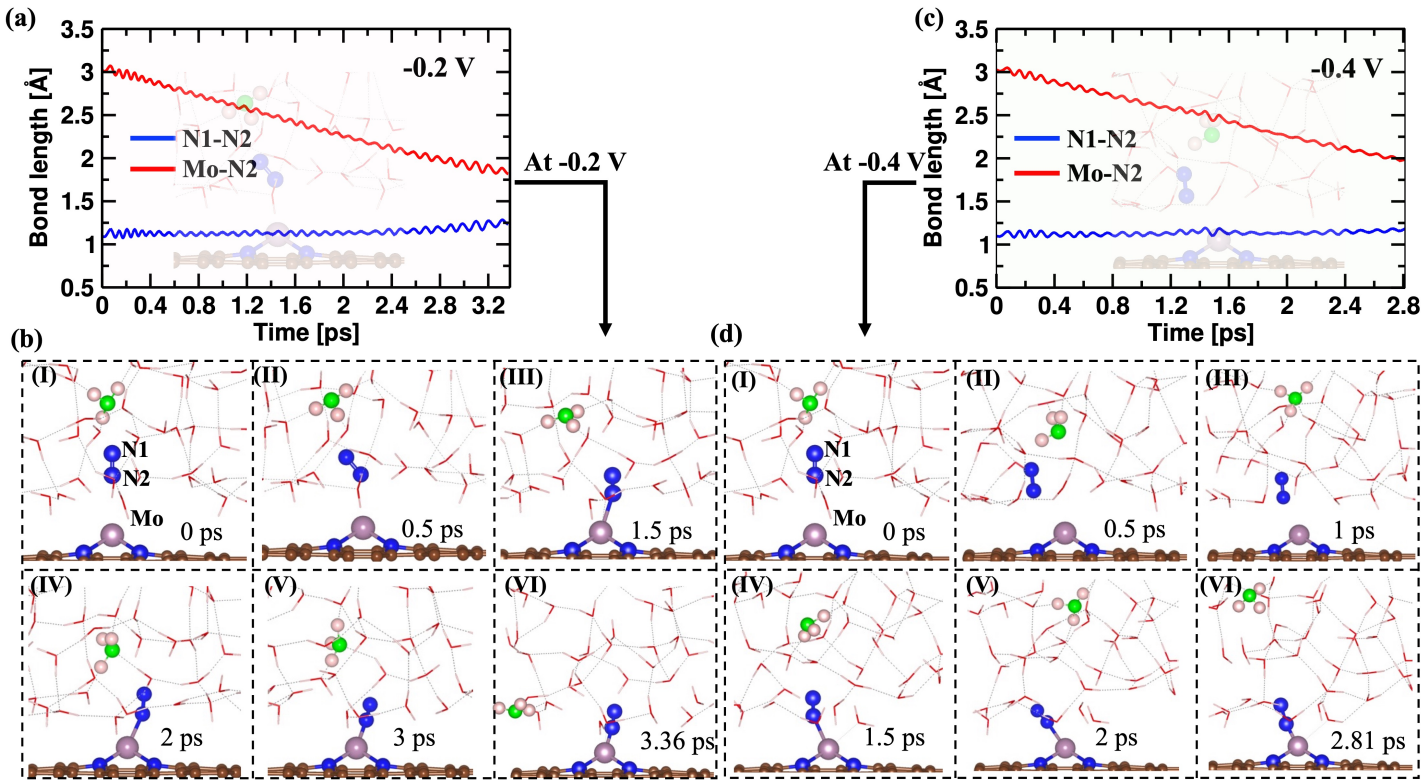

Figure S19. The change in the Mo-N2 and N1-N2 bond length, during the slow growth simulation, with a selective snapshot of *N_2 adsorption at (a) -0.2 and (b) -0.4 V vs RHE.

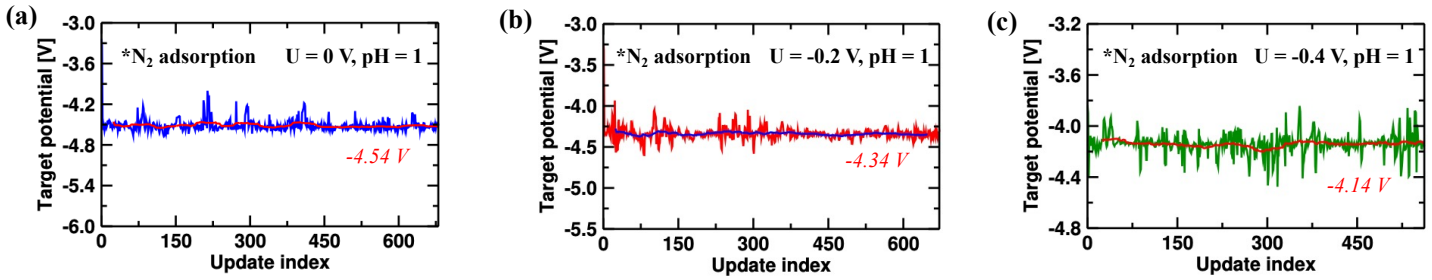

Figure S20. The evolution of the target potential during SG-AIMD simulation of the $*N_2$ adsorption at (a) 0, (b) -0.2, and (c) -0.4 V vs RHE.

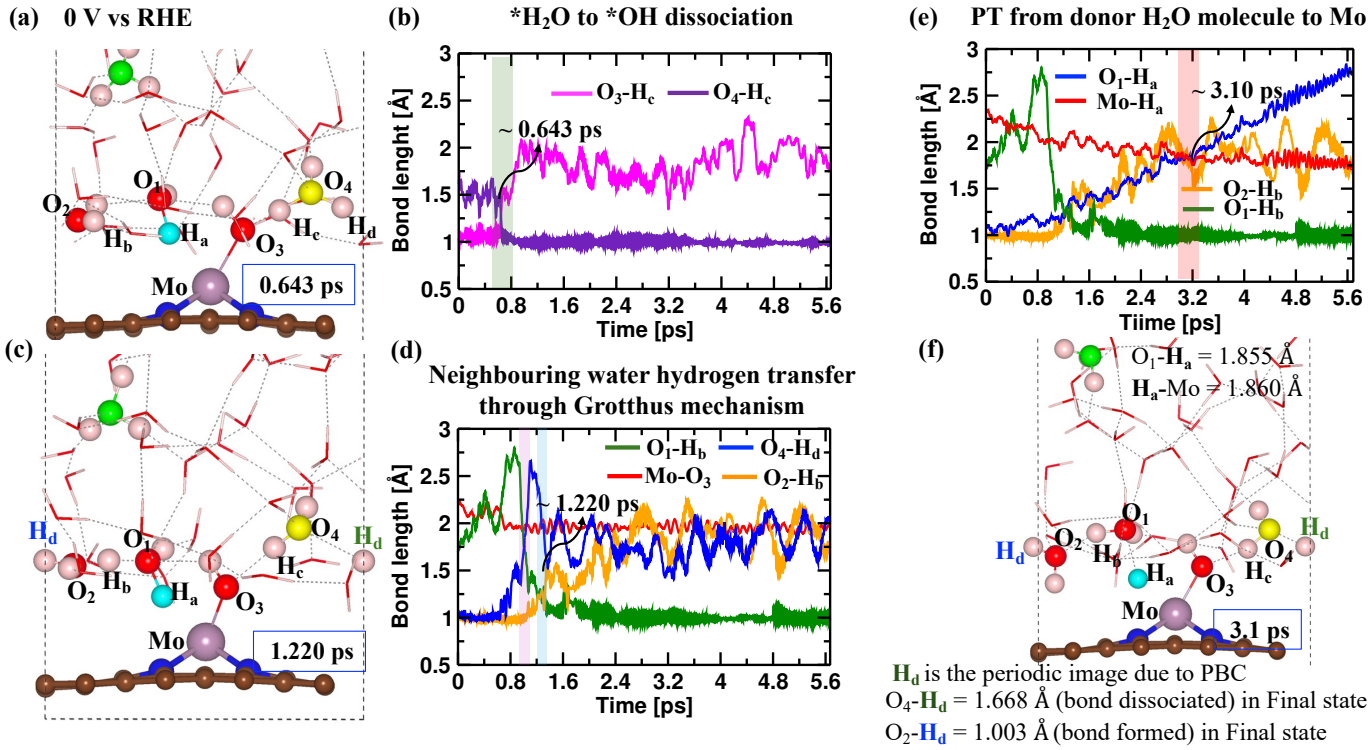

Figure S21. (a) The labeled snapshot at 0 V vs RHE, extracted from SG-AIMD simulation for the *H adsorption, (b) The change in the intermolecular O-H bond length specifically at ~0.650 ps, (c) The labeled snapshot at ~1.220 ps. (d) The change in the bond length of Mo and adsorbed *OH species and other O-H through H-bond network to visualize the time period, PT from H_3O^+, (e) The change in the O-H and Mo-H bond length during the PT at ~3.10 ps (f) The labelled snapshot of PT from water molecule (proton donor) to Mo at ~3.10 ps at 0 V vs RHE in acidic medium.

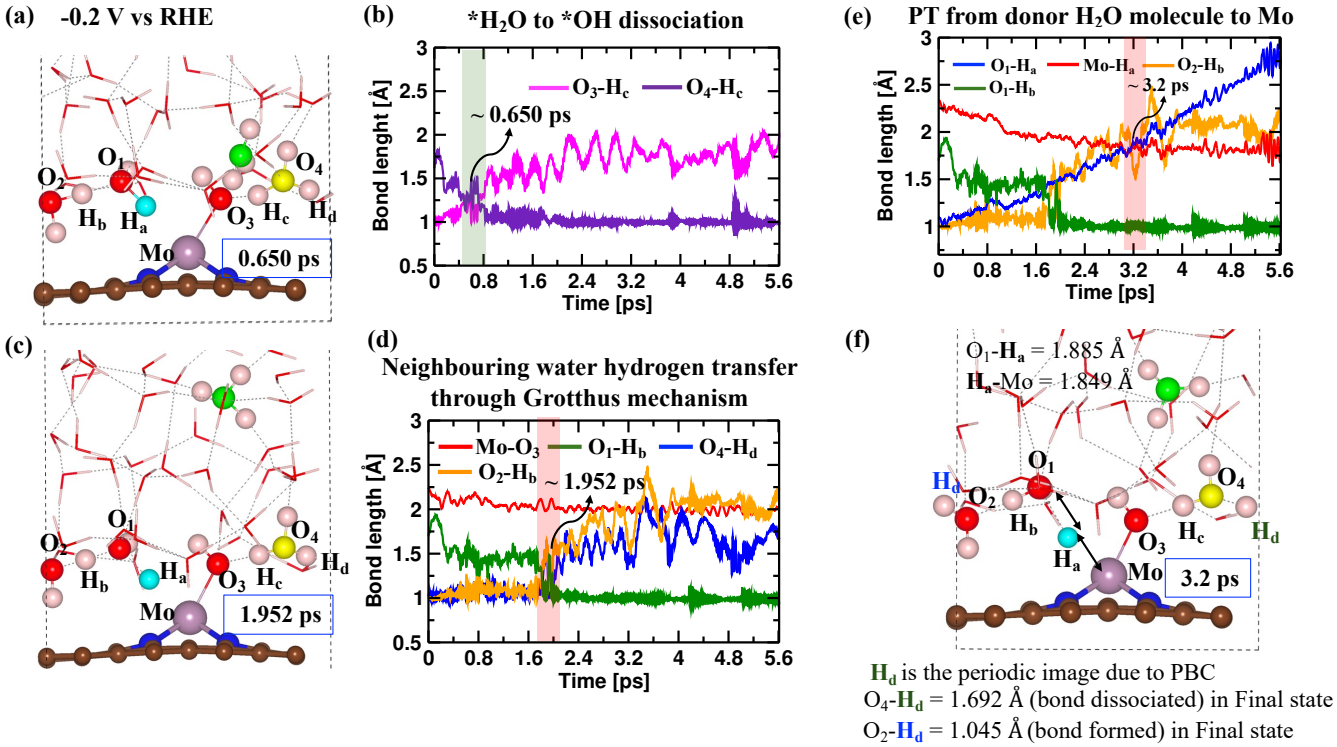

Figure S22. (a) The labeled snapshot at -0.2 V vs RHE, extracted from the SG-AIMD simulation for the *H adsorption (b), The change in the intermolecular O-H bond length specifically at ~0.650 ps, (c) The labeled snapshot at ~1.952 ps. (d) The change in the bond length of Mo and adsorbed *OH species and other O-H through H-bond network to visualize the time period, PT from H_3O^+, (e) The change in the O-H and Mo-H bond length during the PT at ~3.20 ps (f) The labeled snapshot of PT from water molecule (proton donor) to Mo at ~3.20 ps at -0.2 V vs RHE in acidic medium.

