Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supplementary Information

Membrane-modified Electrocatalysts for Nitrate Reduction to Ammonia with High Faradaic Efficiency

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Catalyst	**Electrolyte**	**NH_3 Faradaic Efficiency**
This work (Nafion-modified Cu)	50 mM $NaNO_3$ and 100 mM Na_2SO_4	91 ± 2 %
Fe single atom[1]	500 mM KNO_3 and 100 mM K_2SO_4	75 %
PTCDA/O-Cu[2]	100 mM PBS NO_3^- reduction	77 ± 3 %
Pd-In / c-Al_2O_3[3]	3.28 mM $NaHCO_3$ NO_3^- reduction	71.5 %
Pt[4]	3000 mg L^{-1} NO_3^-	49 %
30 % Cu – 70 % Pd[5]	50 mM KNO_3	58 %
Pd-In / $TinO_{2n-1}$ Pd-Cu / $TinO_{2n-1}$ Pd-Cu / REM[6]	10 mM $NaHCO_3$ buffer NO_3^- reduction	19 ± 1 % 22 ± 2 % < 2.3 %
Co-NAs[7]	1 M KOH 1700 ppm NO_3^-	≥ 96 %
CuFe[8] $Pt_{78}Ru_{22}$/C	100 mM K_2SO_4 100 mM H_2SO_4 1700 ppm NO_3^-	94.5 % ≥ 93.0%
Bi_2O_3-CC[9]	500 mM Na_2SO_4 750 ppm NO_3^-	84.9 %
Co/CoO NSA[10]	100 mM K_2SO_4 200 ppm NO_3^-	93.8 %
Co_3O_4/NiO HNTs[11]	500 mM Na_2SO_4 200 ppm NO_3^-	55 %
Thiourea/Au[12]	500 mM $NaNO_3$	85 %
Co_3O_4/Ti[13]	1 M KOH 50 ppm NO_3^-	80 %
Ir NTs[14]	100 mM $HClO_4$ 17000 ppm NO_3^-	84.7 %

Table S1. Previous literature reports of NH_3-producing NO_3^- reduction catalysts compared to the Nafion-modified Cu electrode presented in this work.

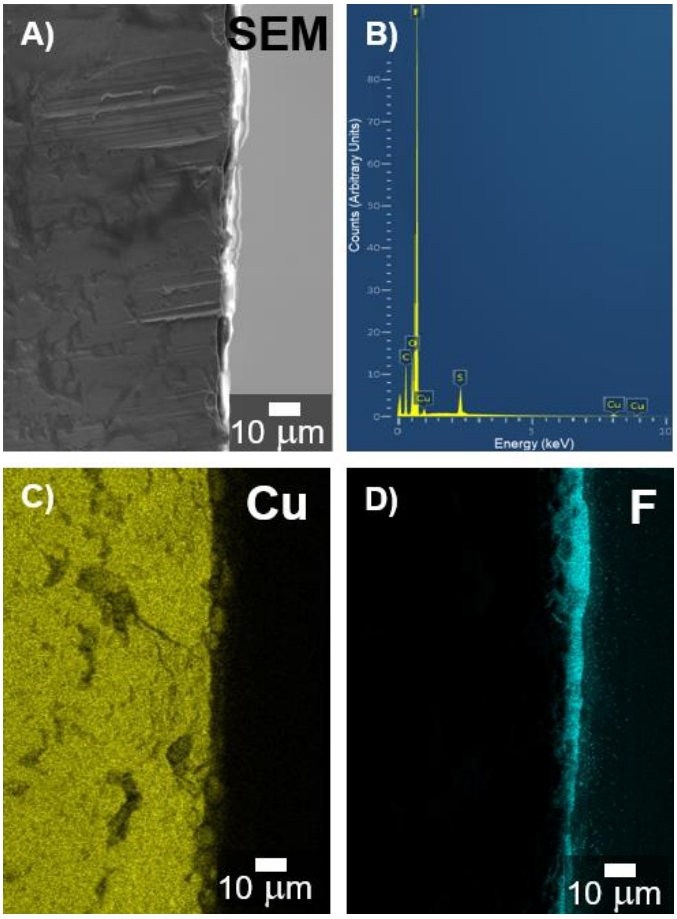

Figure S1: Cross-sectional SEM image of a Cu electrode modified with 6 µm of Nafion (A). The EDX spectrum of this substrate indicates that the electrode contains Cu, F, S, C, and O (B). While Cu originates from the Cu electrode, the other four elements are constituents of Nafion. EDX elemental mapping of Cu (C) and F (D) reveals that the Nafion layer is distributed uniformly on the top of the Cu electrode (Figures 1C and 1D).

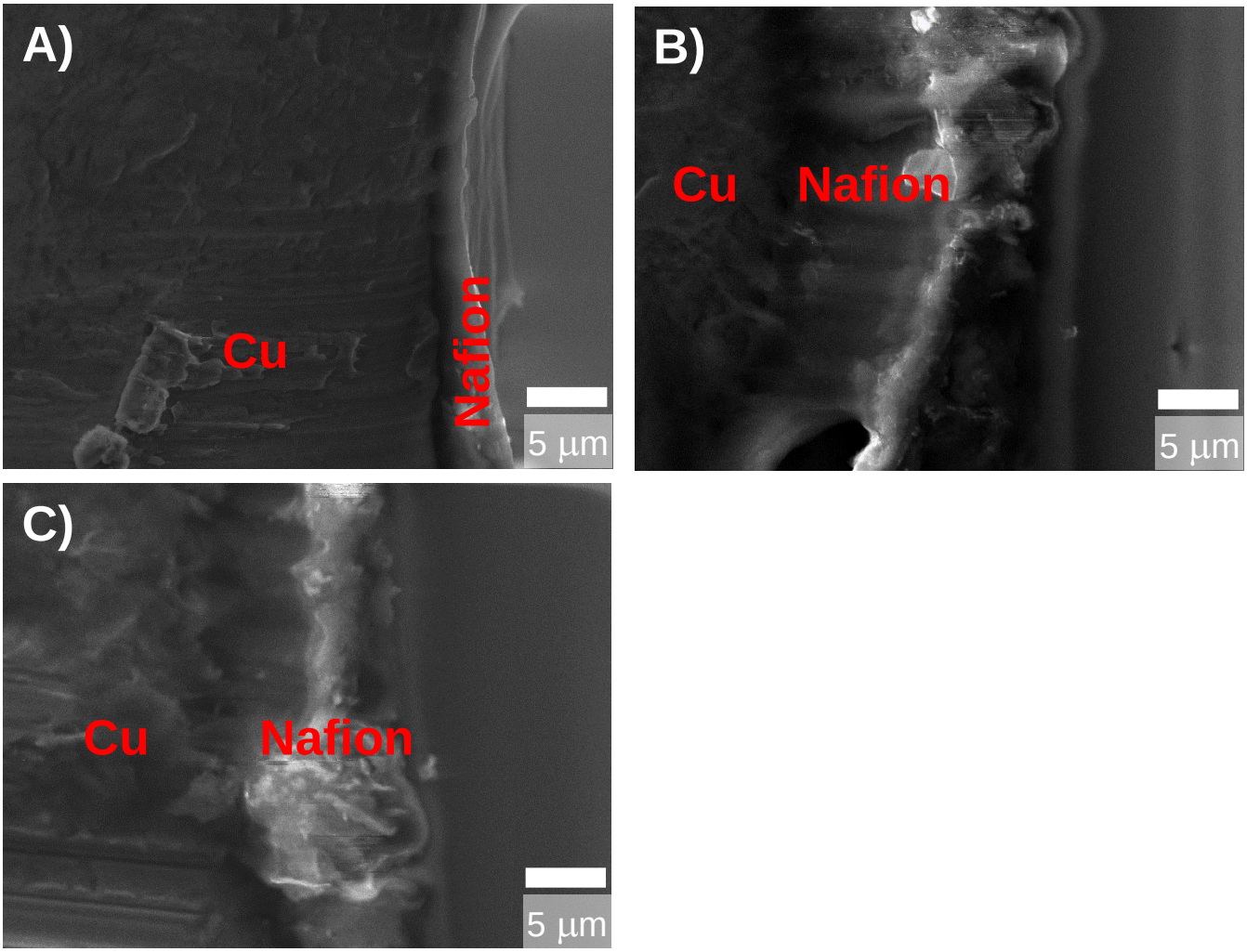

Figure S2: Cross-sectional SEM images of Cu electrodes modified with Nafion layers with thicknesses of about 3 µm (A), 8 µm (B) and 10 µm (C).

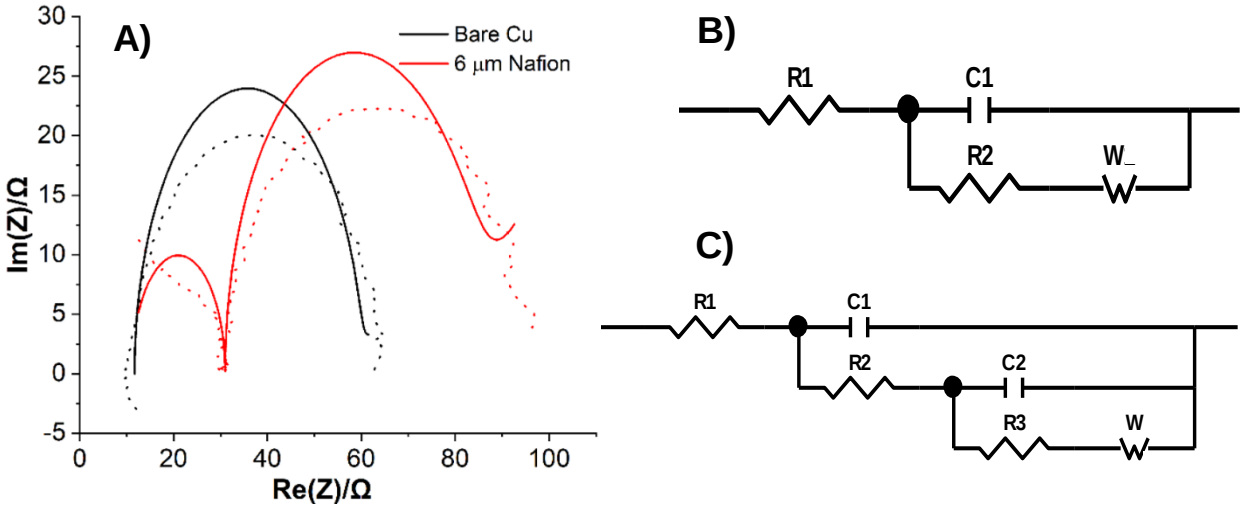

Figure S3: EIS spectra of bare Cu (A, black points) and Cu modified with 6 μm of Nafion (A, red points) in 100 mM KCl at open circuit potential. The best fits are displayed as the solid lines. The equivalent circuits used for fitting the data of bare Cu and Nafion-modified Cu are shown in panels B and C, respectively.

While a standard Randles circuit is used to model the EIS data of the unmodified Cu electrode (Figure S3B), a Randles circuit with one more resistor and capacitor is used to model the EIS data of the Nafion-modified Cu electrode to account for the Nafion layer. R1 is the solution resistance in both circuit diagrams, and it has similar values in both experiments (12 Ω and 11 Ω for bare Cu and Nafion-modified Cu, respectively). This similarity is expected because the presence of Nafion does not significantly alter the resistance of the bulk electrolyte. R2 = 48 Ω and R3 = 52 Ω are the charge transfer resistances of the bare Cu and Nafion-modified Cu electrodes, respectively, which are also similar. The added resistance due to the Nafion is reflected in the R2 = 20 Ω component of the equivalent circuit for the Nafion-modified Cu electrode. C1 = 95 μF and C2 = 230 μF are the double layer capacitances of the bare Cu and Nafion-modified Cu electrodes, respectively. The Nafion-modified Cu electrode possesses a higher double layer capacitance due to the charged nature of the Nafion layer, which increases the quantity of ions that are stored in the double layer above the Nafion. The C1 = 6 nF for the Nafion-modified Cu electrode indicates that some charge is also stored inside the Nafion layer.

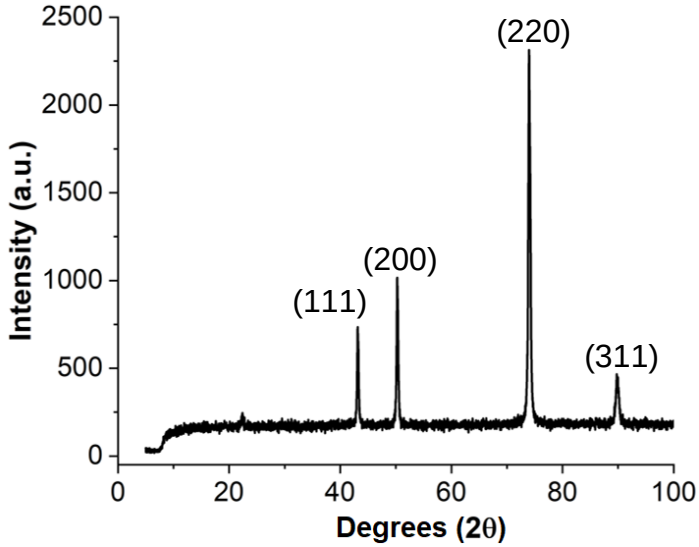

Figure S4: XRD spectrum of an unmodified Cu electrode.

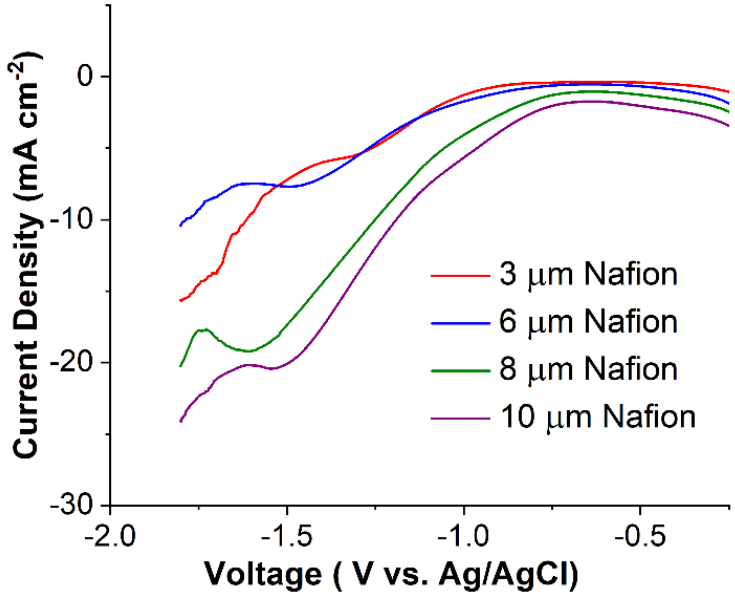

Figure S5: Linear sweep voltammograms at a scan rate of 10 mV s^{-1} in 50 mM $NaNO_3$ and 100 mM Na_2SO_4 of Cu modified with 3 μm (red line), 6 μm (blue line), 8 μm (green line), and 10 μm (purple line) of Nafion. The onset potentials of these LSVs curves (defined as the potential at which 10% of the maximum current is attained) are -1.04 V, -0.88 V, -0.83 V, and -0.75 V for the 3 μm, 6 μm, 8 μm, and 10 μm Nafion layers, respectively.