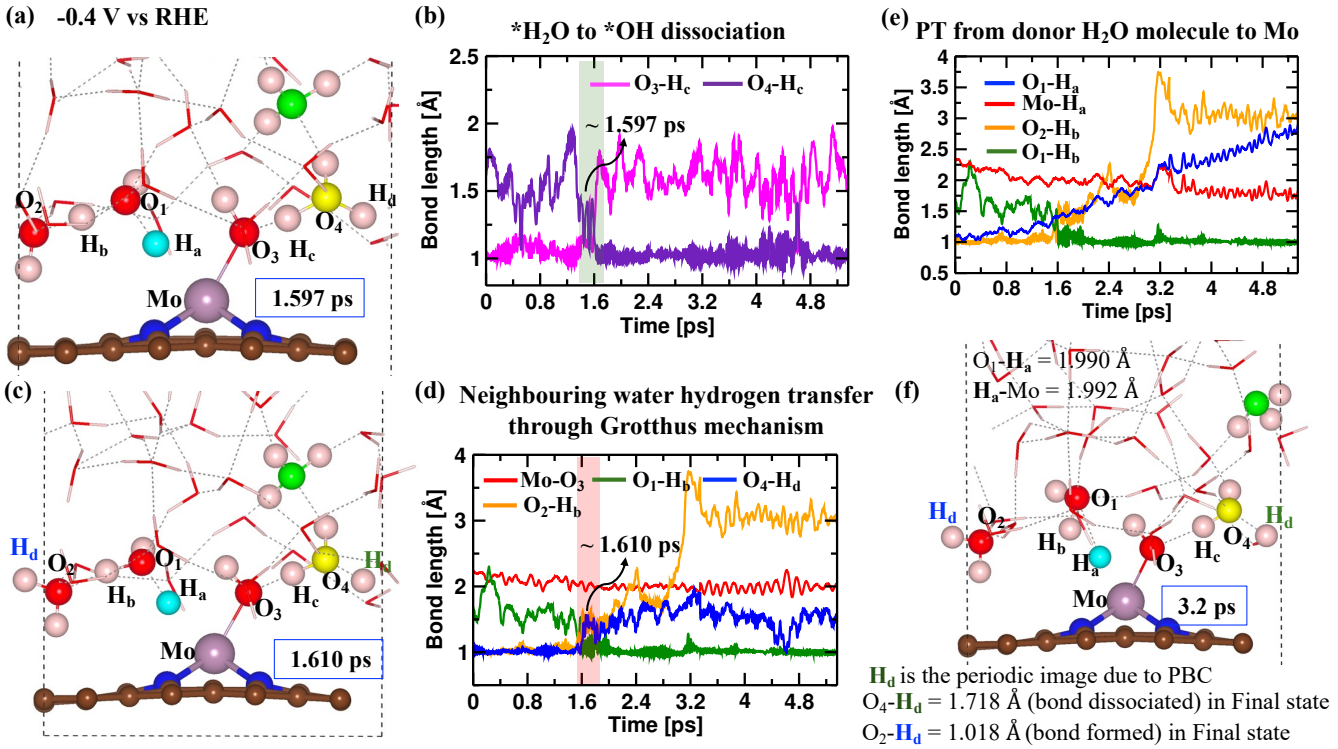

Figure S23. (a) The labeled snapshot at -0.4 V vs RHE extract from SG-AIMD simulation for the *H adsorption, (b) The change in the intermolecular O-H bond length specifically at ~1.597 ps, (c) The labeled snapshot at ~1.610 ps. (d) The change in the bond length of Mo and adsorbed *OH species and other O-H through H-bond network to visualize the time period, PT from H_3O^+, (e) The change in the O-H and Mo-H bond length during the PT at ~3.20 ps (f) The labeled snapshot of PT from water molecule (proton donor) to Mo at ~3.20 ps at -0.4 V vs RHE in acidic medium.

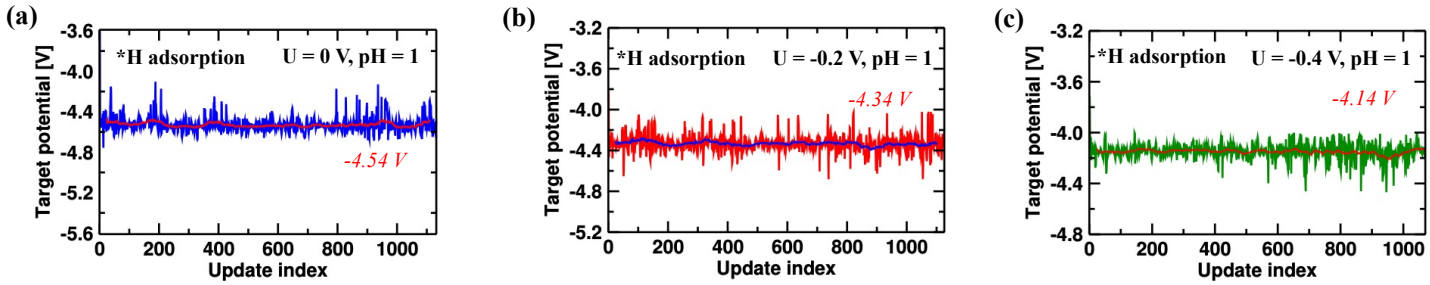

Figure S24. The evolution of the target potential during SG-AIMD simulation of the *H adsorption at (a) 0, (b) -0.2, and (c) -0.4 V vs RHE.

3. Supplementary Tables

Table 1. The MN_4 and MN_3 systems with a range of applied potential and reaction medium were studied through experimental and computational techniques.

Catalysts	References	Potential range (RHE)	medium	Studies

FeN_4	*Nat. Commun.* **2019**, *10,* 1, 341	+0.1 V to -0.4 V	acidic	Exp.
FeN_4	*ACS Catal.* **2022**, 12, 18, 11530–11540	0 to -0.8 V	acidic	Comp.
RuN3	*Adv. Mater.* **2018**, *30,* 40, 1803498	-0.2 to -0.6 V	acidic	Exp.
RuN_4	*ACS Catal.* **2022**, 12, 4, 2505–2512	0, -0.2 V and -0.5 V	acidic	Comp.
MoN_3 and-MoN_3+ vacancy (V_c)	*Small* **2022**, *18* (15), e2106327 *Angew. Chem., Int. Ed.* **2019**, *58* (8), 2321– 2325	0 to -0.2 V -0.15 to -0.45 V	acidic	Exp.
NiN_3	*Small Methods* **2020**, *4* (6), 1900821	-0.3 V (alkaline) and -0.1 V (acidic)	acidic and alkaline	Exp.
NiN_3	ACS Catal. **2025**, 15, 17, 15287–15301	-0.3 V (alkaline) and -0.1 V (acidic)	acidic and alkaline	Comp.
MoN_4	**This Work**	0, -0.2 V and -0.4 V	acidic	Comp.

Table 2. The charge fluctuation at different time steps during the SG-AIMD simulation on $*NH_2$ adsorption on MoN_4/H_2O interface at 0 V vs RHE in acidic medium

Time (ps)	Charge on Mo atom $\|e\|$	Charge of the $H_{transfer}$ $\|e\|$	Charge of the $*NH_2$ $\|e\|$
0	+1.531	+0.425	-1.238
0.5	+1.534	+0.506	-1.325
1	+1.527	+0.532	-1.290
1.5	+1.528	+0.475	-1.239
2	+1.520	+0.437	-1.257
2.5	+1.513	+0.469	-1.297
3	+1.509	+0.462	-1.285
3.5	+1.523	+0.421	-1.254
4	+1.526	+0.418	-1.24
4.5	+1.596	+0.410	-1.211
5	+1.595	+0.399	-1.216
5.1	+1.522	+0.391	-1.209

Table 3. The charge fluctuation at different time steps during the SG-AIMD simulation on $*NH_2$ adsorption on MoN_4/H_2O interface at -0.2 V vs RHE in acidic medium

Time (ps)	Charge on Mo atom $\|e\|$	Charge of the $H_{transfer}$ $\|e\|$	Charge of the $*NH_2$ $\|e\|$
0	+1.578	+0.643	-1.314
0.5	+1.562	+0.670	-1.267
1	+1.540	+0.659	-1.281
1.5	+1.635	+0.626	-1.321
2	+1.692	+0.597	-1.323

2.5	+1.621	+0.585	-1.297
3	+1.644	+0.604	-1.275
3.5	+1.601	+0.553	-1.324
4	+1.544	+0.545	-1.310
4.5	+1.564	+0.541	-1.307
5	+1.574	+0.525	-1.339
5.3	+1.599	+0.498	-1.380

Table 4. The charge fluctuation at different time steps during the SG-AIMD simulation on $*NH_2$ adsorption on MoN_4/H_2O interface at -0.4 V vs RHE in acidic medium

Time (ps)	Charge on Mo atom |*e*|	Charge of the $H_{transfer}$ |*e*|	Charge of the $*NH_2$ |*e*|
0	+1.602	+0.706	-1.439
0.5	+1.600	+0.663	-1.422
1	+1.592	+0.644	-1.386
1.5	+1.609	+0.630	-1.387
2	+1.590	+0.604	-1.366
2.5	+1.582	+0.561	-1.407
3	+1.589	+0.509	-1.433
3.5	+1.593	+0.551	-1.467
4	+1.576	+0.581	-1.446
4.6	+1.566	+0.531	-1.411

Table 5. The charge fluctuation at different time steps during the SG-AIMD simulation on $*N_2$ adsorption on MoN_4/H_2O interface at 0 V vs RHE in acidic medium.

Time (ps)	Charge on Mo atom |*e*|	Charge of the N(2) |*e*|	Charge of the N(1) |*e*|
0	+1.306	-0.893	+0.783
0.5	+1.473	-0.594	+0.361
1	+1.460	0.194	-0.645
1.5	+1.511	0.135	-0.496
2	+1.534	0.075	-0.498
2.5	+1.579	0.016	-0.505
3	+1.562	-0.430	-0.515
3.4	+1.593	-0.531	-0.533

Table 6. The charge fluctuation at different time steps during the SG-AIMD simulation on $*N_2$ adsorption on MoN_4/H_2O interface at -0.2 V vs RHE in acidic medium.

Time (ps)	Charge on Mo atom |*e*|	Charge of the N(2) |*e*|	Charge of the N(1) |*e*|
0	+1.39	-0.887	+0.779
0.5	+1.425	-0.899	+0.695
1	+1.371	-0.751	+0.410

1.5	+1.525	-0.709	+0.151
2	+1.471	-0.618	+0.151
2.5	+1.442	-0.630	-0.096

Table 7. The charge fluctuation at different time steps during the SG-AIMD simulation on $*N_2$ adsorption on MoN_4/H_2O interface at -0.4 V vs RHE in acidic medium.

Time (ps)	Charge on Mo atom $\|e\|$	Charge of the N(2) $\|e\|$	Charge of the N(1) $\|e\|$
0	+1.478	-0.890	+0.781
0.5	+1.572	-0.852	+0.583
1	+1.565	-0.849	+0.446
1.5	+1.592	-0.768	+0.315
2	+1.584	-0.707	-0.047
2.5	+1.573	-0.721	-0.113
2.81	+1.608	-0.658	-0.186

Table 8. The charge fluctuation at different time steps during the SG-AIMD simulation on *H adsorption on MoN_4/H_2O interface at 0 V vs RHE in acidic medium.

Time (ps)	Charge on Mo atom $\|e\|$	Charge of the *OH $\|e\|$	Charge of the $H_{transfer}$ $\|e\|$
0	+1.331	-1.369	+0.429
0.5	+1.340	-1.319	+0.427
1	+1.495	-1.144	+0.354
1.5	+1.496	-1.212	+0.176
2	+1.525	-1.225	+0.01
2.5	+1.566	-1.175	-0.068
3	+1.580	-1.166	-0.141
3.5	+1.593	-1.158	-0.206
4	+1.611	-1.176	-0.283
4.5	+1.607	-1.171	-0.357
5	+1.577	-1.162	-0.258
5.5	+1.686	-1.172	-0.314
5.65	+1.635	-1.214	-0.354
3	+1.479	-0.691	-0.142
3.36	+1.512	-0.678	-0.294

Table 9. The charge fluctuation at different time steps during the SG-AIMD simulation on *H adsorption on MoN_4/H_2O interface at -0.2 V vs RHE in acidic medium.

Time (ps)	Charge on Mo atom $\|e\|$	Charge of the *OH $\|e\|$	Charge of the $H_{transfer}$ $\|e\|$
0	+1.411	-1.399	+0.461
0.5	+1.437	-1.338	+0.375
1	+1.362	-1.272	+0.347

1.5	+1.409	-1.326	+0.167
2	+1.490	-1.221	+0.008
2.5	+1.507	-1.142	-0.157
3	+1.501	-1.181	-0.270
3.5	+1.583	-1.223	-0.382
4	+1.548	-1.200	-0.427
4.5	+1.493	-1.228	-0.371
5	+1.549	-1.252	-0.404
5.35	+1.553	-1.269	-0.408
5.65	+1.599	-1.285	-0.419

Table 10. The charge fluctuation at different time steps during the SG-AIMD simulation on *H adsorption on MoN_4/H_2O interface at -0.4 V vs RHE in acidic medium.

Time (ps)	Charge on Mo atom |*e*|	Charge of the *OH |*e*|	Charge of the $H_{transfer}$ |*e*|
0	+1.340	-1.369	+0.485
0.5	+1.352	-1.300	+0.400
1	+1.474	-1.212	+0.251
1.5	+1.440	-1.265	+0.140
2	+1.531	-1.332	-0.031
2.5	+1.674	-1.262	-0.118
3	+1.698	-1.203	-0.171
3.5	+1.737	-1.284	-0.300
4	+1.724	-1.182	-0.298
4.5	+1.726	-1.158	-0.321
5	+1.778	-1.217	-0.353
5.35	+1.758	-1.283	-0.449

4. Video files of the studied reaction

Video S1. The AIMD trajectory of the Mo leaching from the N-doped graphene surface at 0.0 V vs RHE
Video S2. The AIMD trajectory of the *NH_2 protonation at 0.0 V vs RHE in acidic medium
Video S3. The AIMD trajectory of the *NH_2 protonation at -0.2 V vs RHE in acidic medium
Video S4. The AIMD trajectory of the *NH_2 protonation at -0.4 V vs RHE in acidic medium
Video S5. The AIMD trajectory of the *N_2 adsorption at 0.0 V vs RHE in acidic medium
Video S6. The AIMD trajectory of the *N_2 adsorption at -0.4 V vs RHE in acidic medium
Video S7. The AIMD trajectory of the *H adsorption at 0.0 V vs RHE in acidic medium
Video S8. The AIMD trajectory of the *H adsorption at -0.2 V vs RHE in acidic medium
Video S9. The AIMD trajectory of the *H adsorption at -0.4 V vs RHE in acidic medium

5. References

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The coordinates of Mo leaching on the MoN_4/H_2O interface during the SG-AIMG

At 0 V vs RHE

C
1.0
9.824384 0.0 0.0
0.0 12.762371 0.0
0.0 0.0 25.5
C N Mo O H He
42 4 1 40 80 1
Direct
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At -0.2 V vs RHE

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0.67239179 0.90582075 0.39636240
0.71766505 -0.01391146 0.43646517
0.62965429 0.15632385 0.25909846
0.62870911 0.24568903 0.33896561
0.47006297 0.95629456 0.19952982
0.35310045 0.02940571 0.18383272
0.34711598 0.64280362 0.33950276
0.38470298 0.59583742 0.39778115
0.92611772 0.47870521 0.35833971
0.87400171 0.58583339 0.37570097
0.11443284 1.00970286 0.18056053
0.18324977 0.07687967 0.13757106
1.03192911 0.84201448 0.19969727
0.93361098 0.90286118 0.16135971
0.31271179 0.54944057 0.18478916
0.22506773 0.43764293 0.17647263
0.08904223 0.10867426 0.45110186
0.05604674 -0.00384663 0.47299092
0.36870774 0.52807895 0.48643881
0.42042640 0.43789369 0.44753609
1.02537007 0.72794938 0.25129609
0.12625521 0.82095949 0.25851660
0.93692757 0.16240164 0.39510103
1.02270724 0.26922139 0.40661806
0.61638121 0.50336428 0.47457750
0.74131206 0.50860955 0.51523390
0.44962196 0.21969579 0.16312766
0.52030780 0.26452315 0.21900974
0.07311800 0.38394263 0.12088923
0.06993068 0.34000004 0.17664356
0.23118948 0.64386737 0.26659674
0.28615972 0.53233180 0.26149239
0.41531073 0.35736557 0.37458640
0.35947484 0.27268812 0.40621474
0.61390701 0.78496843 0.22203340
0.74471863 0.75324718 0.26066990
0.57741037 0.23780097 0.53153729
0.57534190 0.15873777 0.57743683
0.49545193 0.43193776 0.55000000

At -0.4 V vs RHE

Frame 683 extracted from XDATCAR
1.0
9.824384 0.0 0.0
0.0 12.762371 0.0
0.0 0.0 25.5
C N Mo O H He
42 4 1 40 80 1
Direct
0.12170330 0.31902779 0.04095263
0.12286877 0.65275731 0.04205020
0.12433451 0.98599241 0.04273894
0.37050883 0.64812565 0.05190071
0.37502911 0.98665844 0.04713208
0.62662565 0.64812565 0.05190071
0.62210425 0.98665844 0.04713208
0.87542995 0.31902779 0.04095263
0.87426540 0.65275731 0.04205020
0.87279864 0.98599241 0.04273894
0.12289117 0.20775850 0.04214176
0.12172784 0.54144242 0.04089157
0.12433665 0.87453193 0.04270788
0.37053326 0.21237355 0.05197314
0.37500865 0.87387391 0.04710267
0.62660010 0.21237355 0.05197314
0.62212552 0.87387391 0.04710267
0.87424219 0.20775850 0.04214176
0.87540552 0.54144242 0.04089157
0.87279793 0.87453193 0.04270788
0.99856693 0.15210113 0.04118694
0.99856693 0.48543182 0.03793733
0.99856693 0.81974572 0.04190933

0.24862841 0.15363603 0.04551278
0.24346056 0.48654682 0.04794792
0.24972161 0.81868808 0.04476129
0.49856673 0.15832176 0.05229408
0.49856673 0.81565581 0.04898659
0.74850606 0.15363603 0.04551278
0.75367280 0.48654682 0.04794792
0.74741276 0.81868808 0.04476129
0.99856693 0.04077957 0.04196314
0.99856693 0.37503776 0.03797400
0.99856693 0.70842792 0.04110027
0.24973169 0.04180156 0.04481710
0.24344946 0.37398153 0.04797357
0.24864969 0.70687727 0.04543039
0.49856673 0.04486807 0.04904224
0.49856673 0.70218692 0.05221804
0.74740157 0.04180156 0.04481710
0.75368390 0.37398153 0.04797357
0.74848469 0.70687727 0.04543039
0.36177535 0.31960911 0.05808553
0.63535902 0.31960911 0.05808553
0.63534060 0.54092848 0.05803294
0.36179266 0.54092848 0.05803294
0.49172265 0.42238646 0.14713869
0.04624713 0.85098289 0.32633918
0.13928218 0.02285127 0.28982975
0.79320301 0.47433300 0.24352671
0.58624315 0.02453935 0.17094374
0.51731571 0.31943231 0.19096379
0.80819234 0.07634700 0.38059360
0.53992548 0.82528834 0.22446643
0.94082310 0.14369385 0.29929792
0.63231729 0.16386944 0.60300045
0.59595499 0.27893727 0.31565389
0.29651219 0.82262663 0.16861211
0.46982608 0.47514452 0.33601207
0.17727783 0.64483875 0.20333672
0.36756431 0.04006386 0.39791237
0.12985865 0.91293411 0.42163516
0.87485375 0.78821739 0.47203058
0.34147887 0.14020739 0.29778361
0.20768407 0.34945770 0.31041148
0.78266186 0.15587222 0.19773013
0.75025200 0.32773114 0.41221753
0.94693431 0.58514029 0.16950344
0.37290137 0.13251525 0.57079906
0.39210233 0.15546281 0.20177765
0.10920681 -0.01395530 0.18583208
0.12506513 0.69823791 0.45121088
0.88550643 0.48530850 0.33393566
0.87757356 0.90927607 0.22592290
0.76799379 0.75152954 0.16979084
0.44548926 0.53661498 0.18306850
0.92375505 0.99047655 0.50256538
0.34941955 0.62474910 0.49614997
0.15114357 0.69549441 0.29563706
0.75768582 0.19112730 0.48690022
0.59748275 0.96543790 0.33350111
0.02408453 0.16587309 0.16537861
0.15636516 0.36163695 0.20728861
0.13940478 0.55084288 0.36713629
0.49124378 0.42623072 0.43930370
0.60923630 0.61256850 0.25162356
0.42739745 0.19314169 0.46634151
0.07914330 0.91176554 0.30654839
0.06453869 0.86616213 0.36304737
0.14883933 0.01083654 0.25133462
0.05171293 0.07395190 0.29545648
0.85760411 0.46353222 0.29879677
0.74729498 0.41879342 0.22843917
0.57478575 0.88831468 0.20639997
0.59398021 0.00103712 0.13459036
0.44777616 0.22785706 0.19773560
0.74860468 0.22773992 0.19834157
0.74494801 0.12891143 0.39383544
0.74490788 0.02213008 0.36454551
0.34655164 0.04840895 0.56693068
0.62095517 0.68911114 0.40287190
0.88056479 0.11659196 0.32822249
0.88447809 0.14381013 0.26819595
0.14612975 0.84769402 0.44096909
0.63326869 0.68682081 0.25503765
0.55872282 0.21030845 0.32371543
0.65303360 0.29394232 0.34664670
0.31691698 0.80909773 0.13246145
0.44534283 0.81583065 0.20864546
0.50635409 0.40952265 0.31970152
0.51066413 0.52506783 0.30909698
0.09872293 0.61075607 0.18705956
0.24885906 0.75418315 0.18132945
0.40459310 0.13881595 0.43816545
0.51854845 0.95991952 0.35529318
0.06750476 0.94962686 0.44539468
0.27786602 1.00650719 0.40488229
0.80468374 0.73484075 0.46726822
-0.03543178 0.74920454 0.47557847
0.35554781 0.07781470 0.36235236
0.25463058 0.09863847 0.29573246
0.29871000 0.21416423 0.30133641
0.11435404 0.33641433 0.32312470
0.87396935 0.16146587 0.17860437
0.66547996 0.07515503 0.17688529
0.67087557 0.36310369 0.42321202
0.77637852 0.27624034 0.44163111
0.90261451 0.52985256 0.19320301
0.93467594 0.55789990 0.13383843
0.54798136 0.12377611 0.59731741
0.59142732 0.21685246 0.62514363
0.46541760 0.09989688 0.18966027
0.37190544 0.14527482 0.24296481
0.17321796 0.92959473 0.17441139
0.01961173 0.95402192 0.19835116
0.11365228 0.65941452 0.41633096
0.21214239 0.66996068 0.46702245
0.85037290 0.44430753 0.36235562
0.04671002 0.51385518 0.35525243
0.84393694 0.84495995 0.20638427
0.88913498 0.87846049 0.26074837
0.80744583 0.68101006 0.16596040
0.66808049 0.74881629 0.17083352
0.24724970 0.58766820 0.20462822
0.23258387 0.37523423 0.18272533
0.88077965 0.92326328 0.49065805
-0.09142429 0.99138816 0.54050569