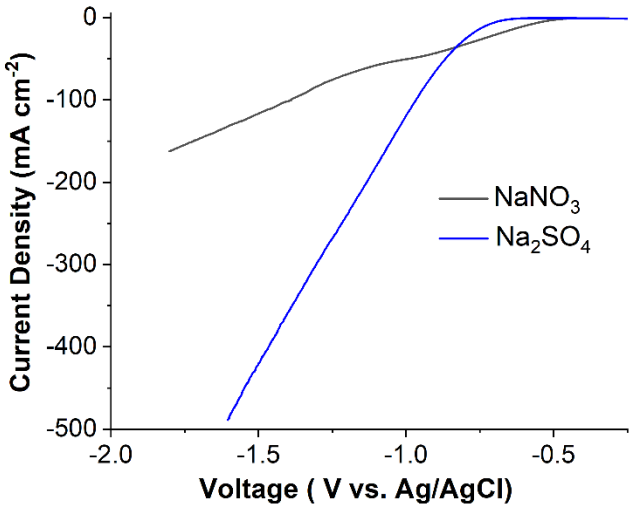

Figure S6: Linear sweep voltammograms at a scan rate of 10 mV s^{-1} of unmodified Cu electrodes at pH 1.0 with 50 mM $NaNO_3$ and 100 mM Na_2SO_4 (black line) and 100 mM Na_2SO_4 (blue line).

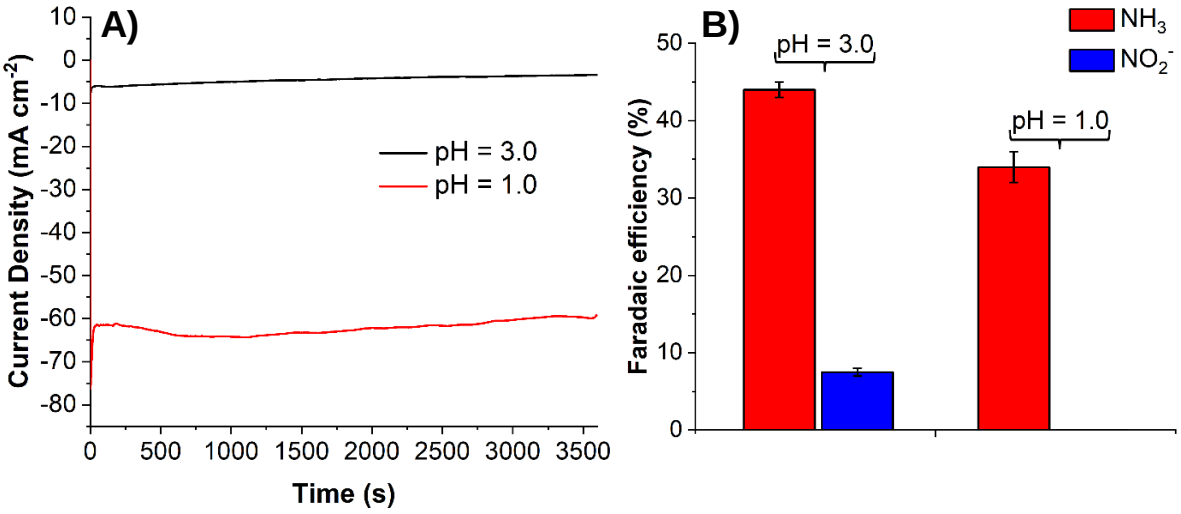

Figure S7: Chronoamperometry of unmodified Cu electrodes in 50 mM $NaNO_3$ and 100 mM Na_2SO_4 at pH 3.0 (A, black line) and pH 1.0 (A, red line) and Faradaic efficiencies of NH_3 (red bars) and NO_2^- (blue bars) production after chronoamperometry (B). In both cases, because no nitrogen-containing products other than NH_3 and NO_2^- were detected, the Faradaic efficiencies for the H_2 evolution reaction are high.

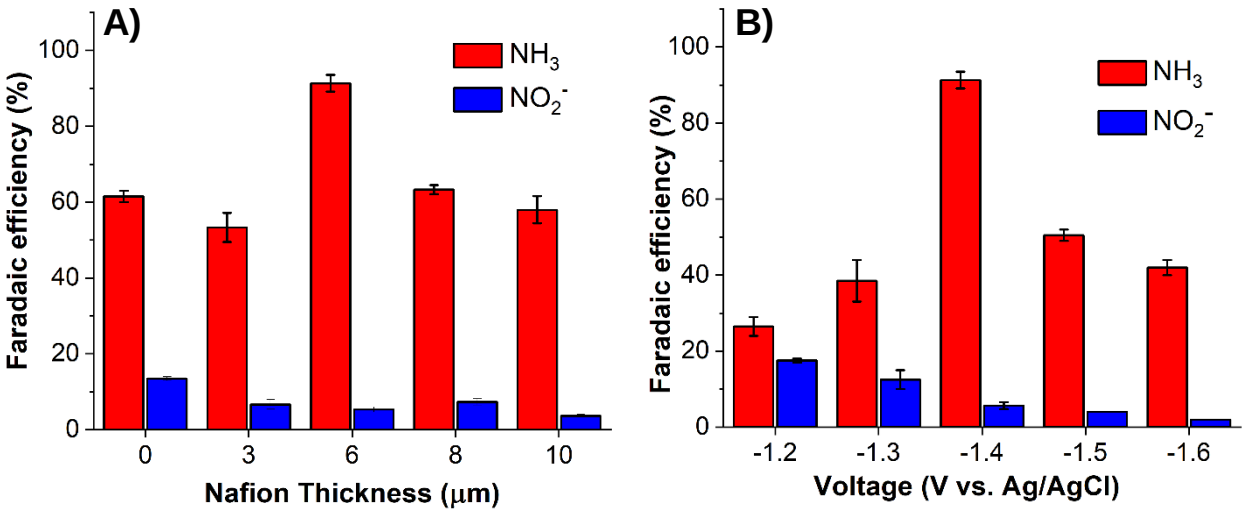

Figure S8: Faradaic efficiencies of NH_3 (red bars) and NO_2^- (blue bars) production after 1 hour of chronoamperometry at -1.4 V vs. Ag/AgCl from Cu electrodes modified with different thickness Nafion (A) and after 1 hour of chronoamperometry at different voltages with 6 μm Nafion (B).

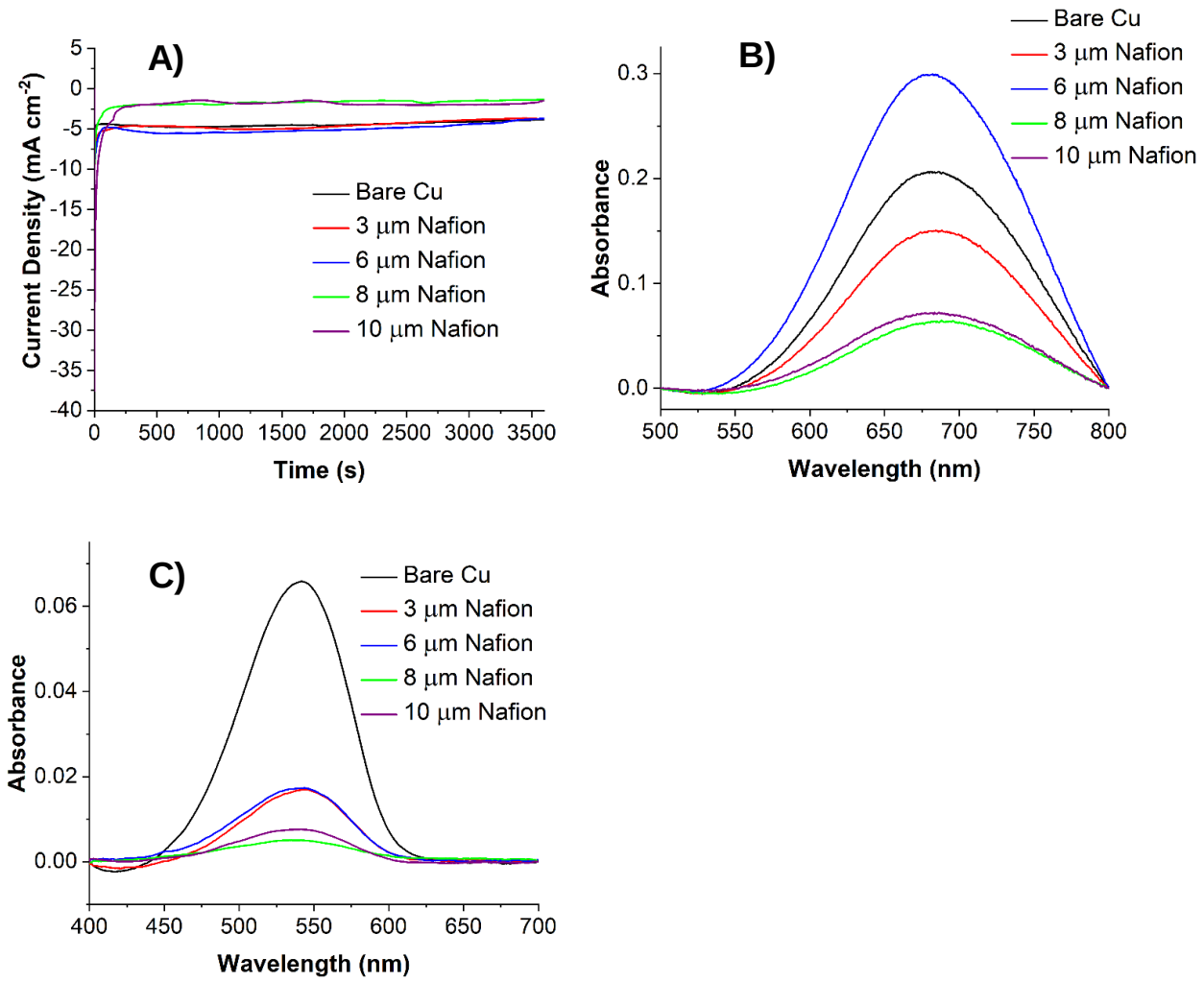

Figure S9: Chronoamperometry curves of unmodified (bare) Cu (black line) and Cu modified with 3 μm (red line), 6 μm (blue line), 8 μm (green line), and 10 μm (purple line) of Nafion at -1.4 V in 50 mM $NaNO_3$ and 100 mM Na_2SO_4 (A), and UV-Vis absorption spectra after chronoamperometry for NH_3 (B) and NO_2^- (C) detection.

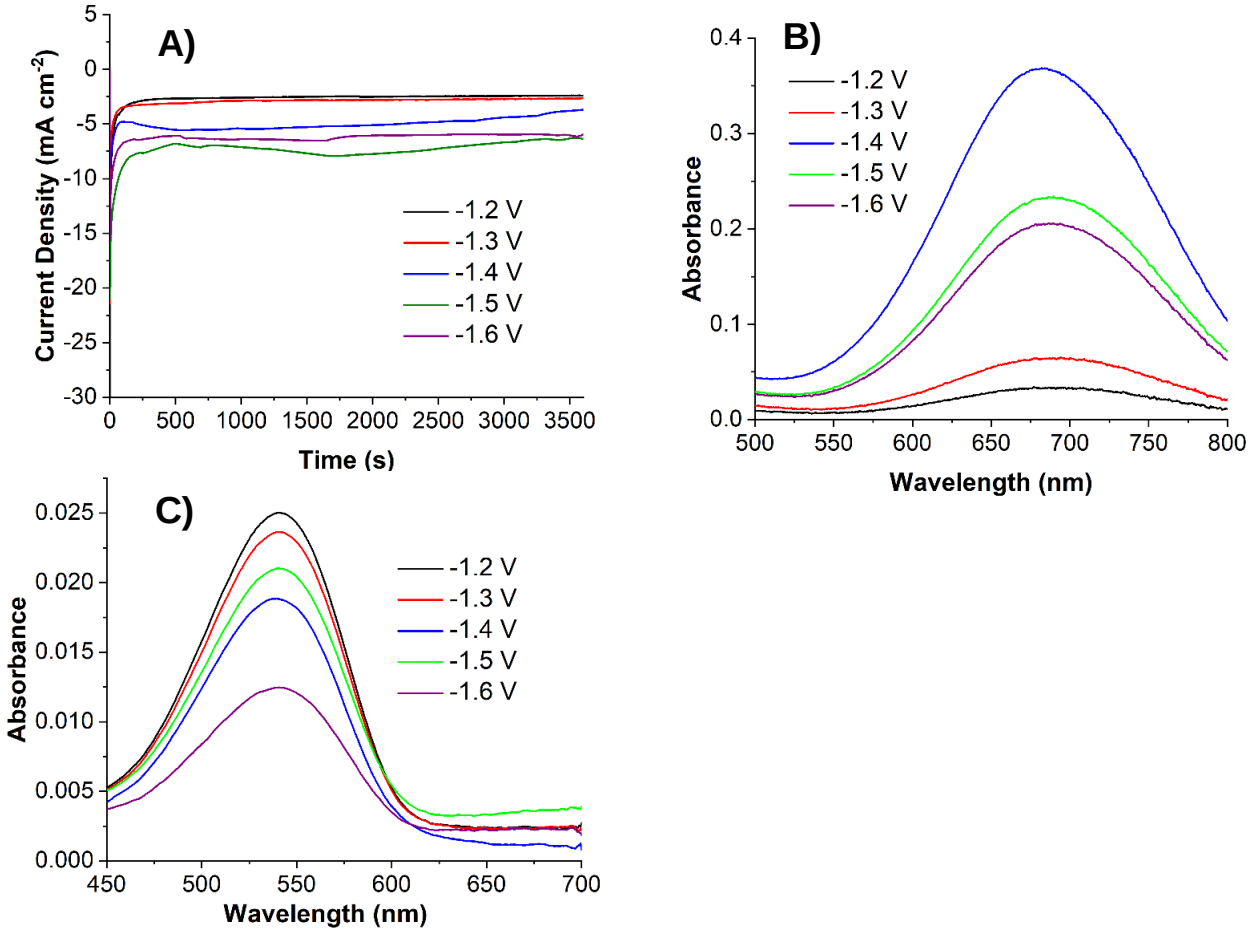

Figure S10: Chronoamperometry curves of Cu modified with 6 μm of Nafion at -1.2 V (black line), -1.3 V (red line), -1.4 V (blue line), -1.5 V (green line), and -1.6 V (purple line) in 50 mM $NaNO_3$ and 100 mM Na_2SO_4 (A), and UV-Vis absorption spectra after chronoamperometry for NH_3 (B) and NO_2^- (C) detection.