0.30434945 0.58313142 0.52309721
0.40021060 0.57019567 0.48089305
0.15034597 0.66979670 0.25700517
0.09031674 0.76997295 0.30836790
0.81499830 0.12869237 0.48581427
0.73482274 0.20331244 0.52394045
0.57523011 0.93482692 0.29841212
0.65042718 0.63542747 0.39708511
0.03329483 0.17731091 0.12744490
0.06669357 0.08980950 0.17048483
0.11574991 0.29423590 0.19525868
0.19459279 0.35875159 0.27140324
0.15992515 0.63752883 0.32392427
0.21407871 0.50418767 0.35279693
0.49141119 0.44677741 0.40014332
0.45854915 0.35767733 0.43945465
0.53064137 0.60741791 0.23028922
0.72540443 0.53983380 0.24875574
0.52526479 0.19195205 0.47003582
0.39538547 0.15252524 0.53534160
0.49545193 0.43193776 0.55000000

The Intial coordinates of the *NH_2 on the MoN_4/H_2O interface during the SG-AIMG

At 0 V vs RHE

C
1.0
9.824384 0.0 0.0
0.0 12.762371 0.0
0.0 0.0 25.0
C N Mo H O
42 5 1 83 40
Selective dynamics
Cartesian
1.128620 3.571834 1.123043 F F F
1.139290 7.831985 1.173802 F F F
1.153170 12.086745 1.216262 F F F
3.578231 7.767404 1.404418 F F F
3.615151 12.096142 1.329628 F F F
6.082321 7.767404 1.404418 F F F
6.045401 12.096142 1.329628 F F F
8.531930 3.571834 1.123043 F F F
8.521249 7.831985 1.173802 F F F
8.507382 12.086745 1.216262 F F F
1.139320 2.156674 1.173241 F F F
1.128741 6.416654 1.123642 F F F
1.153220 10.664243 1.216145 F F F
3.578231 2.221464 1.402227 F F F
3.615212 10.654943 1.329783 F F F
6.082321 2.221464 1.402227 F F F
6.045340 10.654943 1.329783 F F F
8.521232 2.156674 1.173241 F F F
8.531809 6.416654 1.123642 F F F
8.507321 10.664243 1.216145 F F F
9.742464 1.444994 1.160057 F F F
9.742464 5.700932 1.049884 F F F
9.742464 9.966444 1.191449 F F F
2.380030 1.467324 1.269097 F F F
2.330011 5.706925 1.268651 F F F
2.387990 9.947744 1.267566 F F F
4.830271 1.527073 1.425394 F F F
4.830271 9.913444 1.371458 F F F
7.280521 1.467324 1.269097 F F F
7.330538 5.706925 1.268651 F F F
7.272561 9.947744 1.267566 F F F
9.742464 0.022247 1.191690 F F F
9.742464 4.287605 1.049792 F F F
9.742464 8.543544 1.160052 F F F
2.388030 0.040930 1.267375 F F F
2.330181 4.281594 1.267675 F F F
2.380181 8.521294 1.270158 F F F
4.830271 0.075401 1.370925 F F F
4.830271 8.461704 1.427069 F F F
7.272511 0.040930 1.267375 F F F
7.330362 4.281594 1.267675 F F F
7.280360 8.521294 1.270158 F F F
3.506161 3.602114 1.500305 F F F
6.154389 3.602114 1.500305 F F F
6.154361 6.386294 1.503373 F F F
3.506191 6.386294 1.503373 F F F
4.981054 5.191304 4.222055 T T T
4.830271 4.993834 2.243284 F F F
4.188683 5.310773 4.835322 T T T
5.737650 4.742418 4.793166 T T T
4.223842 5.567493 11.071210 T T T
3.699904 7.836371 10.197899 T T T
0.301700 7.980719 9.996396 T T T
4.094494 6.747138 7.094540 T T T
2.577256 2.822992 10.659494 T T T
3.870119 1.853170 10.825474 T T T
4.386713 9.649922 9.215067 T T T
3.204816 10.060800 10.323192 T T T
5.538097 8.736001 7.649890 T T T
4.503438 9.809992 6.944955 T T T
6.952727 11.901425 9.880279 T T T
7.492731 12.133813 11.352346 T T T
9.445427 3.112794 7.067687 T T T
0.921480 2.559847 6.329221 T T T
5.584325 0.426773 7.530723 T T T
4.234885 0.362531 6.867512 T T T
0.211148 1.065254 7.873501 T T T
0.883702 12.541073 8.074581 T T T
0.862992 7.811609 11.496681 T T T
2.517642 6.868455 10.453638 T T T
3.104920 3.625397 6.355751 T T T
2.105300 3.977899 5.190389 T T T
8.296000 9.723591 8.265149 T T T
0.055303 9.685574 8.147983 T T T
8.410424 4.413616 4.790020 T T T
8.595475 5.819297 4.211810 T T T
8.303833 7.552088 5.982581 T T T
8.657995 7.928978 7.509863 T T T
7.013199 9.173326 11.471720 T T T

5.585143 9.166276 10.854670 T T T
6.788607 2.960403 4.881008 T T T
7.225941 3.471594 6.403158 T T T
8.943346 10.129688 5.039671 T T T
8.663093 11.628534 5.500169 T T T
2.773584 0.142775 5.154758 T T T
2.998577 1.670565 5.393808 T T T
7.102849 0.325391 5.501993 T T T
8.438899 0.778452 6.265362 T T T
7.452527 1.194020 10.432626 T T T
8.223443 2.517205 10.946868 T T T
2.183597 8.074685 3.609596 T T T
1.911765 6.968681 4.772582 T T T
2.710817 10.710830 5.112135 T T T
2.752814 9.192289 5.307881 T T T
6.754415 6.925179 10.818500 T T T
7.637584 5.727948 10.239336 T T T
5.132212 7.461700 4.597252 T T T
4.938149 8.993603 4.644793 T T T
6.968579 2.840375 8.958963 T T T
5.819316 3.591599 8.072959 T T T
3.953500 3.602213 8.737972 T T T
3.834167 5.035203 8.012296 T T T
1.042647 11.323702 10.653730 T T T
2.582384 11.891214 10.594448 T T T
0.619209 11.385077 4.331069 T T T
1.677136 12.310436 3.540273 T T T
4.768138 12.658221 10.831174 T T T
4.305497 0.334824 9.421237 T T T
7.324294 8.313295 4.360230 T T T
8.627565 8.231338 3.509644 T T T
6.545953 6.886554 7.296211 T T T
5.994465 6.661321 8.840497 T T T
0.128483 5.847820 10.633615 T T T
9.259131 4.998018 9.346683 T T T
1.093533 2.024613 9.475813 T T T
0.391200 3.430387 10.068343 T T T
8.968923 10.919999 10.017517 T T T
9.460397 12.287304 9.723163 T T T
5.629723 4.979892 11.082689 T T T
4.117443 3.824935 11.156139 T T T
0.400659 5.269270 4.990575 T T T
1.345995 5.665993 6.170737 T T T
5.177453 0.936569 4.411985 T T T
6.399837 0.911751 3.433204 T T T
1.707420 10.953888 8.685999 T T T
2.023133 10.565886 7.095100 T T T
6.485504 10.574099 7.860015 T T T
7.626365 11.770970 7.728229 T T T
8.653830 5.753823 7.454430 T T T
7.889838 4.386948 8.146916 T T T
3.148380 6.696850 8.361821 T T T
3.461702 6.871315 10.178079 T T T
3.165040 6.508910 7.386408 T T T
3.524045 2.799655 10.815070 T T T
4.129603 9.478168 10.121696 T T T
5.201458 9.671278 7.642152 T T T
6.789316 12.444882 10.688689 T T T
9.814246 2.292778 6.667735 T T T
4.703814 0.109432 7.761352 T T T
0.330659 0.411091 8.587236 T T T
0.978647 7.464751 10.554573 T T T
2.477540 3.227776 5.774495 T T T
9.093203 9.132239 8.420671 T T T
9.075970 4.978661 4.292787 T T T
8.211986 7.237966 6.916440 T T T
6.487763 8.762032 10.761164 T T T
7.095023 3.731041 5.401628 T T T
9.041144 11.026124 4.800621 T T T
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7.803946 12.761845 6.175828 T T T
7.803222 2.072673 10.163658 T T T
2.155882 7.958213 4.557656 T T T
3.106696 10.025327 5.716669 T T T
6.757795 6.031436 10.366184 T T T
5.572494 8.272719 4.832142 T T T
6.766259 3.328479 8.138795 T T T
4.106859 4.047019 7.917650 T T T
2.031513 11.097975 10.393623 T T T
1.535340 11.885290 4.427272 T T T
4.023368 0.337910 10.452355 T T T
8.298371 8.313534 4.443306 T T T
5.768717 6.744175 7.874532 T T T
9.485772 4.978083 10.356025 T T T
1.125982 2.758023 10.163505 T T T
9.390659 11.619946 10.486633 T T T
4.710987 4.788533 11.493843 T T T
1.437996 5.403635 5.205954 T T T
6.119475 1.139707 4.293877 T T T
1.345203 10.902318 7.725468 T T T
7.311974 11.019897 8.295527 T T T
8.772881 4.837497 7.872806 T T T

At -0.2 V vs RHE

C
1.0
9.824384 0.0 0.0
0.0 12.762371 0.0
0.0 0.0 25.0
C N Mo H O
42 5 1 83 40
Selective dynamics
Cartesain
1.128620 3.571834 1.123043 F F F
1.139290 7.831985 1.173802 F F F
1.153170 12.086745 1.216262 F F F
3.578231 7.767404 1.404418 F F F
3.615151 12.096142 1.329628 F F F
6.082321 7.767404 1.404418 F F F
6.045401 12.096142 1.329628 F F F
8.531930 3.571834 1.123043 F F F
8.521249 7.831985 1.173802 F F F
8.507382 12.086745 1.216262 F F F
1.139320 2.156674 1.173241 F F F
1.128741 6.416654 1.123642 F F F
1.153220 10.664243 1.216145 F F F
3.578231 2.221464 1.402227 F F F
3.615212 10.654943 1.329783 F F F
6.082321 2.221464 1.402227 F F F
6.045340 10.654943 1.329783 F F F
8.521232 2.156674 1.173241 F F F
8.531809 6.416654 1.123642 F F F
8.507321 10.664243 1.216145 F F F

9.742464 1.444994 1.160057 F F F
9.742464 5.700932 1.049884 F F F
9.742464 9.966444 1.191449 F F F
2.380030 1.467324 1.269097 F F F
2.330011 5.706925 1.268651 F F F
2.387990 9.947744 1.267566 F F F
4.830271 1.527073 1.425394 F F F
4.830271 9.913444 1.371458 F F F
7.280521 1.467324 1.269097 F F F
7.330538 5.706925 1.268651 F F F
7.272561 9.947744 1.267566 F F F
9.742464 0.022247 1.191690 F F F
9.742464 4.287605 1.049792 F F F
9.742464 8.543544 1.160052 F F F
2.388030 0.040930 1.267375 F F F
2.330181 4.281594 1.267675 F F F
2.380181 8.521294 1.270158 F F F
4.830271 0.075401 1.370925 F F F
4.830271 8.461704 1.427069 F F F
7.272511 0.040930 1.267375 F F F
7.330362 4.281594 1.267675 F F F
7.280360 8.521294 1.270158 F F F
3.506161 3.602114 1.500305 F F F
6.154389 3.602114 1.500305 F F F
6.154361 6.386294 1.503373 F F F
3.506191 6.386294 1.503373 F F F
4.669547 4.871287 4.138152 T T T
4.830271 4.993834 2.243284 F F F
4.035429 5.120059 4.874871 T T T
5.527261 4.391745 4.407274 T T T
3.567487 5.982601 10.619231 T T T
3.580547 7.626901 10.146197 T T T
0.354387 8.140995 9.914947 T T T
4.392831 6.475414 7.216400 T T T
2.575733 2.671977 10.783651 T T T
3.913813 1.839621 10.850649 T T T
4.346034 9.309323 9.047894 T T T
3.695541 9.764318 10.380518 T T T
5.774829 8.611197 7.700604 T T T
4.910015 9.428389 6.845132 T T T
7.298411 12.011644 9.949283 T T T
7.631176 12.428587 11.475150 T T T
9.090805 2.569533 6.959236 T T T
0.514351 1.901611 6.183040 T T T
5.201379 0.785313 7.494619 T T T
4.033646 12.581609 7.245452 T T T
0.046426 0.802654 7.904786 T T T
1.219933 12.553982 7.960542 T T T
0.716863 7.773427 11.445642 T T T
2.107916 7.012968 10.289472 T T T
2.566174 2.886298 6.524529 T T T
1.734179 3.464301 5.261331 T T T
9.108426 9.626528 8.524079 T T T
0.661085 9.237368 8.027627 T T T
7.861745 3.828621 4.457816 T T T
7.951188 5.261320 3.703119 T T T
8.616232 7.036822 6.079578 T T T
9.050333 7.491789 7.557938 T T T
7.244591 8.984649 11.656424 T T T
6.169279 9.086063 10.502056 T T T
6.548006 1.731355 4.805279 T T T
6.421742 2.838190 5.853713 T T T
9.488158 9.337625 4.828073 T T T
9.330915 10.889931 5.357821 T T T
2.825860 12.478200 4.998046 T T T
3.052617 1.236499 5.253131 T T T
7.520856 12.175643 5.807115 T T T
8.754246 0.154840 6.078494 T T T
7.094902 1.437764 10.374936 T T T
8.283811 2.520813 10.281134 T T T
2.508144 7.628156 3.569962 T T T
2.009031 6.760526 4.651029 T T T
3.420969 10.200404 4.925411 T T T
3.488915 8.797070 5.230723 T T T
7.037986 7.185627 10.454986 T T T
7.669544 5.628038 10.318896 T T T
5.641136 6.866286 4.313175 T T T
5.590447 8.367058 4.883161 T T T
6.086286 2.488552 8.652206 T T T
4.861931 3.130252 7.684308 T T T
3.261679 3.450436 9.021930 T T T
3.293505 4.820600 7.970685 T T T
1.680114 11.432458 10.632607 T T T
3.121995 11.928954 10.318714 T T T
1.346476 10.793595 4.330439 T T T
2.352350 11.490559 3.302051 T T T
5.150384 0.104212 10.815096 T T T
4.454106 0.362847 9.419666 T T T
7.827248 7.724125 4.224390 T T T
9.241076 7.315744 3.715299 T T T
6.886644 6.460256 7.112052 T T T
6.060268 6.401201 8.467238 T T T
9.726179 5.787499 10.316528 T T T
9.198464 4.809700 9.141474 T T T
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0.285709 3.290058 10.566463 T T T
9.275543 10.912493 10.519306 T T T
9.797808 12.158326 9.774619 T T T
5.328115 5.189249 10.704364 T T T
4.121195 4.250681 11.119689 T T T
0.121215 4.941597 4.578099 T T T
0.762799 5.372687 5.914439 T T T
5.143453 12.759080 5.070838 T T T
6.064591 12.255401 3.909144 T T T
2.323319 10.542547 8.826274 T T T
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6.871313 10.504411 8.278152 T T T
7.891860 11.525620 7.911129 T T T
8.385295 4.964785 7.280060 T T T
7.551173 3.682397 7.806540 T T T
3.026713 7.055405 7.452801 T T T
3.105391 6.732232 10.006189 T T T
3.494231 6.425852 6.865007 T T T
3.549676 2.814790 10.672009 T T T
4.306739 9.019626 10.011407 T T T
5.420373 9.514550 7.703599 T T T
7.018671 12.590589 10.739004 T T T
9.459360 1.690823 6.605356 T T T
4.744258 12.719326 7.878948 T T T
0.592370 0.262568 8.561697 T T T
0.737095 7.376279 10.522183 T T T
1.944859 2.664255 5.783802 T T T
9.686717 8.801364 8.500816 T T T
8.351694 4.746763 4.435930 T T T

8.574580 6.740587 6.986637 T T T
7.153972 8.856876 10.686826 T T T
6.710027 2.702104 4.935651 T T T
0.147142 10.170750 5.046904 T T T
3.411856 0.354536 5.490276 T T T
8.468569 12.000427 6.143423 T T T
7.322327 2.355549 10.061801 T T T
2.180619 7.673563 4.496289 T T T
3.982155 9.619450 5.462104 T T T
6.933315 6.252297 10.135940 T T T
6.193816 7.637292 4.570619 T T T
5.721371 2.608697 7.772029 T T T
3.399262 3.818288 8.077450 T T T
2.552723 11.129693 10.288797 T T T
2.253217 11.118877 4.176379 T T T
4.315959 0.342907 10.416188 T T T
8.756214 7.836519 4.402406 T T T
5.922926 6.681299 7.495917 T T T
9.242285 4.958600 10.186550 T T T
0.900922 2.466280 10.555298 T T T
0.058180 11.621176 10.628543 T T T
4.454781 5.174053 11.172837 T T T
1.022188 5.116640 5.028040 T T T
6.104678 12.596441 4.784931 T T T
2.076587 10.044428 7.934656 T T T
7.709586 10.895835 8.660327 T T T
8.464675 4.052662 7.646786 T T T

At -0.4 V vs RHE

C
1.0
9.824384 0.0 0.0
0.0 12.762371 0.0
0.0 0.0 25.0
C N Mo H O
42 5 1 83 40
Selective dynamics
Cartesian
1.128620 3.571834 1.123043 F F F
1.139290 7.831985 1.173802 F F F
1.153170 12.086745 1.216262 F F F
3.578231 7.767404 1.404418 F F F
3.615151 12.096142 1.329628 F F F
6.082321 7.767404 1.404418 F F F
6.045401 12.096142 1.329628 F F F
8.531930 3.571834 1.123043 F F F
8.521249 7.831985 1.173802 F F F
8.507382 12.086745 1.216262 F F F
1.139320 2.156674 1.173241 F F F
1.128741 6.416654 1.123642 F F F
1.153220 10.664243 1.216145 F F F
3.578231 2.221464 1.402227 F F F
3.615212 10.654943 1.329783 F F F
6.082321 2.221464 1.402227 F F F
6.045340 10.654943 1.329783 F F F
8.521232 2.156674 1.173241 F F F
8.531809 6.416654 1.123642 F F F
8.507321 10.664243 1.216145 F F F
9.742464 1.444994 1.160057 F F F
9.742464 5.700932 1.049884 F F F
9.742464 9.966444 1.191449 F F F
2.380030 1.467324 1.269097 F F F
2.330011 5.706925 1.268651 F F F
2.387990 9.947744 1.267566 F F F
4.830271 1.527073 1.425394 F F F
4.830271 9.913444 1.371458 F F F
7.280521 1.467324 1.269097 F F F
7.330538 5.706925 1.268651 F F F
7.272561 9.947744 1.267566 F F F
9.742464 0.022247 1.191690 F F F
9.742464 4.287605 1.049792 F F F
9.742464 8.543544 1.160052 F F F
2.388030 0.040930 1.267375 F F F
2.330181 4.281594 1.267675 F F F
2.380181 8.521294 1.270158 F F F
4.830271 0.075401 1.370925 F F F
4.830271 8.461704 1.427069 F F F
7.272511 0.040930 1.267375 F F F
7.330362 4.281594 1.267675 F F F
7.280360 8.521294 1.270158 F F F
3.506161 3.602114 1.500305 F F F
6.154389 3.602114 1.500305 F F F
6.154361 6.386294 1.503373 F F F
3.506191 6.386294 1.503373 F F F
4.888199 5.022514 4.197377 T T T
4.830271 4.993834 2.243284 F F F
4.092487 5.362374 4.760690 T T T
5.537471 4.332268 4.682124 T T T
4.556708 5.289885 11.156396 T T T
4.065150 7.321414 10.949249 T T T
0.987172 6.699723 9.918040 T T T
4.371461 6.342336 8.215148 T T T
2.529772 2.394098 10.350142 T T T
3.701720 1.267221 10.623004 T T T
5.463850 9.015374 10.108865 T T T
5.698839 9.366934 11.608544 T T T
7.502366 8.261682 6.779471 T T T
6.112730 8.594391 7.353822 T T T
7.021468 11.779196 9.694183 T T T
7.452386 11.313313 11.078352 T T T
9.798168 2.467270 6.876325 T T T
0.943327 2.296595 5.579949 T T T
5.997001 11.688762 7.913117 T T T
4.866894 12.334970 7.004150 T T T
1.573708 0.896907 7.365385 T T T
2.475076 12.304789 7.474801 T T T
0.831915 6.121883 11.400089 T T T
2.949659 6.315562 10.947531 T T T
3.047972 3.070599 5.924009 T T T
2.955571 3.713752 4.528110 T T T
9.509801 8.292835 9.110640 T T T
0.760766 9.122911 8.343838 T T T
8.616028 4.325657 4.894710 T T T
9.716346 3.733526 3.847435 T T T
9.392796 6.421652 6.192957 T T T
0.121830 6.848073 7.604722 T T T
8.854256 8.046630 11.127020 T T T
7.415282 8.382272 10.547367 T T T
6.946409 2.322181 5.021659 T T T
6.987033 2.970104 6.349575 T T T
9.041562 8.948715 4.509927 T T T
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3.195971 12.625691 5.204230 T T T