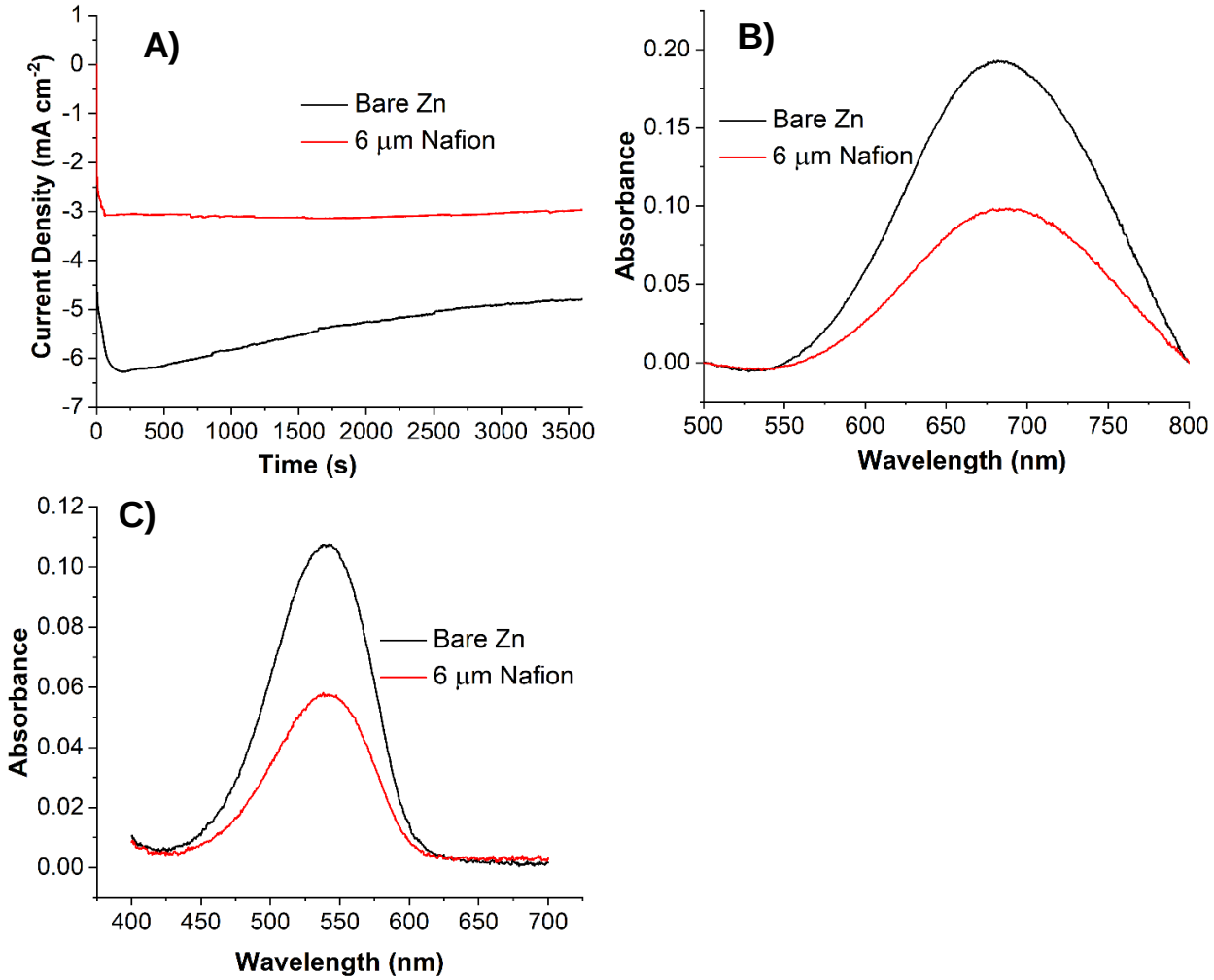

Figure S11: Chronoamperometry curves of unmodified (bare) Zn (black line) and Zn modified with 6 μm of Nafion (red line) at -1.5 V in 50 mM $NaNO_3$ and 100 mM Na_2SO_4 (A), and UV-Vis absorption spectra after chronoamperometry for NH_3 (B) and NO_2^- (C) detection.

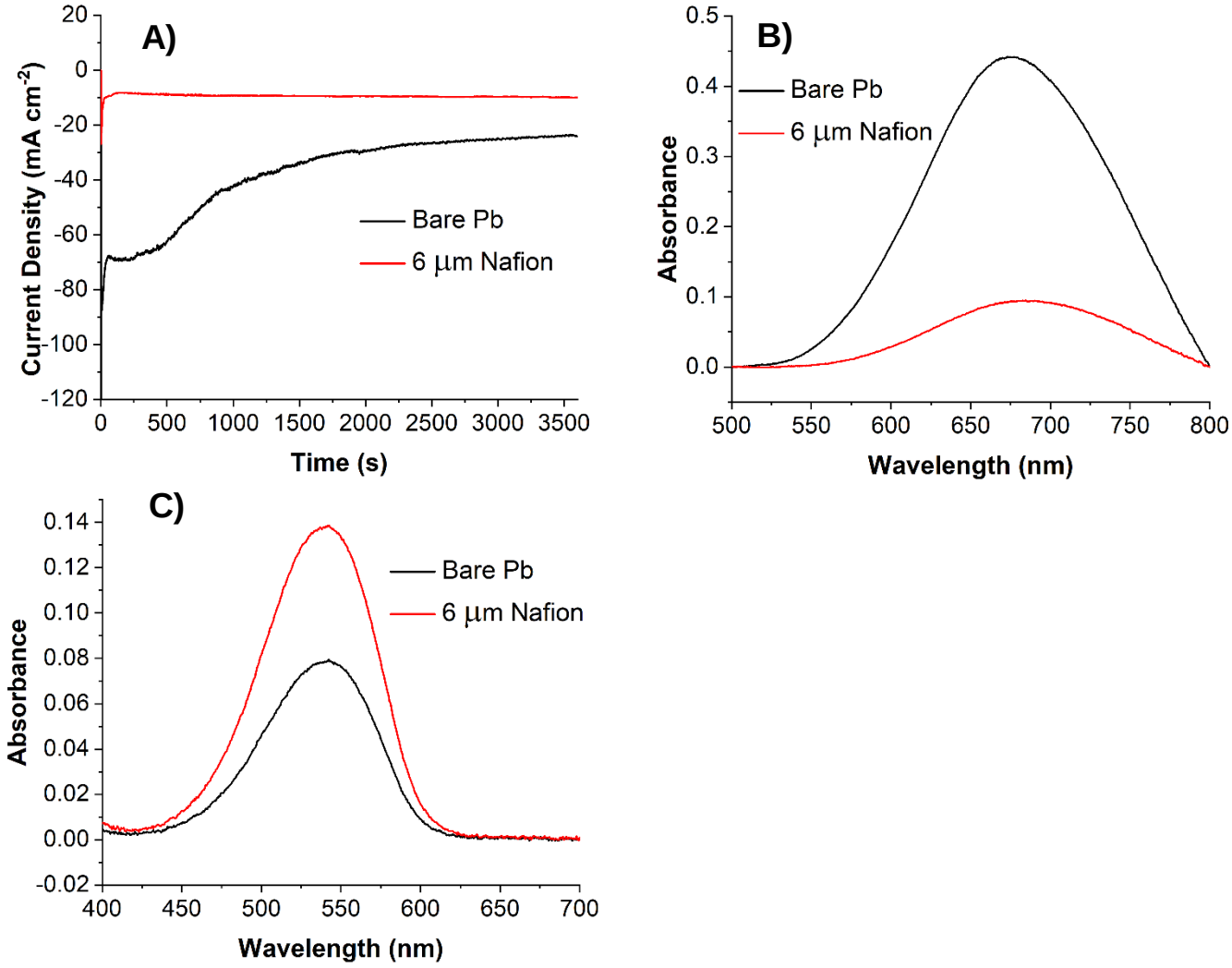

Figure S12: Chronoamperometry curves of unmodified (bare) Pb (black line) and Pb modified with 6 µm of Nafion (red line) at -2.0 V in 50 mM $NaNO_3$ and 100 mM Na_2SO_4 (A), and UV-Vis absorption spectra after chronoamperometry for NH_3 (B) and NO_2^- (C) detection.

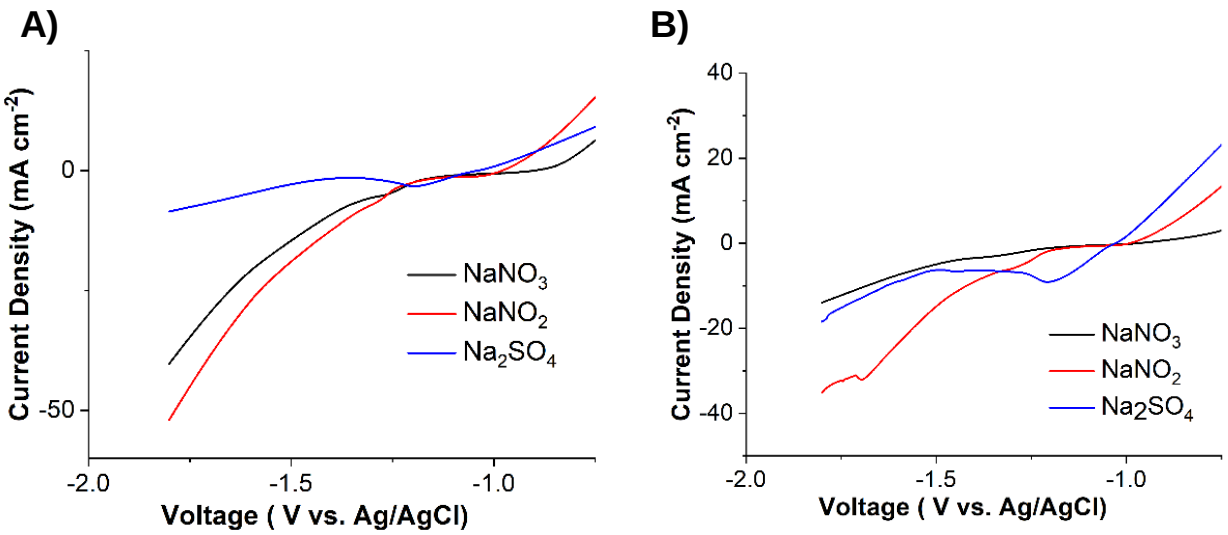

Figure S13: Linear sweep voltammograms at a scan rate of 10 mV s^{-1} of unmodified Zn (A) and Zn modified with 6 μm of Nafion (B) in 50 mM $NaNO_3$ and 100 mM Na_2SO_4 (black line), 50 mM $NaNO_2$ and 100 mM Na_2SO_4 (red line), and 100 mM Na_2SO_4 (blue line). In the presence of 50 mM $NaNO_3$ and 100 mM Na_2SO_4, the onset potentials of the LSVs curves (defined as the potential at which 10% of the maximum current is attained) are -1.24 V and -1.23 V for the unmodified and Nafion-modified Zn electrodes, respectively.

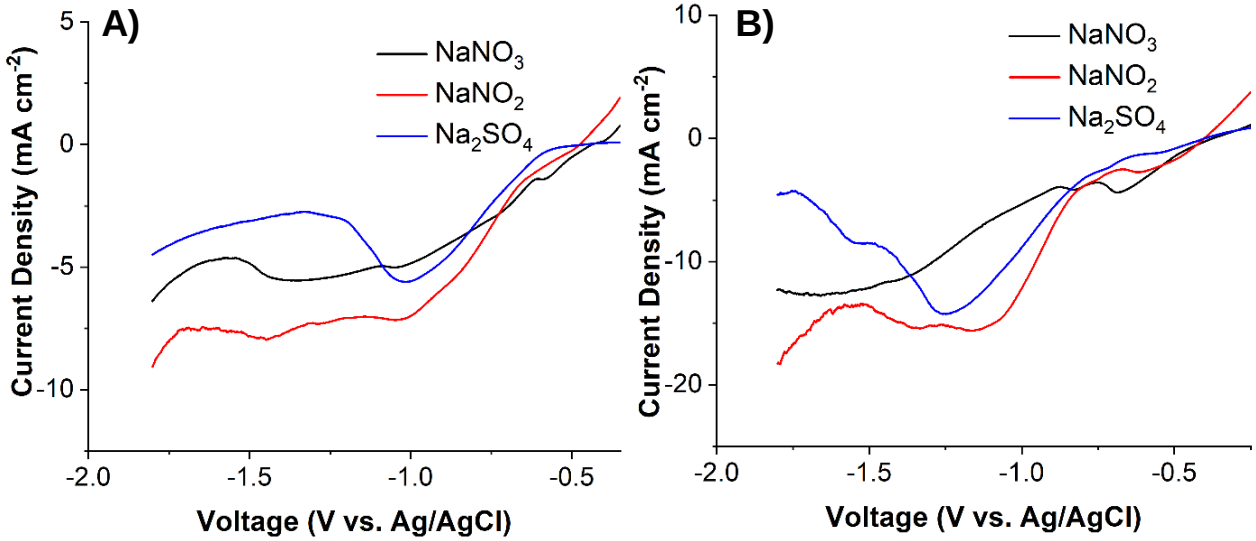

Figure S14: Linear sweep voltammograms at a scan rate of 10 mV s^{-1} of unmodified Pb (A) and Pb modified with 6 μm of Nafion (B) in 50 mM $NaNO_3$ and 100 mM Na_2SO_4 (black line), 50 mM $NaNO_2$ and 100 mM Na_2SO_4 (red line), and 100 mM Na_2SO_4 (blue line). In the presence of 50 mM $NaNO_3$ and 100 mM Na_2SO_4, the onset potentials of the LSVs curves (defined as the potential at which 10% of the maximum current is attained) are -0.5 V and -0.49 V for the unmodified and Nafion-modified Pb electrodes, respectively.