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7.800068 0.055923 5.481615 T T T
9.248449 0.337662 5.964203 T T T
7.271632 0.792161 10.453980 T T T
8.461182 1.494656 9.800833 T T T
1.707731 8.581195 4.237908 T T T
2.403237 7.354282 4.863863 T T T
4.902006 10.035844 3.757013 T T T
3.988791 8.990270 4.559544 T T T
7.799536 4.327379 11.399455 T T T
7.419570 3.115881 10.418378 T T T
5.694355 6.734254 4.942482 T T T
5.854069 8.292913 5.086457 T T T
6.671726 2.333449 8.589382 T T T
5.439729 3.200790 8.035487 T T T
3.050977 2.537553 8.262564 T T T
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2.826787 11.058567 10.546285 T T T
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0.755929 0.357567 9.257904 T T T
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9.597893 11.900841 10.886849 T T T
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4.344133 3.494506 11.298552 T T T
1.147811 5.439200 5.792628 T T T
2.530671 6.054600 6.359586 T T T
5.235444 0.523406 4.767260 T T T
6.277030 0.534484 3.557544 T T T
3.622434 9.415815 9.440012 T T T
4.644417 10.222866 8.500057 T T T
7.437053 10.301985 7.865708 T T T
7.970993 11.701719 7.294238 T T T
9.562936 4.671835 7.837111 T T T
8.220114 3.911232 8.151683 T T T
3.419331 7.594052 8.020002 T T T
3.887479 6.398755 10.757233 T T T
3.472468 6.647002 7.887228 T T T
3.502574 2.264544 10.539933 T T T
5.757646 8.657766 10.958977 T T T
7.076903 8.758566 7.556809 T T T
6.804696 11.924877 10.656810 T T T
0.472926 1.818022 6.321086 T T T
5.019273 11.901426 7.883585 T T T
2.090396 0.287048 7.974582 T T T
1.387360 6.037872 10.569438 T T T
2.678205 2.930468 5.034555 T T T
0.552761 8.186801 8.618522 T T T
9.540044 4.412132 4.548051 T T T
9.649693 6.091632 7.063898 T T T
8.416581 8.289765 10.304172 T T T
7.036258 3.215870 5.361453 T T T
9.366963 9.845850 4.558319 T T T
3.883982 0.540205 5.464779 T T T
8.561500 12.337899 5.951155 T T T
7.528235 1.682494 10.054012 T T T
2.589891 8.207464 4.407130 T T T
4.858658 9.537686 4.576902 T T T
7.205982 4.083093 10.632042 T T T
6.272201 7.430441 5.304654 T T T
6.382849 2.922645 7.848661 T T T
3.059067 3.190032 7.542313 T T T
2.399208 10.241852 10.382117 T T T
1.981618 11.365236 4.752149 T T T
4.095968 12.474760 10.362586 T T T
8.860902 7.168404 4.664835 T T T
6.298644 5.794319 8.351020 T T T
1.011988 3.268568 10.265343 T T T
0.120673 0.610597 9.983239 T T T
9.471810 10.910420 10.823552 T T T
4.931450 4.311903 11.382723 T T T
2.071497 5.797863 5.518396 T T T
6.249538 0.509146 4.519907 T T T
4.462318 9.316588 8.795966 T T T
7.623747 11.250455 8.099948 T T T
9.198368 3.767618 8.216708 T T T

The initial coordinates of the *N_2 adsorption on the MoN_4/H_2O interface during the SG-AIMG

C
1.0
9.824384 0.0 0.0
0.0 12.762371 0.0
0.0 0.0 25.5
C N Mo O H
42 6 1 39 79
Selective dynamics
Cartesian
1.195660 4.071551 1.044292 F F F
1.207110 8.330731 1.072280 F F F
1.221510 12.583601 1.089843 F F F
3.640021 8.271620 1.323468 F F F
3.684430 12.592101 1.201868 F F F
6.156211 8.271620 1.323468 F F F
6.111791 12.592101 1.201868 F F F
8.600560 4.071551 1.044292 F F F
8.589119 8.330731 1.072280 F F F
8.574709 12.583601 1.089843 F F F
1.207330 2.651491 1.074615 F F F
1.195901 6.910089 1.042735 F F F
1.221531 11.161101 1.089051 F F F
3.640261 2.710390 1.325315 F F F
3.684229 11.152703 1.201118 F F F
6.155960 2.710390 1.325315 F F F
6.112000 11.152703 1.201118 F F F

8.588891 2.651491 1.074615 F F F
8.600320 6.910089 1.042735 F F F
8.574702 11.161101 1.089051 F F F
9.810305 1.941171 1.050267 F F F
9.810305 6.195261 0.967402 F F F
9.810305 10.461899 1.068688 F F F
2.442621 1.960760 1.160576 F F F
2.391850 6.209491 1.222672 F F F
2.453361 10.448401 1.141413 F F F
4.898111 2.020561 1.333499 F F F
4.898111 10.409702 1.249158 F F F
7.353611 1.960760 1.160576 F F F
7.404371 6.209491 1.222672 F F F
7.342870 10.448401 1.141413 F F F
9.810305 0.520444 1.070060 F F F
9.810305 4.786371 0.968337 F F F
9.810305 9.041220 1.048057 F F F
2.453460 0.533487 1.142836 F F F
2.391741 4.772891 1.223326 F F F
2.442830 9.021430 1.158475 F F F
4.898111 0.572623 1.250577 F F F
4.898111 8.961570 1.331560 F F F
7.342760 0.533487 1.142836 F F F
7.404480 4.772891 1.223326 F F F
7.353401 9.021430 1.158475 F F F
3.554220 4.078970 1.481181 F F F
6.242011 4.078970 1.481181 F F F
6.241830 6.903530 1.479840 F F F
3.554390 6.903530 1.479840 F F F
4.617460 5.512550 5.406000 T T T
4.617460 5.512550 6.502500 T T T
4.867510 5.512552 2.392877 F F F
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1.997738 0.701767 7.089110 T T T
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6.000479 2.369824 4.331320 T T T
9.247006 6.035772 4.161307 T T T
7.303685 12.491930 7.732092 T T T
6.671867 12.559702 5.277084 T T T
8.998266 1.750214 7.135031 T T T
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6.461675 3.792185 7.391265 T T T
4.266579 11.261488 4.270439 T T T
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4.582947 0.563391 8.031522 T T T
9.298338 4.135593 8.257912 T T T
8.756271 2.798444 4.468282 T T T
7.618437 3.251953 10.927620 T T T
1.570962 6.909314 5.315344 T T T
6.015683 11.990320 10.598979 T T T
6.779794 5.615697 5.207926 T T T
2.440634 0.934175 4.535651 T T T
3.055326 9.052208 10.374797 T T T
7.615322 6.027921 8.791591 T T T
0.210512 12.649403 3.946087 T T T
8.659868 10.650604 5.042878 T T T
6.121023 9.377773 5.345327 T T T
1.492982 0.612270 10.688263 T T T
2.182424 6.493875 10.991201 T T T
2.425901 9.509807 5.507486 T T T
8.154966 0.687985 10.879870 T T T
9.137517 6.909671 10.818303 T T T
2.303312 3.790718 5.249270 T T T
1.733377 4.897445 7.596224 T T T
3.487009 8.741402 7.814323 T T T
3.573079 5.274719 9.038791 T T T
7.122611 9.641215 7.879786 T T T
5.123001 3.604705 10.149618 T T T
0.919032 11.902620 6.663508 T T T
0.642134 10.866118 7.859379 T T T
2.279431 0.691574 6.136625 T T T
1.068707 1.058652 7.076452 T T T
8.744507 7.347163 7.882723 T T T
0.098515 8.221951 8.146599 T T T
6.149559 1.431283 4.551744 T T T
5.575101 2.415043 3.424016 T T T
8.338358 5.853726 4.580790 T T T
9.071854 6.321428 3.222057 T T T
6.764089 12.618489 8.529761 T T T
7.362146 11.481346 7.740952 T T T
6.574501 12.606464 6.271491 T T T
5.932819 12.044986 4.933816 T T T
8.370199 1.015606 7.342532 T T T
8.805584 2.023739 6.182329 T T T
4.856220 9.237280 10.460295 T T T
5.944830 9.245915 9.293423 T T T
6.231116 2.849977 7.138514 T T T
6.139547 3.790443 8.337834 T T T
4.395245 10.860062 3.360289 T T T
3.385546 10.836859 4.483689 T T T
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1.659407 10.149487 9.864170 T T T
8.317287 9.454831 12.026097 T T T
7.418324 9.503633 10.734322 T T T
4.600199 0.733024 8.998325 T T T
3.635179 0.447972 7.965889 T T T
0.790030 4.566876 7.902028 T T T
8.976659 3.261234 7.856744 T T T
9.144853 3.621604 4.178908 T T T
7.841153 2.789005 4.215430 T T T
8.007618 3.574254 10.084952 T T T
8.032327 2.343604 11.009521 T T T
0.650742 6.690582 4.929478 T T T
1.540692 6.498432 6.231140 T T T
5.919029 10.994472 10.605109 T T T
5.180520 12.487145 10.831546 T T T
6.220567 5.502169 4.287090 T T T
6.807882 4.685398 5.581677 T T T
3.074378 0.285118 4.147599 T T T
1.625950 0.590970 4.186265 T T T
3.184645 8.998323 9.353266 T T T
2.782181 8.111628 10.555232 T T T
8.531344 4.916247 8.258920 T T T
7.819045 6.231480 9.712206 T T T
9.614767 11.801725 4.280012 T T T
9.425151 0.653287 4.133419 T T T
9.246040 10.521666 5.786468 T T T

7.939471 11.258456 5.249082 T T T
5.378470 9.896741 5.018949 T T T
6.923326 9.534355 4.801518 T T T
0.771266 0.681952 11.333576 T T T
1.219023 12.495853 10.317780 T T T
2.243044 6.251795 11.984053 T T T
3.075054 5.793401 9.777966 T T T
2.043711 8.546929 5.239921 T T T
1.740781 10.048082 5.979728 T T T
7.341974 0.109761 11.081030 T T T
8.395198 0.347057 9.982932 T T T
8.972068 7.902246 10.788808 T T T
9.005580 6.575454 11.730467 T T T
1.888103 4.418253 4.551890 T T T
2.356275 2.920836 4.868315 T T T
1.940106 4.233611 6.873507 T T T
2.684062 5.027889 8.318839 T T T
3.044652 9.093979 6.930263 T T T
4.222973 8.113264 7.517743 T T T
4.938358 6.202205 7.662287 T T T
4.195273 4.601235 9.484854 T T T
6.589061 9.449995 7.071817 T T T
7.975226 9.136332 7.730687 T T T
5.882757 3.765800 10.760240 T T T
4.869412 2.707403 10.525936 T T T
1.223509 6.681596 10.879746 T T T

The selective coordinates of the *H adsorption at 0 V vs RHE on the MoN_4/H_2O interface during the SG-AIMG