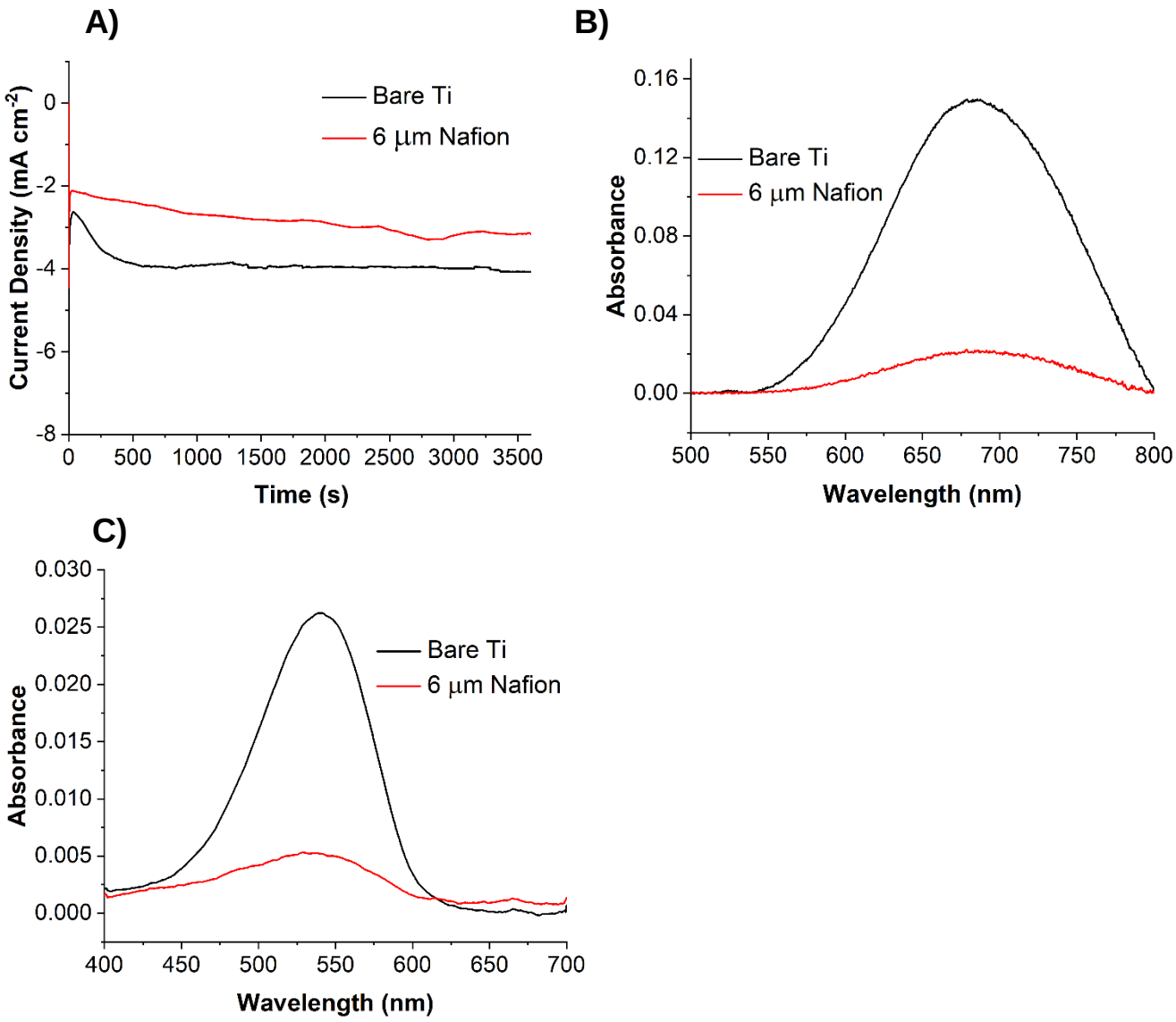

Figure S15: Chronoamperometry curves of unmodified (bare) Ti (black line) and Ti modified with 6 μm of Nafion (red line) at -1.6 V in 50 mM $NaNO_3$ and 100 mM Na_2SO_4 (A), and UV-Vis absorption spectra after chronoamperometry for NH_3 (B) and NO_2^- (C) detection.

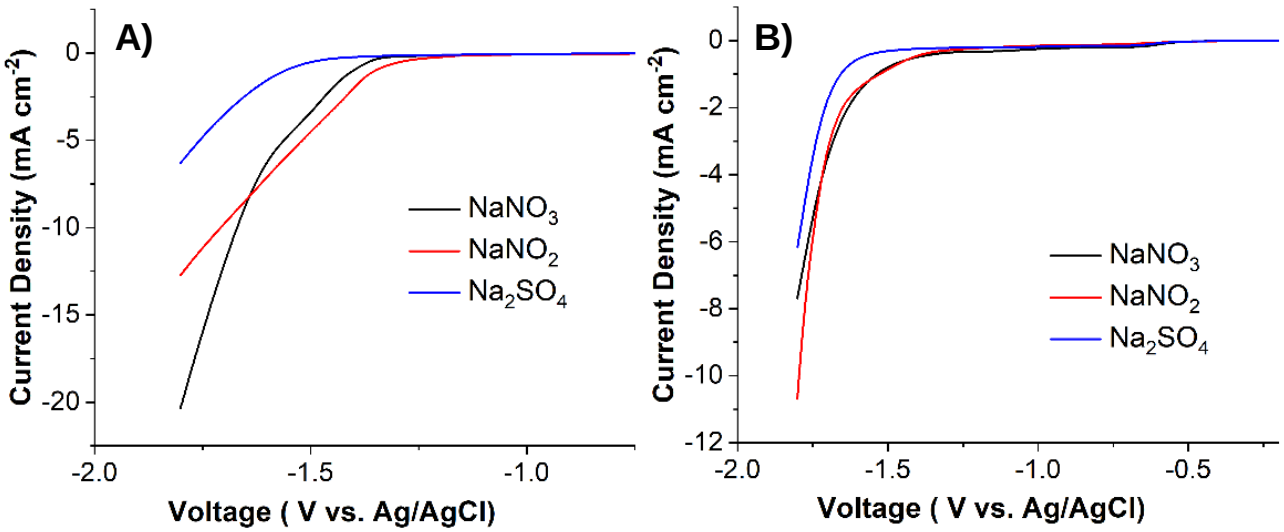

Figure S16: Linear sweep voltammograms at a scan rate of 10 mV s^{-1} of unmodified Ti (A) and Ti modified with 6 μm of Nafion (B) in 50 mM $NaNO_3$ and 100 mM Na_2SO_4 (black line), 50 mM $NaNO_2$ and 100 mM Na_2SO_4 (red line), and 100 mM Na_2SO_4 (blue line). In the presence of 50 mM $NaNO_3$ and 100 mM Na_2SO_4, the onset potentials of the LSVs curves (defined as the potential at which 10% of the maximum current is attained) are -1.45 V and -1.48 V for the unmodified and Nafion-modified Ti electrodes, respectively.

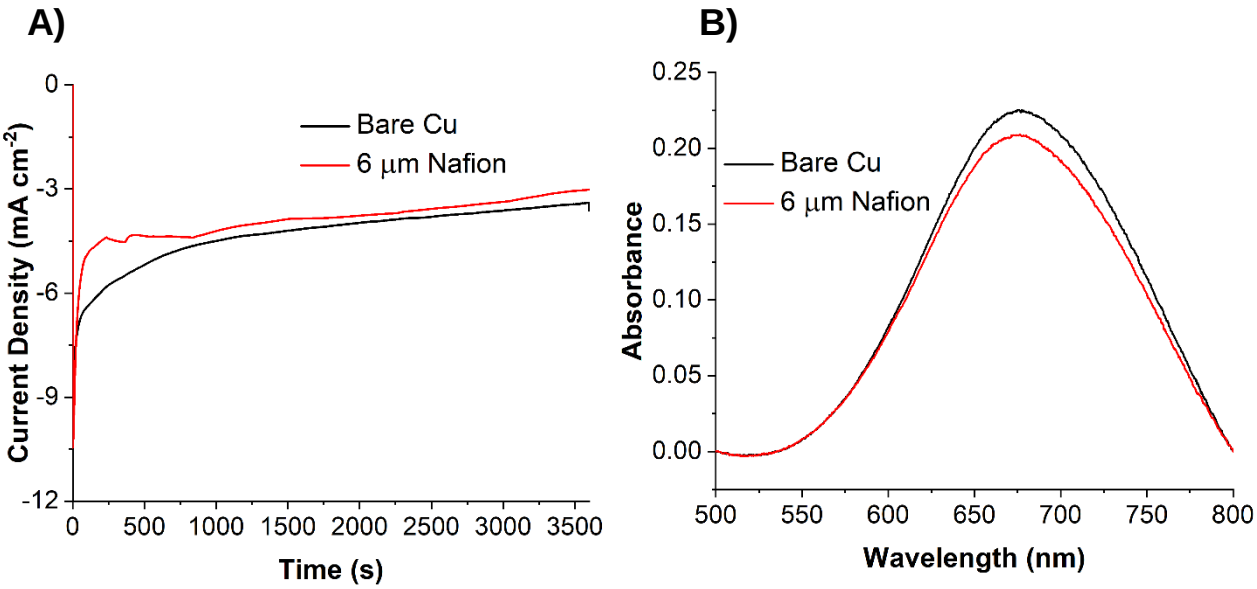

Figure S17: Chronoamperometry curves of unmodified (bare) Cu (black line) and Cu modified with 6 μm of Nafion (red line) at -1.4 V in 50 mM $NaNO_2$ and 100 mM Na_2SO_4 (A), and UV-Vis absorption spectra after chronoamperometry for NH_3 (B) detection.

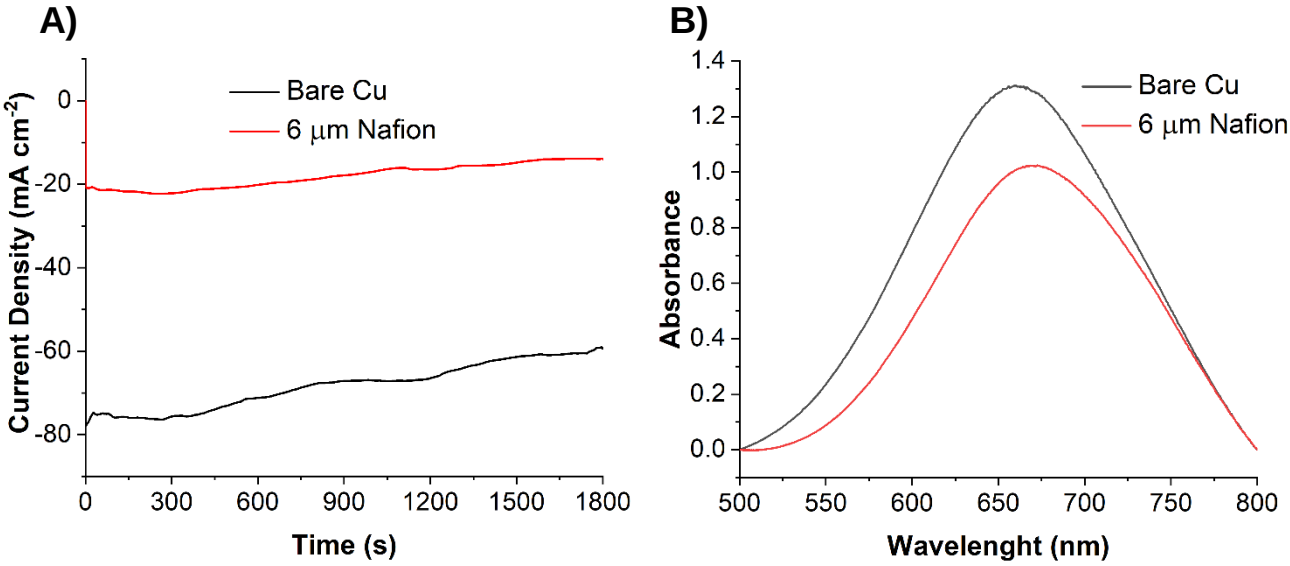

Figure S18: Chronoamperometry curves of unmodified (bare) Cu (black line) and Cu modified with 6 μm of Nafion (red line) at -1.4 V in 2 mM NO and 100 mM Na_2SO_4 (A), and UV-Vis absorption spectra after chronoamperometry for NH_3 (B) detection.

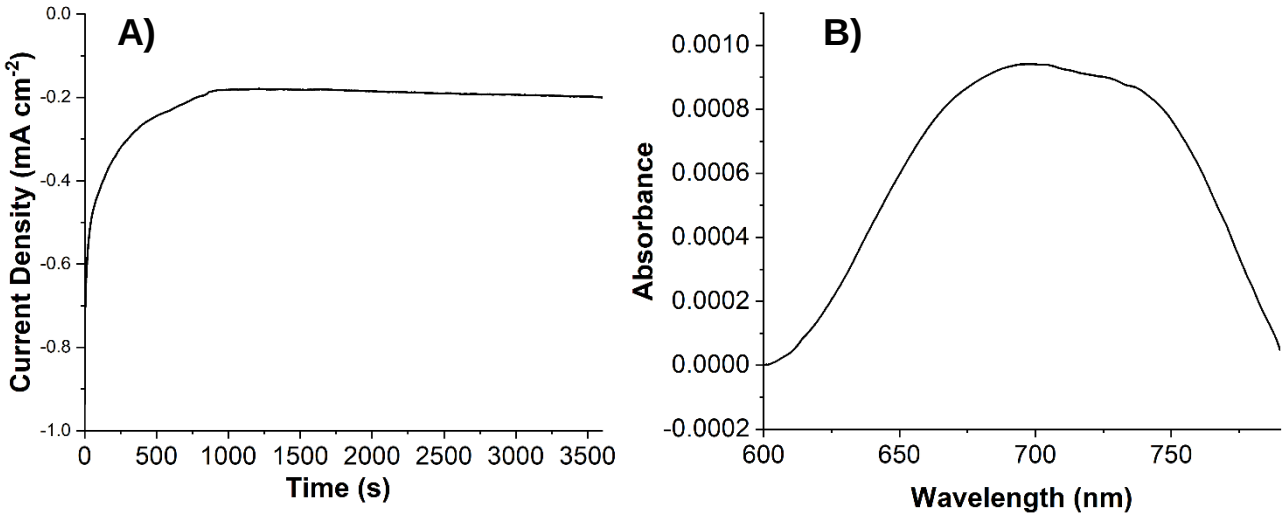

Figure S19: Chronoamperometry curve of Cu modified with 6 μm of Nafion at -1.4 V in groundwater obtained from a well in Silver Springs, Nevada, United States, and UV-Vis absorption spectrum after chronoamperometry for NH_3 detection (B).

Pseudopotentials and plane wave basis sets:

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C 12.01070 C.pbe-n-kjpaw_psl.1.0.0.UPF
F 18.99840 F.pbe-n-kjpaw_psl.1.0.0.UPF
S 32.06500 S.pbe-nl-kjpaw_psl.1.0.0.UPF

FIRST PROTONATION ON CU111 Surfaces

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Cu 6.395065014 11.077118519 27.073685965

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H 4.710914626 5.385579142 29.600230492
H 4.522678373 7.714491231 29.750959041
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H 6.666814554 4.155203909 29.976130476
End final coordinates

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ATOMIC_POSITIONS (angstrom)
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Cu -1.278850839 3.691702335 22.978979452 0 0 0
Cu -2.557695540 5.906724349 22.978979452 0 0 0
Cu -3.836538707 8.121746364 22.978979452 0 0 0
Cu -5.115383407 10.336769913 22.978979452 0 0 0
Cu -6.394226574 12.551793462 22.978979452 0 0 0
Cu 2.557677125 1.476680320 22.978979452 0 0 0
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Cu -1.278852374 8.121746364 22.978979452 0 0 0
Cu -2.557697075 10.336769913 22.978979452 0 0 0
Cu -3.836540241 12.551793462 22.978979452 0 0 0
Cu 5.115363457 1.476680320 22.978979452 0 0 0
Cu 3.836518757 3.691702335 22.978979452 0 0 0
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End final coordinates

NO-Cu111-Nafion
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Cu -2.543831652 10.324276993 22.997134664
Cu -3.830183976 12.548026314 22.998185068
Cu 5.116905282 1.460617413 22.977400029
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Cu 0.002634983 10.323030853 23.015167627
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Cu 0.023462013 2.933397111 25.091483298
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Cu -5.107855789 11.802099145 25.029854759
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Cu 1.301051879 5.167883407 25.124890456
Cu 0.007117410 7.367208157 25.132914161
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Cu -2.550006019 11.800731022 25.039996215
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End final coordinates

NOH-Cu111-Nafion
CELL_PARAMETERS (angstrom)
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ATOMIC_POSITIONS (angstrom)
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Cu 10.226286219 2.952893869 25.014780052
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Cu 7.673226139 7.385716112 24.995013399

Cu 6.398678941 9.607551753 25.000239354
Cu 5.113936367 11.815530956 25.025449462
Cu 14.061609478 0.735040977 25.025411913
Cu 12.782136913 2.950267320 25.012334804
Cu 11.500799877 5.174945113 25.008749915
Cu 10.229925335 7.391140549 25.011847300
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Cu 8.952607645 2.221341807 27.071022454
Cu 7.704126151 4.438382934 27.037013358
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End final coordinates

SECOND PROTONATION ON CU111 Surfaces

NOH-w-Eigen-Cu111
CELL_PARAMETERS (angstrom)
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ATOMIC_POSITIONS (angstrom)
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Cu -1.278850839 3.691702335 22.978979452 0 0 0
Cu -2.557695540 5.906724349 22.978979452 0 0 0
Cu -3.836538707 8.121746364 22.978979452 0 0 0
Cu -5.115383407 10.336769913 22.978979452 0 0 0
Cu -6.394226574 12.551793462 22.978979452 0 0 0
Cu 2.557677125 1.476680320 22.978979452 0 0 0
Cu 1.278832424 3.691702335 22.978979452 0 0 0
Cu -0.000009208 5.906724349 22.978979452 0 0 0
Cu -1.278852374 8.121746364 22.978979452 0 0 0
Cu -2.557697075 10.336769913 22.978979452 0 0 0
Cu -3.836540241 12.551793462 22.978979452 0 0 0
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Cu 3.836518757 3.691702335 22.978979452 0 0 0
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End final coordinates

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ATOMIC_POSITIONS (angstrom)
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Cu -1.278850839 3.691702335 22.978979452 0 0 0
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End final coordinates

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0.000000000 0.000000000 50.000000000

ATOMIC_POSITIONS (angstrom)
Cu -0.000007673 1.476683389 22.979020887 0 0 0
Cu -1.278852374 3.691708473 22.979020887 0 0 0
Cu -2.557700144 5.906735091 22.979020887 0 0 0
Cu -3.836544845 8.121760175 22.979020887 0 0 0

Cu	-5.115392615	10.336788328	22.979020887	0	0	0
Cu	-6.394237316	12.551816481	22.979020887	0	0	0
Cu	2.557681729	1.476683389	22.979020887	0	0	0
Cu	1.278833959	3.691708473	22.979020887	0	0	0
Cu	-0.000009208	5.906735091	22.979020887	0	0	0
Cu	-1.278853909	8.121760175	22.979020887	0	0	0
Cu	-2.557701679	10.336788328	22.979020887	0	0	0
Cu	-3.836546380	12.551816481	22.979020887	0	0	0
Cu	5.115372665	1.476683389	22.979020887	0	0	0
Cu	3.836524895	3.691708473	22.979020887	0	0	0
Cu	2.557680194	5.906735091	22.979020887	0	0	0
Cu	1.278832424	8.121760175	22.979020887	0	0	0
Cu	-0.000012277	10.336788328	22.979020887	0	0	0
Cu	-1.278856978	12.551816481	22.979020887	0	0	0
Cu	7.673062067	1.476683389	22.979020887	0	0	0
Cu	6.394215831	3.691708473	22.979020887	0	0	0
Cu	5.115371131	5.906735091	22.979020887	0	0	0
Cu	3.836523360	8.121760175	22.979020887	0	0	0
Cu	2.557678660	10.336788328	22.979020887	0	0	0
Cu	1.278830889	12.551816481	22.979020887	0	0	0
Cu	10.230753003	1.476683389	22.979020887	0	0	0
Cu	8.951905233	3.691708473	22.979020887	0	0	0
Cu	7.673062067	5.906735091	22.979020887	0	0	0
Cu	6.394214297	8.121760175	22.979020887	0	0	0
Cu	5.115369596	10.336788328	22.979020887	0	0	0
Cu	3.836521826	12.551816481	22.979020887	0	0	0
Cu	12.788443940	1.476683389	22.979020887	0	0	0
Cu	11.509596170	3.691708473	22.979020887	0	0	0
Cu	10.230751469	5.906735091	22.979020887	0	0	0
Cu	8.951905233	8.121760175	22.979020887	0	0	0
Cu	7.673060532	10.336788328	22.979020887	0	0	0
Cu	6.394212762	12.551816481	22.979020887	0	0	0
N	2.509659042	1.501735133	28.132059268			
O	2.503860957	4.077383182	29.313646378			
H	2.315982535	3.104635631	29.211693101			
Cu	1.277112664	0.733376132	25.040150145			
Cu	-0.006415846	2.955232770	25.025241498			
Cu	-1.288021834	5.182724562	25.006008360			
Cu	-2.560959079	7.390087697	25.018305632			
Cu	-3.838254211	9.592975352	25.018361691			
Cu	-5.115347459	11.828616033	25.046823122			
Cu	3.832245737	0.734105029	25.039637642			
Cu	2.554011489	2.972369706	25.071056127			
Cu	1.288957133	5.162601380	25.056796972			
Cu	-0.006620803	7.387788998	25.019827973			
Cu	-1.283518060	9.599310394	25.026071844			
Cu	-2.563752083	11.807681765	25.026311199			
Cu	6.391849972	0.736126598	25.013043628			
Cu	5.103091818	2.967963422	25.054980587			
Cu	3.833754838	5.169868869	25.115904278			
Cu	2.565523821	7.381863974	25.047221903			
Cu	1.270218321	9.598596467	25.020633733			
Cu	-0.000230303	11.810728781	25.026227685			
Cu	8.948013869	0.733861058	25.015386563			
Cu	7.681925553	2.972938798	25.033591056			
Cu	6.395354293	5.152367374	25.066773220			
Cu	5.102926518	7.371734503	25.032706358			
Cu	3.828345026	9.602768308	25.013818740			
Cu	2.555063244	11.814505596	25.026629041			
Cu	11.505616014	0.740019595	25.027266895			
Cu	10.230323586	2.956360919	25.015107459			
Cu	8.938877196	5.167641773	25.047494229			
Cu	7.676065697	7.384072094	24.999531890			
Cu	6.395744787	9.606040609	24.999765086			
Cu	5.110388827	11.815906337	25.025171733			
Cu	14.063817240	0.743643267	25.029203486			
Cu	12.772442687	2.958676258	25.008888632			
Cu	11.500371214	5.178748881	25.007153089			
Cu	10.229153372	7.385564527	25.013094770			
Cu	8.959259815	9.599029686	25.003282116			
Cu	7.676284843	11.812745703	25.026597064			
Cu	-0.052690209	-0.032382992	27.073352875			
Cu	-1.336434674	2.227819107	27.050683704			
Cu	-2.575946104	4.442128835	27.038246977			
Cu	-3.842255751	6.657295657	27.056058040			
Cu	-5.121462916	8.854321957	27.070017835			
Cu	-6.401677026	11.045149276	27.058481301			
Cu	2.545885878	-0.084345091	27.177508631			
Cu	1.154526746	2.215501694	27.087589249			
Cu	-0.067061567	4.449778125	27.041119171			
Cu	-1.300557688	6.657354452	27.069923597			
Cu	-2.564201317	8.857454354	27.073199883			
Cu	-3.836432765	11.047906838	27.057514980			
Cu	5.156131110	-0.039785169	27.066048457			
Cu	3.899420982	2.186500132	27.102072091			
Cu	2.500239867	4.479163752	27.182141722			
Cu	1.242446258	6.680195463	27.056191317			
Cu	-0.010858689	8.867520373	27.070738852			
Cu	-1.276207586	11.066850060	27.074924240			
Cu	7.684567150	-0.008819793	27.073678798			
Cu	6.427942296	2.181858220	27.017251405			
Cu	5.146417203	4.429156888	27.132251747			
Cu	3.833281378	6.715053024	27.147288836			
Cu	2.540904609	8.897315904	27.060347630			
Cu	1.276183374	11.079724594	27.074487580			
Cu	10.231856753	-0.004182565	27.070178850			
Cu	8.978453246	2.187716869	27.039756313			
Cu	7.727237894	4.429553725	27.161032988			
Cu	6.429186477	6.686434659	27.025010601			
Cu	5.127104676	8.896988857	27.015066019			
Cu	3.835623358	11.078754871	27.077439588			
Cu	12.773058024	-0.002200001	27.076712768			
Cu	11.498738963	2.219983584	27.076146165			
Cu	10.257617973	4.431917166	27.054321779			
Cu	8.962044152	6.672840241	27.060589029			
Cu	7.671742108	8.873644228	27.021983576			
Cu	6.385753231	11.074911335	27.072657633			
O	4.057496597	6.928210136	29.452461708			
H	3.177474495	6.955388092	29.868560618			
H	4.942052570	5.477290365	29.507218364			
H	4.571000298	7.765313414	29.727344290			
O	5.492330746	9.008416140	30.151158528			
H	5.413226561	9.706335957	29.465098316			
H	6.456213614	8.780990191	30.166009696			
O	11.850201156	5.152179379	30.115616750			
O	9.238044521	5.728396208	30.704396750			
O	8.291562550	8.360178114	30.157688386			
O	7.758021454	4.130741248	29.411879678			
H	10.202364717	5.622451506	30.476804649			
H	12.304634357	5.789329723	29.524392057			
H	8.993976513	6.672265466	30.563397328			
H	8.389372594	4.787563117	29.929583496			
H	8.809658984	9.113959903	30.495269799			
H	8.478446119	8.358870371	29.179410139			
H	11.826117426	4.341427307	29.563794367			
O	5.164645034	4.527091331	29.304147438			
H	6.123078696	4.349587097	29.539320349			
H	3.468142774	4.089439998	29.538282261			
H	8.099334024	3.226027785	29.536914536			

End final coordinates

N-OH_2-Cu111-Nafion

CELL_PARAMETERS (angstrom)

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 15.346059799   0.000000000   0.000000000
 -7.673035145  13.290086719   0.000000000
  0.000000000   0.000000000  50.000000000
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ATOMIC_POSITIONS (angstrom)