At 0.65 ps

Frame 650 extracted from XDATCAR
1.0
9.824384 0.0 0.0
0.0 12.762371 0.0
0.0 0.0 25.5
C N Mo O H
42 4 1 40 81
Direct
0.12170330 0.31902779 0.04095263
0.12286877 0.65275731 0.04205020
0.12433451 0.98599241 0.04273894
0.37050883 0.64812565 0.05190071
0.37502911 0.98665844 0.04713208
0.62662565 0.64812565 0.05190071
0.62210425 0.98665844 0.04713208
0.87542995 0.31902779 0.04095263
0.87426540 0.65275731 0.04205020
0.87279864 0.98599241 0.04273894
0.12289117 0.20775850 0.04214176
0.12172784 0.54144242 0.04089157
0.12433665 0.87453193 0.04270788
0.37053326 0.21237355 0.05197314
0.37500865 0.87387391 0.04710267
0.62660010 0.21237355 0.05197314
0.62212552 0.87387391 0.04710267
0.87424219 0.20775850 0.04214176
0.87540552 0.54144242 0.04089157
0.87279793 0.87453193 0.04270788
0.99856693 0.15210113 0.04118694
0.99856693 0.48543182 0.03793733
0.99856693 0.81974572 0.04190933
0.24862841 0.15363603 0.04551278
0.24346056 0.48654682 0.04794792
0.24972161 0.81868808 0.04476129
0.49856673 0.15832176 0.05229408
0.49856673 0.81565581 0.04898659
0.74850606 0.15363603 0.04551278
0.75367280 0.48654682 0.04794792
0.74741276 0.81868808 0.04476129
0.99856693 0.04077957 0.04196314
0.99856693 0.37503776 0.03797400
0.99856693 0.70842792 0.04110027
0.24973169 0.04180156 0.04481710
0.24344946 0.37398153 0.04797357
0.24864969 0.70687727 0.04543039
0.49856673 0.04486807 0.04904224
0.49856673 0.70218692 0.05221804
0.74740157 0.04180156 0.04481710
0.75368390 0.37398153 0.04797357
0.74848469 0.70687727 0.04543039
0.36177535 0.31960911 0.05808553
0.63535902 0.31960911 0.05808553
0.63534060 0.54092848 0.05803294
0.36179266 0.54092848 0.05803294
0.49545193 0.43193792 0.09383831
0.07251988 0.83539369 0.29910839
0.14334025 0.03400933 0.30198466
0.91038382 0.63721524 0.33021202
0.59961923 0.10547203 0.16860271
0.92814855 0.49782716 0.17626203
0.70520923 0.98186541 0.28513655
0.64287127 0.90367648 0.18949817
0.87674476 0.13977338 0.27603759
0.64247827 0.80386493 0.43761276
0.46268594 0.20945415 0.25759820
0.41746772 0.78288868 0.17658118
0.57852674 0.47726460 0.29728580
0.39154247 0.45691406 0.16506472
0.32068257 0.09015262 0.49606122
0.13645838 0.78556471 0.40202718
0.88220156 0.72869565 0.48170571
0.45747404 0.03253022 0.33887902
0.91238067 0.35514825 0.29317020
0.84864023 0.19565129 0.17127626
0.75323294 0.34264869 0.44513670
0.17090621 0.50463915 0.21152975
0.57797237 1.02830063 0.43904203
0.66295415 0.39331807 0.20423194
0.27822946 0.02495994 0.18772452
0.41581426 0.68604816 0.41306904
0.78992145 0.44663781 0.36156695
0.01253587 1.02239818 0.15034030
0.92455370 0.83765186 0.20069748

0.75600995 0.66246690 0.15855732
0.13619970 0.02049615 0.42762825
0.29741698 0.48924018 0.45085496
0.25771723 0.70927662 0.25826433
0.84231250 0.12671828 0.40138671
1.05106173 0.52185913 0.49561409
0.17968624 0.22134689 0.20504144
0.17791720 0.35944998 0.27844662
0.49673490 0.67889958 0.31199392
0.40604437 0.39543998 0.36281836
0.70000671 0.79761684 0.33433539
0.44427218 0.25071335 0.44131142
0.09813969 0.90705859 0.28857710
0.08824718 0.82918794 0.33662962
0.19435483 0.04715701 0.26924592
0.06077977 0.07004380 0.29321119
0.87845230 0.58099078 0.35471903
-0.00053415 0.65550195 0.34515358
0.61805858 0.02910250 0.16967574
0.54525169 0.12614756 0.13705205
0.86708731 0.45147873 0.19557044
0.87595592 0.56249175 0.17462378
0.61261132 0.99542117 0.30029260
0.72528600 0.91672368 0.30544539
0.65379807 0.90331035 0.22764906
0.55688483 0.85859172 0.18290578
0.80835874 0.08275225 0.28431166
0.86031055 0.15688257 0.23933320
0.56172902 0.76641933 0.43977350
0.67987626 0.80103646 0.40091200
0.50169659 0.16398815 0.22949308
0.49774964 0.16745382 0.28616196
0.37112361 0.78270776 0.14228829
0.35086459 0.77245519 0.20462570
0.69733618 0.46366716 0.34358981
0.61477994 0.43584646 0.26658034
0.45562348 0.45344814 0.19446865
0.27242162 0.47825007 0.18939455
0.30002527 0.10283419 0.53397090
0.23851439 0.07009820 0.47741569
0.07275471 0.76616044 0.43124150
0.23176417 0.76222679 0.41019395
0.91130829 0.78031190 0.51043491
0.79153210 0.75424107 0.46797534
0.50518173 0.01797811 0.37265538
0.35734913 0.02692944 0.34640627
0.01848770 0.35518678 0.29386211
0.87713987 0.27783225 0.28854884
0.83349585 0.26972913 0.15921905
0.75569926 0.15859217 0.16914155
0.66039279 0.32977934 0.45566917
0.79500427 0.27875800 0.43164816
0.06764889 0.49484686 0.19330477
0.16697706 0.45511203 0.24423686
0.60146168 0.95292162 0.43897114
0.49823154 1.03553771 0.46217486
0.63080520 0.41294508 0.16046732
0.64134577 0.31741053 0.20917712
0.35473283 -0.01261415 0.17518063
0.19765875 0.01208348 0.16529685
0.47502376 0.66990073 0.38329924
0.36542871 0.61913381 0.41896564
0.85339003 0.39724202 0.33352132
0.76482230 0.40725877 0.39387497
0.97708791 0.95705440 0.16616900
0.93804063 0.07676268 0.15212436
0.94351952 0.83993649 0.23874608
0.83052353 0.86571566 0.20350606
0.65552841 0.66298795 0.15500866
0.78248428 0.73093081 0.17210611
0.05666888 0.05738410 0.41445270
0.12647929 0.94849608 0.41545635
0.35983754 0.46257864 0.47674322
0.36375364 0.43165724 0.39197396
0.22595915 0.64747561 0.24106351
0.17911634 0.76251265 0.26921235
0.77243815 0.08766772 0.41909237
0.82644288 0.12704789 0.36437569
1.01820991 0.59055766 0.50619535
0.97160924 0.47825990 0.48600697
0.09246465 0.18895091 0.20618564
0.24599558 0.15973151 0.19927597
0.19173070 0.29915680 0.25144821
0.24638100 0.36783890 0.30651149
0.40788166 0.69736910 0.29089861
0.52580469 0.61649132 0.29448498
0.50282833 0.44620413 0.31229451
0.41236447 0.32507873 0.37810597
0.61472496 0.75261391 0.32213569
0.77781148 0.75043288 0.32194483
0.51875001 0.19978379 0.43554448
0.40256506 0.20390219 0.46995929
0.20587258 0.50151425 0.46889996

At 3.2 ps

Frame 1404 extracted from XDATCAR
1.0
9.824384 0.0 0.0
0.0 12.762371 0.0
0.0 0.0 25.5
C N Mo O H
42 4 1 40 81
Direct
0.12170330 0.31902779 0.04095263
0.12286877 0.65275731 0.04205020
0.12433451 0.98599241 0.04273894
0.37050883 0.64812565 0.05190071
0.37502911 0.98665844 0.04713208
0.62662565 0.64812565 0.05190071
0.62210425 0.98665844 0.04713208
0.87542995 0.31902779 0.04095263
0.87426540 0.65275731 0.04205020
0.87279864 0.98599241 0.04273894
0.12289117 0.20775850 0.04214176
0.12172784 0.54144242 0.04089157
0.12433665 0.87453193 0.04270788
0.37053326 0.21237355 0.05197314
0.37500865 0.87387391 0.04710267
0.62660010 0.21237355 0.05197314
0.62212552 0.87387391 0.04710267
0.87424219 0.20775850 0.04214176
0.87540552 0.54144242 0.04089157

0.87279793 0.87453193 0.04270788
0.99856693 0.15210113 0.04118694
0.99856693 0.48543182 0.03793733
0.99856693 0.81974572 0.04190933
0.24862841 0.15363603 0.04551278
0.24346056 0.48654682 0.04794792
0.24972161 0.81868808 0.04476129
0.49856673 0.15832176 0.05229408
0.49856673 0.81565581 0.04898659
0.74850606 0.15363603 0.04551278
0.75367280 0.48654682 0.04794792
0.74741276 0.81868808 0.04476129
0.99856693 0.04077957 0.04196314
0.99856693 0.37503776 0.03797400
0.99856693 0.70842792 0.04110027
0.24973169 0.04180156 0.04481710
0.24344946 0.37398153 0.04797357
0.24864969 0.70687727 0.04543039
0.49856673 0.04486807 0.04904224
0.49856673 0.70218692 0.05221804
0.74740157 0.04180156 0.04481710
0.75368390 0.37398153 0.04797357
0.74848469 0.70687727 0.04543039
0.36177535 0.31960911 0.05808553
0.63535902 0.31960911 0.05808553
0.63534060 0.54092848 0.05803294
0.36179266 0.54092848 0.05803294
0.49545193 0.43193792 0.09383831
0.12856804 0.74021410 0.28939129
0.22593605 0.94864459 0.31421947
0.87739292 0.58857858 0.38463693
0.70274126 0.05731088 0.16781868
0.94842621 0.35743680 0.17999539
0.70401121 0.91215525 0.32872652
0.66927868 0.90472441 0.22655199
0.95985242 0.08061766 0.30496935
0.72982629 0.82153845 0.46027934
0.59121320 0.22105763 0.20757067
0.50127956 0.78084447 0.18651430
0.61126487 0.41529275 0.30397127
0.38660860 0.44568294 0.15938706
0.26957934 -0.02617790 0.52920222
0.10846838 0.70445503 0.38817426
0.10239915 0.87412122 0.43517538
0.47316184 0.03722796 0.36942639
0.02430397 0.26399999 0.32884736
0.95769297 0.13872696 0.20391445
0.79687040 0.31951821 0.45841593
0.15923390 0.45001313 0.20793368
0.52830625 -0.00412537 0.47387353
0.68794334 0.40221201 0.21074311
0.32041291 0.98348019 0.21040453
0.34530679 0.60566966 0.41543306
0.82198807 0.38182741 0.36414627
0.09866073 0.91442054 0.17038396
0.92496305 0.78023100 0.21650538
0.71075876 0.64396146 0.17172144
0.10865384 0.16511286 0.52260646
0.19321363 0.28812454 0.41605816
0.32828374 0.65443149 0.22768962
0.87125340 -0.02837729 0.41823985
0.03400489 0.38262876 0.48561543
0.32899318 0.17702998 0.18714924
0.26934797 0.29165918 0.27447154
0.49200116 0.59160988 0.32655318
0.44898100 0.26798452 0.35379775
0.68862244 0.72378798 0.37326479
0.80824479 0.12824660 0.48237960
0.16959234 0.80926804 0.29590775
0.11476798 0.72258241 0.32876947
0.27660435 0.96828920 0.28465820
0.14285449 -0.00721222 0.31372392
0.87288642 0.50263669 0.37027228
0.96913663 0.63370146 0.38886071
0.68808651 0.99099769 0.19394078
0.65733198 0.04211418 0.13282242
0.79182522 0.39883375 0.20746690
0.94080124 0.36858180 0.14300082
0.62087992 0.94982628 0.34257645
0.69509454 0.83729791 0.34219799
0.67611478 0.90327933 0.26569636
0.60073442 0.84600668 0.21015359
0.88959335 0.02478617 0.30901512
0.96120640 0.09520675 0.26615435
0.76044919 0.77254954 0.48452598
0.70595465 0.77670733 0.42693754
0.64481068 0.15979787 0.18942927
0.49493291 0.21930649 0.19980014
0.56804134 0.73096443 0.17176218
0.42444894 0.73732416 0.20434180
0.73984498 0.40468405 0.33977435
0.64216719 0.40193214 0.26475682
0.42125915 0.43782894 0.19464294
0.24231138 0.43684714 0.18077784
0.26874279 -0.07521638 0.55741923
0.23282031 0.03438199 0.54479526
0.12042434 0.76745555 0.40915734
0.18177303 0.65854346 0.40027042
0.05336682 0.92570903 0.41586135
1.11824553 0.90656114 0.46851538
0.49411647 0.02782631 0.40630183
0.38177804 0.00866645 0.36810476
0.11085545 0.26841251 0.30684822
-0.00859772 0.18740715 0.32610371
-0.04997243 0.21352635 0.19906635
0.86938292 0.12042738 0.18786601
0.80911528 0.24066741 0.46211618
0.89632748 0.34950071 0.47177617
0.03524583 0.39756531 0.19013384
0.18957241 0.41868360 0.24224273
0.57463558 0.93419024 0.48017777
0.44450100 -0.01477278 0.49487436
0.62341156 0.43527338 0.14515429
0.65635139 0.32559613 0.20959639
0.39145431 0.94332172 0.19312357
0.22056488 0.95630487 0.19509874
0.40264085 0.58858633 0.38405466
0.40502430 0.64203231 0.43851306
0.89040860 0.33828056 0.34399035
0.78468488 0.34124120 0.42271578
0.02339187 0.87449625 0.18889626
0.06280533 0.97664613 0.15551075
0.98585971 0.76178795 0.24883324
0.84935709 0.81971138 0.22967989