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Cu     -0.000007673   1.476680320  22.978979452   0  0  0
Cu     -1.278850839   3.691702335  22.978979452   0  0  0
Cu     -2.557695540   5.906724349  22.978979452   0  0  0
Cu     -3.836538707   8.121746364  22.978979452   0  0  0
Cu     -5.115383407  10.336769913  22.978979452   0  0  0
Cu     -6.394226574  12.551793462  22.978979452   0  0  0
Cu      2.557677125   1.476680320  22.978979452   0  0  0
Cu      1.278832424   3.691702335  22.978979452   0  0  0
Cu     -0.000009208   5.906724349  22.978979452   0  0  0
Cu     -1.278852374   8.121746364  22.978979452   0  0  0
Cu     -2.557697075  10.336769913  22.978979452   0  0  0
Cu     -3.836540241  12.551793462  22.978979452   0  0  0
Cu      5.115363457   1.476680320  22.978979452   0  0  0
Cu      3.836518757   3.691702335  22.978979452   0  0  0
Cu      2.557675590   5.906724349  22.978979452   0  0  0
Cu      1.278830889   8.121746364  22.978979452   0  0  0
Cu     -0.000012277  10.336769913  22.978979452   0  0  0
Cu     -1.278855443  12.551793462  22.978979452   0  0  0
Cu      7.673048255   1.476680320  22.978979452   0  0  0
Cu      6.394205089   3.691702335  22.978979452   0  0  0
Cu      5.115361923   5.906724349  22.978979452   0  0  0
Cu      3.836517222   8.121746364  22.978979452   0  0  0
Cu      2.557674056  10.336769913  22.978979452   0  0  0
Cu      1.278829355  12.551793462  22.978979452   0  0  0
Cu     10.230734588   1.476680320  22.978979452   0  0  0
Cu      8.951889887   3.691702335  22.978979452   0  0  0
Cu      7.673048255   5.906724349  22.978979452   0  0  0
Cu      6.394203555   8.121746364  22.978979452   0  0  0
Cu      5.115360388  10.336769913  22.978979452   0  0  0
Cu      3.836515687  12.551793462  22.978979452   0  0  0
Cu     12.788420921   1.476680320  22.978979452   0  0  0
Cu     11.509576220   3.691702335  22.978979452   0  0  0
Cu     10.230733053   5.906724349  22.978979452   0  0  0
Cu      8.951889887   8.121746364  22.978979452   0  0  0
Cu      7.673046721  10.336769913  22.978979452   0  0  0
Cu      6.394202020  12.551793462  22.978979452   0  0  0
N       0.071763587   2.982193098  28.142137216
O       2.443508518   4.234700834  29.257217266
H       3.186402301   3.713793703  29.618542736
Cu      1.287189096   0.737671777  25.029176927
Cu      0.002951052   2.953905286  25.033281282
Cu     -1.272802414   5.186213006  25.040140636
Cu     -2.557739570   7.387715241  25.037196880
Cu     -3.841829933   9.594401027  25.020014706
Cu     -5.114559110  11.797833993  25.017676151
Cu      3.841685039   0.730970823  25.014037662
Cu      2.555420544   2.965485685  25.056574805
Cu      1.286845141   5.182155203  25.087282135
Cu     -0.000814901   7.380822466  25.065001524
Cu     -1.286356232   9.597902032  25.023461354
Cu     -2.560406491  11.806610133  25.026657703
Cu      6.394737807   0.733837236  25.020510492
Cu      5.122645832   2.974675036  25.043713303
Cu      3.833812027   5.168351819  25.119322965
Cu      2.566363621   7.376119706  25.072272880
Cu      1.276999851   9.599991330  25.019859193
Cu     -0.002071219  11.811776315  25.026659409
Cu      8.952305131   0.736951298  25.025512802
Cu      7.672988127   2.947238767  25.007591295
Cu      6.373793583   5.164588895  25.034910397
Cu      5.100003868   7.372576256  25.039065005
Cu      3.836268897   9.601062280  25.010323105
Cu      2.559994557  11.812886076  25.027091256
Cu     11.510011237   0.736539251  25.027935489
Cu     10.228790938   2.950685200  25.015938253
Cu      8.954778146   5.170550294  24.995185943
Cu      7.670097322   7.382328647  24.996386635
Cu      6.396995230   9.602846569  24.997521995
Cu      5.116796651  11.811115638  25.021508385
Cu     14.070710821   0.751446064  25.056549292
Cu     12.805198237   2.937742668  25.041638694
Cu     11.508285495   5.164952559  25.007821493
Cu     10.226435821   7.386406231  25.006444225
Cu      8.952580986   9.598740507  25.007508750
Cu      7.672778967  11.817997702  25.021577499
Cu      0.000929611  -0.062631166  27.074084980
Cu     -1.338480950   2.180919557  27.224587270
Cu     -2.622428880   4.435156636  27.030687454
Cu     -3.877774663   6.643616894  27.046177584
Cu     -5.127002082   8.851987641  27.062319362
Cu     -6.393169145  11.052606847  27.069956242
Cu      2.590314054  -0.045496976  27.048967942
Cu      1.339774384   2.105706217  27.119430832
Cu     -0.056916088   4.500066973  27.098660604
Cu     -1.330317771   6.682784784  27.114546774
Cu     -2.581742557   8.879945752  27.066311175
Cu     -3.839856714  11.059122969  27.071988323
Cu      5.134341781  -0.019507998  27.071888782
Cu      3.876982888   2.155950998  27.027731927
Cu      2.583264332   4.427348119  27.153852068
Cu      1.260592266   6.707659885  27.118377685
Cu     -0.015028472   8.923132620  27.055574710
Cu     -1.286810142  11.082037172  27.078772413
Cu      7.679212904  -0.003099409  27.075210665
Cu      6.430726000   2.186910818  27.055658362
Cu      5.174404201   4.397363277  27.159146313
Cu      3.873597598   6.701224443  27.159831823
Cu      2.563701844   8.924031574  27.046307953
Cu      1.279155487  11.093537361  27.077246177
Cu     10.222647188  -0.001684820  27.072196474
Cu      8.953640692   2.216666997  27.068781804
Cu      7.707301679   4.427162951  27.010732869
Cu      6.443682063   6.664201214  27.037900552
Cu      5.137311170   8.897799122  27.021097155
Cu      3.845915467  11.084781443  27.074568041
Cu     12.770950618  -0.010464352  27.064224168
Cu     11.488173764   2.203966585  27.065930040
Cu     10.215044474   4.424712020  27.063535164
Cu      8.949073563   6.639761676  27.043756414
Cu      7.673883573   8.865382367  27.025805625
Cu      6.396248286  11.068280171  27.071657013
O       0.148761553   5.303536458  30.959418322
S      -0.019034396   6.538700123  30.217769672
C      -0.104666754   7.935345573  31.495089041
C      -1.231121106   7.798750099  32.571805848
O      -1.006854092   6.640182165  33.293938167
C      -1.641975061   6.433503644  34.513074397
F      -1.049309637   7.130894222  35.504862843
F      -2.950928595   6.770771081  34.481936121
F      -1.530111536   5.125459568  34.780641939
F      -1.217815462   8.908242780  33.364371713
F      -2.450181161   7.768020956  31.951633354
F      -0.306891538   9.105115419  30.832230818
F       1.096083548   7.990504363  32.133444203
O      -1.310445786   6.672835621  29.468302524
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O 1.140081761 6.983676134 29.384640715
O 3.949005753 6.796823975 29.368783832
H 3.003368085 6.808403341 29.651271925
H 4.853727872 5.334020584 29.562144415
H 4.410088699 7.634159896 29.688523948
O 5.396250821 8.904068998 30.172105870
H 5.365820060 9.609884276 29.489644897
H 6.341452133 8.637863109 30.204452513
O 11.795211172 5.260115856 30.119407453
O 9.600087133 5.873206557 30.987914251
O 8.292117984 7.980340576 30.052849730
O 8.037719223 3.890034382 30.138938183
H 10.632445952 5.690589514 30.573928582
H 12.586776924 5.861806294 30.023573449
H 9.165981917 6.721551307 30.635920633
H 9.009946589 5.097080799 30.716071607
H 8.832129237 8.791798322 29.955328766
H 8.144931046 7.719279673 29.096249559
H 11.657363065 4.897380754 29.205324018
H 8.303229786 3.721552169 29.189188372
O 5.192634984 4.414280350 29.372599338
H 6.115605258 4.338807244 29.700794756
H 1.603618158 3.722824489 29.357512034
H 8.085139237 3.013450932 30.566048854
End final coordinates

NB: We accounted for water loss before moving to the next protonation step.

THIRD PROTONATION ON CU111 Surfaces

N-Eigen-Cu111
CELL_PARAMETERS (angstrom)
15.346059799 0.000000000 0.000000000
-7.673035145 13.290086719 0.000000000
0.000000000 0.000000000 50.000000000

ATOMIC_POSITIONS (angstrom)
Cu -0.000007673 1.476686458 22.979062321 0 0 0
Cu -1.278853909 3.691714611 22.979062321 0 0 0
Cu -2.557704748 5.906745834 22.979062321 0 0 0
Cu -3.836550983 8.121773987 22.979062321 0 0 0
Cu -5.115401823 10.336806743 22.979062321 0 0 0
Cu -6.394248058 12.551839500 22.979062321 0 0 0
Cu 2.557686333 1.476686458 22.979062321 0 0 0
Cu 1.278835493 3.691714611 22.979062321 0 0 0
Cu -0.000009208 5.906745834 22.979062321 0 0 0
Cu -1.278855443 8.121773987 22.979062321 0 0 0
Cu -2.557706282 10.336806743 22.979062321 0 0 0
Cu -3.836552518 12.551839500 22.979062321 0 0 0
Cu 5.115381873 1.476686458 22.979062321 0 0 0
Cu 3.836531033 3.691714611 22.979062321 0 0 0
Cu 2.557684798 5.906745834 22.979062321 0 0 0
Cu 1.278833959 8.121773987 22.979062321 0 0 0
Cu -0.000012277 10.336806743 22.979062321 0 0 0
Cu -1.278858512 12.551839500 22.979062321 0 0 0
Cu 7.673075878 1.476686458 22.979062321 0 0 0
Cu 6.394226574 3.691714611 22.979062321 0 0 0
Cu 5.115380338 5.906745834 22.979062321 0 0 0
Cu 3.836529499 8.121773987 22.979062321 0 0 0
Cu 2.557683263 10.336806743 22.979062321 0 0 0
Cu 1.278832424 12.551839500 22.979062321 0 0 0
Cu 10.230771419 1.476686458 22.979062321 0 0 0
Cu 8.951920579 3.691714611 22.979062321 0 0 0
Cu 7.673075878 5.906745834 22.979062321 0 0 0
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End final coordinates

NH-Cu111
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O 7.786097391 4.185853628 29.394116321
H 10.221737889 5.608743383 30.522927486
H 12.291595926 5.698885699 29.504273034
H 9.025557590 6.674298565 30.612425793
H 8.416961980 4.823182865 29.934127246
H 8.785146464 9.105900752 30.468527663
H 8.458784788 8.303187985 29.182195981
H 11.759408764 4.271293508 29.556329716
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H 6.095599005 4.415185635 29.533553232
H 8.085594280 3.271643280 29.555250185
End final coordinates

NH-Cu111-Nafion
CELL_PARAMETERS (angstrom)
15.346059799 0.000000000 0.000000000
-7.673035145 13.290086719 0.000000000
0.000000000 0.000000000 50.000000000

ATOMIC_POSITIONS (angstrom)
Cu -0.000007673 1.476683389 22.979020887 0 0 0
Cu -1.278852374 3.691708473 22.979020887 0 0 0
Cu -2.557700144 5.906735091 22.979020887 0 0 0
Cu -3.836544845 8.121760175 22.979020887 0 0 0
Cu -5.115392615 10.336788328 22.979020887 0 0 0
Cu -6.394237316 12.551816481 22.979020887 0 0 0
Cu 2.557681729 1.476683389 22.979020887 0 0 0
Cu 1.278833959 3.691708473 22.979020887 0 0 0
Cu -0.000009208 5.906735091 22.979020887 0 0 0
Cu -1.278853909 8.121760175 22.979020887 0 0 0
Cu -2.557701679 10.336788328 22.979020887 0 0 0
Cu -3.836546380 12.551816481 22.979020887 0 0 0
Cu 5.115372665 1.476683389 22.979020887 0 0 0
Cu 3.836524895 3.691708473 22.979020887 0 0 0
Cu 2.557680194 5.906735091 22.979020887 0 0 0
Cu 1.278832424 8.121760175 22.979020887 0 0 0
Cu -0.000012277 10.336788328 22.979020887 0 0 0
Cu -1.278856978 12.551816481 22.979020887 0 0 0
Cu 7.673062067 1.476683389 22.979020887 0 0 0
Cu 6.394215831 3.691708473 22.979020887 0 0 0
Cu 5.115371131 5.906735091 22.979020887 0 0 0
Cu 3.836523360 8.121760175 22.979020887 0 0 0
Cu 2.557678660 10.336788328 22.979020887 0 0 0
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Cu 7.673062067 5.906735091 22.979020887 0 0 0
Cu 6.394214297 8.121760175 22.979020887 0 0 0
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Cu 8.951905233 8.121760175 22.979020887 0 0 0
Cu 7.673060532 10.336788328 22.979020887 0 0 0
Cu 6.394212762 12.551816481 22.979020887 0 0 0
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Cu 0.002100868 2.955409058 25.042467963
Cu -1.267704256 5.169873695 25.061348373
Cu -2.559604660 7.381266563 25.036948927
Cu -3.844228442 9.596646383 25.019699696
Cu -5.120269676 11.806680771 25.017679282
Cu 3.828821951 0.734229177 25.023043806
Cu 2.547234418 2.960976561 25.043444775
Cu 1.273081139 5.178879367 25.062102399
Cu -0.013503676 7.376161954 25.063850532
Cu -1.290437215 9.600157841 25.021622813
Cu -2.564463363 11.810833038 25.024226476
Cu 6.390695677 0.731924166 25.021247184
Cu 5.108617784 2.972060233 25.055957358
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Cu 5.161506840 4.409451944 27.166319483
Cu 3.861006869 6.697611778 27.159374958
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Cu 7.699914160 4.427135362 27.014813890
Cu 6.435088607 6.666124132 27.043073146
Cu 5.128361290 8.891378829 27.026196838
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Cu 12.778442479 -0.007261451 27.076053143
Cu 11.490232229 2.213664571 27.081019354
Cu 10.210109370 4.425514970 27.061832228
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Cu 7.668531575 8.865530017 27.030727781
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C -0.220948158 8.005305021 31.459823626
C -1.347148356 7.856427736 32.535705467
O -1.044202660 6.767778148 33.333048565
C -1.677282250 6.590277116 34.558891741
F -1.153253832 7.394747978 35.506891584
F -3.007749615 6.821633171 34.496628081
F -1.466776696 5.314611258 34.909597865
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F -2.554606943 7.695157435 31.911750565
F -0.502438312 9.113957481 30.723766441
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O 1.114332700 7.024801728 29.410745168
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O 11.766406536 5.163493412 30.132212029
O 9.549140026 5.795467106 30.957026354
O 8.250140469 7.917520713 30.058916887
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H 8.097284176 7.676154784 29.097988079
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H 8.174302834 3.648174636 29.206351581
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End final coordinates

Fourth-protonation on Cu(111) surfaces

NH-Eigen-Cu111
CELL_PARAMETERS (angstrom)
15.346059799 0.000000000 0.000000000
-7.673035145 13.290086719 0.000000000
0.000000000 0.000000000 50.000000000

ATOMIC_POSITIONS (angstrom)
Cu -0.000007673 1.476686458 22.979062321 0 0 0
Cu -1.278853909 3.691714611 22.979062321 0 0 0
Cu -2.557704748 5.906745834 22.979062321 0 0 0
Cu -3.836550983 8.121773987 22.979062321 0 0 0
Cu -5.115401823 10.336806743 22.979062321 0 0 0
Cu -6.394248058 12.551839500 22.979062321 0 0 0
Cu 2.557686333 1.476686458 22.979062321 0 0 0
Cu 1.278835493 3.691714611 22.979062321 0 0 0
Cu -0.000009208 5.906745834 22.979062321 0 0 0
Cu -1.278855443 8.121773987 22.979062321 0 0 0
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Cu 0.019482450 2.950090705 25.052373736
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Cu -2.554698319 7.386477354 25.017315588
Cu -3.835866662 9.598737331 25.024104869
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Cu 2.567349343 2.959717613 25.037388168
Cu 1.298076196 5.162631647 25.054274057
Cu -0.005379281 7.391026643 25.019304623
Cu -1.281137283 9.598675458 25.024694923
Cu -2.556381658 11.806709991 25.022088729
Cu 6.401495300 0.733734940 25.022935416
Cu 5.098683606 2.954466551 25.074061308
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Cu 1.273602672 9.601531461 25.022303462
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Cu 8.957442934 0.741211721 25.027342482
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Cu 6.379566372 5.161200730 25.030789565
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Cu -3.839233180 6.654377127 27.050681801
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Cu -6.393763815 11.066811070 27.073749198
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Cu 1.235581253 2.185747451 27.165884214
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Cu -1.294953341 6.653077738 27.077602886
Cu -2.562703779 8.857909545 27.073046241
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Cu 3.910024365 2.146695149 27.199448150
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End final coordinates

NH-Eigen-Cu111-Nafion
CELL_PARAMETERS (angstrom)
15.346059799 0.000000000 0.000000000
-7.673035145 13.290086719 0.000000000
0.000000000 0.000000000 50.000000000

ATOMIC_POSITIONS (angstrom)
Cu -0.000007673 1.476683389 22.979020887 0 0 0
Cu -1.278852374 3.691708473 22.979020887 0 0 0
Cu -2.557700144 5.906735091 22.979020887 0 0 0
Cu -3.836544845 8.121760175 22.979020887 0 0 0
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Cu 1.278832424 8.121760175 22.979020887 0 0 0
Cu -0.000012277 10.336788328 22.979020887 0 0 0
Cu -1.278856978 12.551816481 22.979020887 0 0 0

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Cu	5.115371131	5.906735091	22.979020887	0	0	0
Cu	3.836523360	8.121760175	22.979020887	0	0	0
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Cu	6.394214297	8.121760175	22.979020887	0	0	0
Cu	5.115369596	10.336788328	22.979020887	0	0	0
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Cu	-2.551495931	7.384408264	25.037244499			
Cu	-3.836652761	9.597830547	25.021963291			
Cu	-5.114780362	11.807835936	25.021270584			
Cu	3.832687942	0.739691659	25.034773648			
Cu	2.550676944	2.959426840	25.055229835			
Cu	1.280480975	5.176616972	25.074732252			
Cu	-0.000190438	7.375168962	25.075867127			
Cu	-1.279739587	9.601077800	25.025143798			
Cu	-2.558119506	11.816091012	25.027417184			
Cu	6.397957228	0.739134572	25.029918506			
Cu	5.116905400	2.955176028	25.025053524			
Cu	3.814512480	5.158988385	25.052529452			
Cu	2.550440101	7.381232516	25.052255363			
Cu	1.279984934	9.604735019	25.027299661			
Cu	0.000897059	11.816910530	25.025890203			
Cu	8.954212031	0.741850113	25.026745348			
Cu	7.674577908	2.950603896	25.014717348			
Cu	6.401860625	5.178443756	25.001439610			
Cu	5.122654394	7.385655083	25.006325092			
Cu	3.836244087	9.603406758	25.012051506			
Cu	2.562073783	11.815570937	25.026663492			
Cu	11.509673474	0.737710061	25.030521294			
Cu	10.232214967	2.951355341	25.021730015			
Cu	8.958305230	5.172561120	25.003018229			
Cu	7.677776242	7.386874810	25.004322033			
Cu	6.399185552	9.603313278	25.004835755			
Cu	5.118352415	11.814437416	25.026855592			
Cu	14.074942486	0.733445177	25.034189773			
Cu	12.791492377	2.951068806	25.022519081			
Cu	11.501010175	5.175268462	25.006213424			
Cu	10.231557596	7.391186945	25.010765078			
Cu	8.957835506	9.598735371	25.012992135			
Cu	7.677194795	11.806381047	25.023347766			
Cu	-0.002500080	-0.035459344	27.068265524			
Cu	-1.318922547	2.189760146	27.076906022			
Cu	-2.600660772	4.427797353	27.026388317			
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Cu	2.565798300	-0.028605205	27.066876661			
Cu	1.279127369	2.129932615	27.197831221			
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Cu	-1.318127283	6.665277455	27.128052858			
Cu	-2.568199820	8.875653675	27.068976402			
Cu	-3.835157155	11.070521663	27.070954675			
Cu	5.124956347	0.001649824	27.078306004			
Cu	3.884173576	2.202409902	27.081426551			
Cu	2.654399469	4.471340286	27.190193936			
Cu	1.298261743	6.697519340	27.156318726			
Cu	-0.001339210	8.898951756	27.067256393			
Cu	-1.278669409	11.085488764	27.072579768			
Cu	7.678697329	0.008596628	27.076815817			
Cu	6.410191994	2.228716509	27.084333907			
Cu	5.160494067	4.450363840	27.032290688			
Cu	3.884320022	6.668187456	27.054067429			
Cu	2.578537006	8.887397715	27.068484301			
Cu	1.284554731	11.089297375	27.076707215			
Cu	10.230220587	0.005078910	27.074294890			
Cu	8.947892564	2.227984874	27.075796628			
Cu	7.685403598	4.442805976	27.026015529			
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Cu	3.845504541	11.075069757	27.076465738			
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S	0.056041344	6.484692596	30.399003760			
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End final coordinates

NH_2-Cu111

CELL_PARAMETERS (angstrom)

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Cu     -2.557700144   5.906735091  22.979020887   0  0  0
Cu     -3.836544845   8.121760175  22.979020887   0  0  0
Cu     -5.115392615  10.336788328  22.979020887   0  0  0
Cu     -6.394237316  12.551816481  22.979020887   0  0  0
Cu      2.557681729   1.476683389  22.979020887   0  0  0
Cu      1.278833959   3.691708473  22.979020887   0  0  0
Cu     -0.000009208   5.906735091  22.979020887   0  0  0
Cu     -1.278853909   8.121760175  22.979020887   0  0  0
Cu     -2.557701679  10.336788328  22.979020887   0  0  0
Cu     -3.836546380  12.551816481  22.979020887   0  0  0
Cu      5.115372665   1.476683389  22.979020887   0  0  0
Cu      3.836524895   3.691708473  22.979020887   0  0  0
Cu      2.557680194   5.906735091  22.979020887   0  0  0
Cu      1.278832424   8.121760175  22.979020887   0  0  0
Cu     -0.000012277  10.336788328  22.979020887   0  0  0
Cu     -1.278856978  12.551816481  22.979020887   0  0  0
Cu      7.673062067   1.476683389  22.979020887   0  0  0
Cu      6.394215831   3.691708473  22.979020887   0  0  0
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Cu     10.230753003   1.476683389  22.979020887   0  0  0
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Cu      6.394214297   8.121760175  22.979020887   0  0  0
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Cu      8.951905233   8.121760175  22.979020887   0  0  0
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Cu      0.023440184   2.948798508  25.053549283
Cu     -1.283306989   5.175823673  25.000566508
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Cu     -5.116817156  11.809471381  25.021071797
Cu      3.836066108   0.720810017  25.006782442
Cu      2.556263206   2.963746839  25.056384068
Cu      1.294786846   5.166205727  25.035408145
Cu     -0.004854267   7.388154777  25.018001982
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Cu      8.936273962   5.159897016  25.049982084
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Cu      5.118743888  11.815538923  25.024204274
Cu     14.074993770   0.737353704  25.030336174
Cu     12.793564023   2.951299477  25.016861961
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Cu     10.227661594   7.382855049  25.013006708
Cu      8.957225065   9.598966785  25.010679472
Cu      7.679324351  11.817987317  25.023689046
Cu      0.000803707  -0.007953426  27.075368278
Cu     -1.290775331   2.212047517  27.068250939
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End final coordinates

NH_2-Cu111-Nafion
CELL_PARAMETERS (angstrom)
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Cu 11.499776188 2.217249276 27.078726567
Cu 10.220506395 4.426749751 27.062580985
Cu 8.952379494 6.642550266 27.044903700
Cu 7.676416731 8.869356583 27.030780263
Cu 6.401661325 11.077369790 27.073084188
O 0.235935668 5.348644578 31.048206974
S -0.019979997 6.550045441 30.268149817
C -0.217065651 8.004343890 31.473719055
C -1.347687296 7.857230650 32.544902998
O -1.046416561 6.766941574 33.341608395
C -1.680642355 6.588314779 34.566548819

F -1.157193245 7.391962726 35.516076921
F -3.010796055 6.819948142 34.503325182
F -1.470216237 5.311938156 34.916057050
F -1.427176564 9.013404142 33.263709544
F -2.553228205 7.697732460 31.918583090
F -0.494905708 9.111747664 30.734793964
F 0.967096644 8.188673184 32.116481292
O -1.307037015 6.570662101 29.510518429
O 1.120475676 7.020137375 29.425214188
O 3.853203358 6.753987291 29.386248477
H 2.900168980 6.859427854 29.630555325
H 4.641986778 5.227432757 29.552163053
H 4.365033745 7.560246768 29.710228915
O 5.356648853 8.819539120 30.202014620
H 5.321613248 9.526850312 29.521614386
H 6.302761339 8.555656632 30.230177204
O 11.764093327 5.164140440 30.136513574
O 9.540524514 5.792644614 30.954206347
O 8.250128799 7.917205761 30.056305673
O 7.922501153 3.854114969 30.156567325
H 10.564165037 5.604457081 30.564126729
H 12.554372352 5.764920722 30.059478164
H 9.119152380 6.650828728 30.606517335
H 8.936762770 5.023275000 30.680376336
H 8.790674516 8.730186110 29.971467866
H 8.096840643 7.674230696 29.095759400
H 11.659747902 4.790966823 29.223407236
H 8.153315366 3.653166877 29.204714206
O 5.053928513 4.345617180 29.334622782
H 5.959460164 4.329255603 29.712064605
H 7.954569850 2.988913205 30.606511043
H 2.626728088 3.044049154 29.305909469
End final coordinates

Fifth-protonation on Cu111 surfaces

NH_2-Eigen-Cu111
CELL_PARAMETERS (angstrom)
15.346059799 0.000000000 0.000000000
-7.673035145 13.290086719 0.000000000
0.000000000 0.000000000 50.000000000

ATOMIC_POSITIONS (angstrom)
Cu -0.000007673 1.476689528 22.979103755 0 0 0
Cu -1.278855443 3.691720750 22.979103755 0 0 0
Cu -2.557709352 5.906756576 22.979103755 0 0 0
Cu -3.836557122 8.121787798 22.979103755 0 0 0
Cu -5.115411030 10.336825159 22.979103755 0 0 0
Cu -6.394258800 12.551862519 22.979103755 0 0 0
Cu 2.557690936 1.476689528 22.979103755 0 0 0
Cu 1.278837028 3.691720750 22.979103755 0 0 0
Cu -0.000009208 5.906756576 22.979103755 0 0 0
Cu -1.278856978 8.121787798 22.979103755 0 0 0
Cu -2.557710886 10.336825159 22.979103755 0 0 0
Cu -3.836558656 12.551862519 22.979103755 0 0 0
Cu 5.115391080 1.476689528 22.979103755 0 0 0
Cu 3.836537172 3.691720750 22.979103755 0 0 0
Cu 2.557689402 5.906756576 22.979103755 0 0 0
Cu 1.278835493 8.121787798 22.979103755 0 0 0
Cu -0.000012277 10.336825159 22.979103755 0 0 0
Cu -1.278860047 12.551862519 22.979103755 0 0 0
Cu 7.673089690 1.476689528 22.979103755 0 0 0
Cu 6.394237316 3.691720750 22.979103755 0 0 0
Cu 5.115389546 5.906756576 22.979103755 0 0 0
Cu 3.836535637 8.121787798 22.979103755 0 0 0
Cu 2.557687867 10.336825159 22.979103755 0 0 0
Cu 1.278833959 12.551862519 22.979103755 0 0 0
Cu 10.230789834 1.476689528 22.979103755 0 0 0
Cu 8.951935925 3.691720750 22.979103755 0 0 0
Cu 7.673089690 5.906756576 22.979103755 0 0 0
Cu 6.394235781 8.121787798 22.979103755 0 0 0
Cu 5.115388011 10.336825159 22.979103755 0 0 0
Cu 3.836534103 12.551862519 22.979103755 0 0 0
Cu 12.788489978 1.476689528 22.979103755 0 0 0
Cu 11.509636069 3.691720750 22.979103755 0 0 0
Cu 10.230788299 5.906756576 22.979103755 0 0 0
Cu 8.951935925 8.121787798 22.979103755 0 0 0
Cu 7.673088155 10.336825159 22.979103755 0 0 0
Cu 6.394234247 12.551862519 22.979103755 0 0 0
N 1.863211691 3.334065644 28.730368724
H 1.129448025 3.753224961 29.308704583
Cu 1.287089253 0.774454668 25.076491810
Cu 0.019584464 2.946008252 25.050729941
Cu -1.276858754 5.174952764 25.002623749
Cu -2.551485336 7.388720579 25.019648788
Cu -3.832403829 9.600398261 25.027094575
Cu -5.113901476 11.816358655 25.025022768
Cu 3.835586459 0.731809141 25.020433502
Cu 2.557022691 2.959228058 25.069990193
Cu 1.301228296 5.156099617 25.054495870
Cu 0.005777629 7.384849906 25.022896797
Cu -1.275914222 9.598936223 25.027641781
Cu -2.553449648 11.813103448 25.026433063
Cu 6.400006552 0.737201609 25.026465510
Cu 5.122871431 2.958475850 25.008300825
Cu 3.809098512 5.162662183 25.104019202
Cu 2.578299540 7.378133845 25.052590795
Cu 1.279766109 9.598973440 25.023707250
Cu 0.004701928 11.812141151 25.027234938
Cu 8.958792793 0.740472137 25.028017223
Cu 7.678154252 2.949967150 25.015526425
Cu 6.397616067 5.173781217 25.007160193
Cu 5.107670864 7.370351421 25.038847790
Cu 3.836325806 9.603479345 25.017400944
Cu 2.562015441 11.815428018 25.027375133
Cu 11.512902392 0.741050922 25.031558970
Cu 10.234549989 2.952359200 25.021434163
Cu 8.960933899 5.173014044 25.009008292
Cu 7.679181383 7.387465407 25.002949851
Cu 6.400880943 9.604444278 25.002480657
Cu 5.118797440 11.816045408 25.026417631
Cu 14.072502470 0.736271075 25.031566999
Cu 12.790724891 2.952484334 25.019077263
Cu 11.510743252 5.172180246 25.012296340
Cu 10.236231796 7.390339109 25.013703466
Cu 8.962806599 9.605474495 25.012655774
Cu 7.680521821 11.818412654 25.025343546
Cu -0.001254919 -0.008365045 27.076671112
Cu -1.302183438 2.211193658 27.070770488
Cu -2.567079616 4.436391930 27.047081244
Cu -3.836539851 6.654795199 27.053336788
Cu -5.117278802 8.859294053 27.074146684
Cu -6.389477968 11.070021771 27.072601867
Cu 2.579061536 -0.018885187 27.074015943
Cu 1.262292645 2.183517975 27.222552813
Cu -0.068673888 4.473970367 27.017402073
Cu -1.289770801 6.657871136 27.078023989
Cu -2.557111342 8.859523042 27.076816518
Cu -3.830882102 11.067954567 27.074531837
Cu 5.135782497 -0.012675869 27.077163990
Cu 3.926510919 2.179996079 27.026764340
Cu 2.589003009 4.434328279 27.238218136

Cu 1.274197379 6.664242443 27.064723096
Cu 0.005345927 8.863719682 27.075523228
Cu -1.271464548 11.072021942 27.073911664
Cu 7.685041623 0.001964469 27.074486335
Cu 6.428665146 2.217127974 27.079655148
Cu 5.172073867 4.420237671 27.037117166
Cu 3.866452357 6.658548658 27.167622408
Cu 2.559987585 8.881740219 27.062433390
Cu 1.284961101 11.080681882 27.076482943
Cu 10.235740367 0.005628345 27.076465490
Cu 8.960943531 2.226433927 27.078319571
Cu 7.697681108 4.439986152 27.034981569
Cu 6.437580213 6.650611119 27.044954185
Cu 5.133671626 8.881992225 27.021017888
Cu 3.845951258 11.077516704 27.080483775
Cu 12.787599993 -0.000630429 27.076399542
Cu 11.507523340 2.226434322 27.081485340
Cu 10.234201114 4.435946813 27.060148278
Cu 8.965546299 6.651628532 27.052315408
Cu 7.678824038 8.869159475 27.028656750
Cu 6.400715468 11.076076091 27.071057333
O 4.017690587 6.831284110 29.489765830
H 3.099341180 7.051278913 29.732358935
H 4.707702109 5.253839851 29.995198370
H 4.578316631 7.642926926 29.726745325
O 5.538584912 8.919305959 30.147348805
H 5.485938794 9.607798522 29.447308225
H 6.489846354 8.661842491 30.165226058
O 11.650601258 5.081023754 30.099281930
O 9.226169581 5.674006309 30.876822477
O 8.363317885 8.105407895 30.110034533
O 7.666051938 3.918960871 30.235719924
H 10.170095143 5.473272791 30.535687502
H 12.046848046 5.756607385 29.503488951
H 8.943754269 6.589850387 30.577346955
H 8.477161683 4.872008010 30.537150014
H 8.938558573 8.855091959 30.355384320
H 8.437010624 8.071138037 29.111877282
H 11.623215836 4.291872071 29.511653485
O 5.083188951 4.354585130 30.192207799
H 6.672542666 4.162310916 30.235865439
H 7.854347294 3.575126578 29.328491420
H 4.795167854 3.809193593 29.427703812
H 2.511723602 2.865465052 29.369261414
End final coordinates