0.70829671 0.57194663 0.18431703
0.80204829 0.67807720 0.18235080
0.12002547 0.23493244 0.53598986
0.01162913 0.16123085 0.51532685
0.19973317 0.22133812 0.43322050
0.37359369 0.29528713 0.37846910
0.28507287 0.60063910 0.20912677
0.25631885 0.68257766 0.25015117
0.83666109 0.92057930 0.44263540
0.80867378 -0.03867143 0.38701987
0.10219781 0.34921905 0.45872615
0.04514275 0.45892634 0.48209957
0.25137794 0.19678008 0.16072449
0.32672399 0.09924537 0.19355107
0.29446032 0.24722267 0.24340956
0.35519389 0.28647010 0.29490905
0.44008414 0.60944040 0.29492487
0.53186549 0.51964684 0.31637623
0.55263707 0.35475189 0.31347015
0.47842393 0.19652779 0.36233178
0.60511989 0.68408670 0.35879765
0.76614509 0.64774378 0.37634028
0.81281792 0.07724024 0.45286729
0.72231103 0.12202311 0.50014386
0.14140712 0.27719622 0.38125248

At 5.6 ps

Frame 158 extracted from XDATCAR
1.0
9.824384 0.0 0.0
0.0 12.762371 0.0
0.0 0.0 25.5
C N Mo O H
42 4 1 40 81
Direct
0.12170330 0.31902779 0.04095263
0.12286877 0.65275731 0.04205020
0.12433451 0.98599241 0.04273894
0.37050883 0.64812565 0.05190071
0.37502911 0.98665844 0.04713208
0.62662565 0.64812565 0.05190071
0.62210425 0.98665844 0.04713208
0.87542995 0.31902779 0.04095263
0.87426540 0.65275731 0.04205020
0.87279864 0.98599241 0.04273894
0.12289117 0.20775850 0.04214176
0.12172784 0.54144242 0.04089157
0.12433665 0.87453193 0.04270788
0.37053326 0.21237355 0.05197314
0.37500865 0.87387391 0.04710267
0.62660010 0.21237355 0.05197314
0.62212552 0.87387391 0.04710267
0.87424219 0.20775850 0.04214176
0.87540552 0.54144242 0.04089157
0.87279793 0.87453193 0.04270788
0.99856693 0.15210113 0.04118694
0.99856693 0.48543182 0.03793733
0.99856693 0.81974572 0.04190933
0.24862841 0.15363603 0.04551278
0.24346056 0.48654682 0.04794792
0.24972161 0.81868808 0.04476129
0.49856673 0.15832176 0.05229408
0.49856673 0.81565581 0.04898659
0.74850606 0.15363603 0.04551278
0.75367280 0.48654682 0.04794792
0.74741276 0.81868808 0.04476129
0.99856693 0.04077957 0.04196314
0.99856693 0.37503776 0.03797400
0.99856693 0.70842792 0.04110027
0.24973169 0.04180156 0.04481710
0.24344946 0.37398153 0.04797357
0.24864969 0.70687727 0.04543039
0.49856673 0.04486807 0.04904224
0.49856673 0.70218692 0.05221804
0.74740157 0.04180156 0.04481710
0.75368390 0.37398153 0.04797357
0.74848469 0.70687727 0.04543039
0.36177535 0.31960911 0.05808553
0.63535902 0.31960911 0.05808553
0.63534060 0.54092848 0.05803294
0.36179266 0.54092848 0.05803294
0.49545193 0.43193792 0.09383831
0.09140269 0.69190568 0.29959032
0.10848276 0.89794027 0.28109575
0.82369121 0.55216313 0.39253356
0.67081274 0.98959186 0.18309455
0.86551873 0.33613332 0.18056106
0.69187781 0.92320794 0.38903153
0.53138338 0.90585713 0.25297884
0.88309929 0.01135793 0.31433790
0.47866011 0.73806318 0.43365079
0.51228235 0.16700944 0.18138022
0.41135624 0.73376408 0.19162734
0.57708063 0.33158470 0.32359405
0.38657977 0.40343419 0.15615163
0.26082516 0.96703104 0.49600061
0.06052012 0.65978734 0.39975784
0.05816098 0.85345414 0.44302185
0.34517630 1.00022550 0.32373338
0.99273851 0.20063619 0.34045653
0.85524777 0.10387489 0.22289839
0.78764496 0.29651163 0.46707497
0.14673049 0.41163079 0.20993981
0.42835993 0.93094086 0.41067197
0.62573213 0.32209090 0.23002806
0.15448655 0.87749314 0.17856537
0.29185344 0.57420292 0.43027525
0.79240134 0.33251178 0.37473644
0.86618213 0.82357132 0.16978640
0.84101655 0.71832539 0.25803089
0.68783426 0.63967995 0.16993470
0.12996386 0.14417206 0.51864378
0.16565849 0.25437482 0.41295259
0.28887201 0.57257860 0.25291508
0.78582882 0.92631527 0.49063129
0.02474513 0.39903544 0.46972803
0.14341992 0.11796508 0.18047326
0.17209460 0.23736899 0.26562310
0.42101201 0.51675019 0.34159933
0.36941441 0.19744857 0.33966044
0.64512570 0.67363415 0.34961099

0.86705979 0.09764158 0.53265578
0.10575009 0.77009104 0.29036474
0.06527817 0.66829802 0.36042982
0.11032157 0.88708759 0.24121097
0.03068146 0.94318564 0.29132212
0.82364172 0.47923664 0.37421372
0.91498887 0.57782340 0.39794509
0.61142885 0.95319628 0.20976034
0.74137281 0.92925869 0.17052396
0.72105984 0.34016417 0.21236281
0.84791993 0.36045206 0.14405738
0.59294761 0.92988262 0.39674812
0.69494764 0.85722501 0.36975328
0.45727365 0.93242008 0.27482407
0.48987181 0.84311474 0.23861239
0.80665446 0.98810417 0.33853228
0.84452797 0.05504976 0.28787444
0.41689575 0.68045840 0.44202497
0.53793392 0.70545854 0.40695642
0.55104062 0.09634361 0.17784257
0.42062219 0.16574628 0.16773149
0.49982934 0.70892961 0.17746459
0.37665506 0.66883129 0.21249978
0.67786348 0.32580470 0.35058547
0.60266288 0.33371244 0.28304429
0.44468184 0.38893312 0.18896507
0.21616104 0.41091110 0.18086058
0.30570462 0.93394809 0.52653579
0.20663550 0.03138457 0.50732816
0.06521818 0.73586258 0.41170633
0.19265012 0.60334579 0.42540545
0.98594413 0.87351750 0.46841024
0.13975712 0.88194322 0.45889571
0.37417435 0.97898887 0.35663606
0.26998199 0.96407125 0.30772343
0.05668046 0.20942343 0.31077398
0.95758220 0.13053039 0.33098850
0.83519094 0.17537544 0.20973852
0.77929232 0.05247837 0.20898277
0.81027171 0.23196779 0.49156337
0.86882093 0.35136781 0.48130906
0.95424179 0.36854323 0.18721395
0.15377512 0.34264418 0.22941948
0.43106773 0.85070524 0.41521576
0.37731421 0.96336191 0.44458664
0.61544875 0.45070428 0.14354528
0.58204248 0.25923704 0.21218913
0.23215900 0.82850136 0.16928443
0.06548111 0.85248839 0.16605997
0.36157056 0.51556275 0.37540775
0.30148544 0.55019710 0.46571108
0.88016511 0.31156560 0.35359818
0.79274391 0.30315455 0.41094485
0.85302166 0.80300327 0.20650162
0.81235873 0.76746229 0.14977331
0.92975924 0.69056099 0.27553643
0.78345302 0.72878528 0.28645416
0.65633903 0.57436398 0.15737839
0.73741344 0.63165279 0.20445301
0.14655863 0.20602173 0.54466012
0.02426872 0.13309088 0.52659813
0.15318465 0.21337721 0.44690974
0.31531288 0.20325752 0.37198079
0.24160564 0.51283272 0.23715583
0.16064672 0.64822498 0.27997849
0.73605835 0.88046900 0.51680376
0.73840076 0.91326093 0.45559503
0.09552731 0.35784227 0.44829759
0.04091387 0.47146375 0.47088990
0.05766364 0.09482937 0.19047553
0.19654797 0.05288874 0.17380811
0.18272518 0.18037114 0.23846044
0.25961439 0.24934973 0.28585607
0.34608587 0.54575372 0.28391830
0.47438179 0.44933971 0.34151599
0.50316388 0.27402771 0.33320651
0.37215578 0.11983355 0.33077739
0.56231523 0.64157585 0.33693415
0.71643026 0.61954592 0.36161313
0.82534650 0.03510095 0.51872794
0.82703983 0.10961702 0.56717893
0.08924377 0.23175416 0.39101060

Input file used in calculation

INCAR for the DFT calculation

Global Parameters
ALGO=Fast
ISTART = 0
ISPIN = 2
ENCUT = 550
PREC = Accurate
LREAL= Auto

Electronic Relaxation
ISMEAR = 0
SIGMA = 0.05
EDIFF = 1E-05
EDIFFG = -0.01
NELM = 150
NELMIN = 6

Ionic Relaxation
NSW = 1000
IBRION = 2
ISIF = 2
IVDW = 11

LSOL = .TRUE.
EB_K = 78
LAMBDA_D_K = 3.04

INCAR for the AIMD simulation

ISTART = 0
IVDW= 11
ICHARG = 2
LREAL = Auto
PREC = Accurate
ENCUT = 400
EDIFF = 1E-05
NSW = 5000
ISPIN = 2
ISMEAR = 0
EDIFFG = -0.05
SIGMA = 0.05
ISIF = 2
ALGO=VeryFast
ISMEAR=0
SIGMA=0.05
IBRION=0
POTIM=1.0
TEBEG=300.00
TEEND=300.00
SMASS = 0
MDALGO = 2
NWRITE = 0
NBLOCK =1
LWAVE = .FALSE
LCHARG = .FALSE

INCAR for the constant potential AIMD slow growth in the acidic medium

ISTART = 0
IVDW= 11
LREAL = Auto
ICHARG = 2
PREC = Accurate
ENCUT = 400
EDIFF = 1E-05
NSW = 500
ISIF = 2
ISMEAR = 0
EDIFFG = -0.05
SIGMA = 0.05
NELM = 120
NELMIN = 4
ALGO=VeryFast
ISMEAR=0
SIGMA=0.0516
ISPIN =2
IBRION=0
POTIM=0.5
TEBEG=300.00
TEEND=300.00
SMASS = 0
MDALGO = 2
NWRITE = 0
NBLOCK =1
LWAVE = .FALSE
LCHARG = .FALSE
LBLUEOUT=.TRUE.
INCREM = -0.0004
# CP-VASP Parameters
LCEP = .TRUE.
NESCHEME = 2
CAP_MAX = 2.0
NEADJUST = 5
TARGETMU = -4.6
FERMICONVERGE = 0.01
LSOL = .TRUE.
EB_K = 78
LAMBDA_D_K = 3.04