NH_2-Eigen-Cu111-Nafion
CELL_PARAMETERS (angstrom)
15.346059799 0.000000000 0.000000000
-7.673035145 13.290086719 0.000000000
0.000000000 0.000000000 50.000000000

ATOMIC_POSITIONS (angstrom)
Cu -0.000007673 1.476683389 22.979020887 0 0 0
Cu -1.278852374 3.691708473 22.979020887 0 0 0
Cu -2.557700144 5.906735091 22.979020887 0 0 0
Cu -3.836544845 8.121760175 22.979020887 0 0 0
Cu -5.115392615 10.336788328 22.979020887 0 0 0
Cu -6.394237316 12.551816481 22.979020887 0 0 0
Cu 2.557681729 1.476683389 22.979020887 0 0 0
Cu 1.278833959 3.691708473 22.979020887 0 0 0
Cu -0.000009208 5.906735091 22.979020887 0 0 0
Cu -1.278853909 8.121760175 22.979020887 0 0 0
Cu -2.557701679 10.336788328 22.979020887 0 0 0
Cu -3.836546380 12.551816481 22.979020887 0 0 0
Cu 5.115372665 1.476683389 22.979020887 0 0 0
Cu 3.836524895 3.691708473 22.979020887 0 0 0
Cu 2.557680194 5.906735091 22.979020887 0 0 0
Cu 1.278832424 8.121760175 22.979020887 0 0 0
Cu -0.000012277 10.336788328 22.979020887 0 0 0
Cu -1.278856978 12.551816481 22.979020887 0 0 0
Cu 7.673062067 1.476683389 22.979020887 0 0 0
Cu 6.394215831 3.691708473 22.979020887 0 0 0
Cu 5.115371131 5.906735091 22.979020887 0 0 0
Cu 3.836523360 8.121760175 22.979020887 0 0 0
Cu 2.557678660 10.336788328 22.979020887 0 0 0
Cu 1.278830889 12.551816481 22.979020887 0 0 0
Cu 10.230753003 1.476683389 22.979020887 0 0 0
Cu 8.951905233 3.691708473 22.979020887 0 0 0
Cu 7.673062067 5.906735091 22.979020887 0 0 0
Cu 6.394214297 8.121760175 22.979020887 0 0 0
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Cu 12.788443940 1.476683389 22.979020887 0 0 0
Cu 11.509596170 3.691708473 22.979020887 0 0 0
Cu 10.230751469 5.906735091 22.979020887 0 0 0
Cu 8.951905233 8.121760175 22.979020887 0 0 0
Cu 7.673060532 10.336788328 22.979020887 0 0 0
Cu 6.394212762 12.551816481 22.979020887 0 0 0
N 1.860031894 3.352632206 28.722397231
H 1.161314833 3.796719596 29.328121503
Cu 1.284397613 0.778239254 25.076230865
Cu 0.015336501 2.948497292 25.041161728
Cu -1.282161672 5.185256893 25.017006302
Cu -2.551069514 7.387341716 25.039433215
Cu -3.837437493 9.605105993 25.023702583
Cu -5.116041852 11.821297738 25.024745428
Cu 3.835537335 0.735495487 25.019785914
Cu 2.550161513 2.959791440 25.069345729
Cu 1.297218976 5.168716700 25.075178209
Cu 0.000712778 7.377071764 25.061910416
Cu -1.280194254 9.601598168 25.024014789
Cu -2.554385745 11.817344878 25.025771740
Cu 6.401053614 0.739813641 25.028958979
Cu 5.126113662 2.958766755 25.006576921
Cu 3.806680876 5.147952059 25.063568123
Cu 2.553047243 7.382974308 25.042993650
Cu 1.281028005 9.598791762 25.026950220
Cu 0.005390832 11.813352636 25.027194533
Cu 8.958710892 0.740489547 25.028150133
Cu 7.676772197 2.951575920 25.013815598
Cu 6.398244186 5.180419261 25.000780333
Cu 5.116105708 7.379585894 25.009423139
Cu 3.837417228 9.602764980 25.013301518
Cu 2.563237866 11.814036641 25.027069375
Cu 11.512022215 0.740843867 25.029821328
Cu 10.229578083 2.953506483 25.020240682
Cu 8.956939118 5.175312595 25.004577321
Cu 7.674150606 7.390691978 25.006983352
Cu 6.397837784 9.607534143 25.007137358
Cu 5.118719308 11.814836842 25.028086423
Cu 14.071008255 0.736432854 25.028558046
Cu 12.786832648 2.952258644 25.012572121
Cu 11.503410748 5.175797064 25.009150830
Cu 10.230887895 7.395673299 25.013626339
Cu 8.956965422 9.609319302 25.015901319
Cu 7.679059854 11.821379658 25.027241117
Cu -0.003923966 -0.004044892 27.075491930
Cu -1.310829198 2.210119280 27.064346686
Cu -2.588924250 4.424925242 27.031984471
Cu -3.861215562 6.649181381 27.054706959
Cu -5.121969116 8.865765746 27.072556776

Cu	-6.390567649	11.076696274	27.073976786
Cu	2.575055111	-0.007260691	27.072039301
Cu	1.248892926	2.199999675	27.223826470
Cu	-0.077212499	4.456100268	27.007669826
Cu	-1.305171519	6.658045925	27.129059220
Cu	-2.567790324	8.875068328	27.069359872
Cu	-3.834453442	11.078527348	27.074605069
Cu	5.134998330	-0.003498280	27.077205169
Cu	3.924433327	2.188386386	27.022468796
Cu	2.611801413	4.439565488	27.235658001
Cu	1.295052762	6.671784332	27.126373300
Cu	-0.000291497	8.892414307	27.062331547
Cu	-1.274604979	11.082245240	27.074937108
Cu	7.684826944	0.005880234	27.076300807
Cu	6.425589899	2.229649510	27.083863095
Cu	5.164467233	4.440688351	27.026504711
Cu	3.866506168	6.651574395	27.058963738
Cu	2.579399632	8.878815450	27.067085491
Cu	1.288617489	11.082825517	27.077304732
Cu	10.235154977	0.004150554	27.075309983
Cu	8.953131896	2.228649892	27.079437243
Cu	7.687644393	4.446276628	27.030021526
Cu	6.412582446	6.657681802	27.063006174
Cu	5.124164496	8.862986480	27.030168711
Cu	3.848553265	11.073364820	27.080424294
Cu	12.786757025	-0.000991567	27.073199606
Cu	11.498779448	2.222176440	27.076348260
Cu	10.221913638	4.436886117	27.059211438
Cu	8.949629727	6.652086687	27.048295572
Cu	7.672276958	8.871569287	27.037404128
Cu	6.399034420	11.071653807	27.074238514
O	0.224786205	5.231289000	31.129529065
S	0.037631679	6.465879605	30.381289516
C	-0.094200272	7.887744525	31.635637338
C	-1.257681654	7.786161178	32.676351154
O	-1.051671495	6.658555349	33.451694316
C	-1.728810809	6.497311624	34.655831455
F	-1.182397649	7.245760096	35.636344449
F	-3.039891513	6.815921635	34.562912230
F	-1.611780784	5.203404831	34.983355206
F	-1.278996907	8.926317491	33.424680754
F	-2.455373844	7.723335023	32.017670158
F	-0.275440620	9.037509855	30.932719941
F	1.084305909	7.965876060	32.310976777
O	-1.223483197	6.579492698	29.601341129
O	1.233406877	6.892723348	29.578585433
O	3.650355092	6.548885238	30.639489734
H	2.746683339	6.653782308	30.191876126
H	4.105163446	5.632918232	30.421804875
H	4.301136342	7.350708606	30.443130613
O	5.254108489	8.482019628	30.304297810
H	5.106241106	8.940523734	29.442637323
H	6.209469413	8.236841700	30.290511450
O	11.731345588	5.206212984	30.135663732
O	9.460569725	5.718016300	30.911731387
O	8.121875235	7.840630791	30.074869036
O	7.705545629	3.827416997	30.218577862
H	10.497334265	5.567876518	30.538395705
H	12.515724093	5.814267366	30.129382682
H	9.026692246	6.576552041	30.583787684
H	8.851456714	4.953113669	30.643687169
H	8.608223621	8.690592197	30.094988922
H	8.041015776	7.665775858	29.088087027
H	11.678280384	4.876104313	29.199778530
H	7.770551669	3.704679164	29.226365491
O	4.759767583	4.302193243	30.193810778
H	5.739498023	4.232396101	30.275976839
H	4.578322005	4.062803057	29.249412224
H	7.858313133	2.931750307	30.576259988
H	2.503119578	2.859317356	29.347540489

End final coordinates

NH_3-Cu111

CELL_PARAMETERS (angstrom)

15.346059799	0.000000000	0.000000000
-7.673035145	13.290086719	0.000000000
0.000000000	0.000000000	50.000000000

ATOMIC_POSITIONS (angstrom)

Cu	-0.000007673	1.476683389	22.979020887	0	0	0
Cu	-1.278852374	3.691708473	22.979020887	0	0	0
Cu	-2.557700144	5.906735091	22.979020887	0	0	0
Cu	-3.836544845	8.121760175	22.979020887	0	0	0
Cu	-5.115392615	10.336788328	22.979020887	0	0	0
Cu	-6.394237316	12.551816481	22.979020887	0	0	0
Cu	2.557681729	1.476683389	22.979020887	0	0	0
Cu	1.278833959	3.691708473	22.979020887	0	0	0
Cu	-0.000009208	5.906735091	22.979020887	0	0	0
Cu	-1.278853909	8.121760175	22.979020887	0	0	0
Cu	-2.557701679	10.336788328	22.979020887	0	0	0
Cu	-3.836546380	12.551816481	22.979020887	0	0	0
Cu	5.115372665	1.476683389	22.979020887	0	0	0
Cu	3.836524895	3.691708473	22.979020887	0	0	0
Cu	2.557680194	5.906735091	22.979020887	0	0	0
Cu	1.278832424	8.121760175	22.979020887	0	0	0
Cu	-0.000012277	10.336788328	22.979020887	0	0	0
Cu	-1.278856978	12.551816481	22.979020887	0	0	0
Cu	7.673062067	1.476683389	22.979020887	0	0	0
Cu	6.394215831	3.691708473	22.979020887	0	0	0
Cu	5.115371131	5.906735091	22.979020887	0	0	0
Cu	3.836523360	8.121760175	22.979020887	0	0	0
Cu	2.557678660	10.336788328	22.979020887	0	0	0
Cu	1.278830889	12.551816481	22.979020887	0	0	0
Cu	10.230753003	1.476683389	22.979020887	0	0	0
Cu	8.951905233	3.691708473	22.979020887	0	0	0
Cu	7.673062067	5.906735091	22.979020887	0	0	0
Cu	6.394214297	8.121760175	22.979020887	0	0	0
Cu	5.115369596	10.336788328	22.979020887	0	0	0
Cu	3.836521826	12.551816481	22.979020887	0	0	0
Cu	12.788443940	1.476683389	22.979020887	0	0	0
Cu	11.509596170	3.691708473	22.979020887	0	0	0
Cu	10.230751469	5.906735091	22.979020887	0	0	0
Cu	8.951905233	8.121760175	22.979020887	0	0	0
Cu	7.673060532	10.336788328	22.979020887	0	0	0
Cu	6.394212762	12.551816481	22.979020887	0	0	0
N	1.560913431	2.354121527	29.333999521			
H	0.920148092	3.043007133	29.738277002			
Cu	1.283400996	0.761275819	25.063324838			
Cu	0.021636047	2.944183507	25.063872710			
Cu	-1.282774246	5.169733226	25.010710600			
Cu	-2.558541999	7.382769857	25.020289047			
Cu	-3.835990979	9.593234163	25.025998030			
Cu	-5.114920786	11.808559210	25.017126949			
Cu	3.840396601	0.726536907	25.008994356			
Cu	2.546901672	2.946625695	25.043147327			
Cu	1.271349962	5.175585489	25.007055554			
Cu	-0.004408036	7.386520724	25.019006846			
Cu	-1.281377822	9.593719245	25.026571180			
Cu	-2.556608203	11.804065545	25.023972153			
Cu	6.397910042	0.726805575	25.010834407			
Cu	5.119460278	2.971552482	25.034956552			
Cu	3.858681129	5.177921185	25.060746156			

Cu	2.568299996	7.377574570	25.040933434
Cu	1.274633263	9.596033447	25.019531640
Cu	0.001382039	11.805876791	25.025150532
Cu	8.954385844	0.729410032	25.017629289
Cu	7.678616025	2.963179106	25.047492695
Cu	6.396429723	5.145658731	25.089424715
Cu	5.109481684	7.374238026	25.036816976
Cu	3.834341628	9.600642409	25.015079091
Cu	2.560298533	11.809874390	25.026636903
Cu	11.513408654	0.736122138	25.028374341
Cu	10.235424886	2.948241063	25.019774017
Cu	8.935612456	5.156036525	25.054270635
Cu	7.674597058	7.377499242	25.004986917
Cu	6.399329599	9.604766683	25.001682663
Cu	5.119123457	11.815061603	25.024518555
Cu	14.071901266	0.738459763	25.026589460
Cu	12.791831300	2.949641997	25.015375897
Cu	11.503803527	5.168185665	25.011516780
Cu	10.228601493	7.380701444	25.016135866
Cu	8.960480292	9.600209477	25.011620233
Cu	7.679399158	11.815908303	25.021259613
Cu	-0.005367434	-0.013897381	27.065344279
Cu	-1.293199129	2.212936098	27.066083151
Cu	-2.553006756	4.427188757	27.044669017
Cu	-3.841855326	6.644262289	27.054713892
Cu	-5.118234195	8.856257922	27.075824083
Cu	-6.390904773	11.069746032	27.071953108
Cu	2.575600652	-0.034541266	27.054426375
Cu	1.294038660	2.221498409	27.224189582
Cu	-0.022537058	4.460635029	27.055018766
Cu	-1.294341526	6.648993904	27.076653561
Cu	-2.562527699	8.850995750	27.077747370
Cu	-3.834413046	11.059369402	27.074844144
Cu	5.122743134	-0.022619293	27.070601599
Cu	3.859120208	2.169711746	27.012297784
Cu	2.519176360	4.466146714	27.009879004
Cu	1.255391502	6.657410958	27.060433981
Cu	-0.002659380	8.858186121	27.073218261
Cu	-1.277180481	11.064046118	27.072597896
Cu	7.682566898	-0.014968573	27.072732742
Cu	6.408092976	2.163010577	27.034784428
Cu	5.079663834	4.403923420	27.155610880
Cu	3.836699480	6.689418069	27.141846900
Cu	2.548557395	8.886219105	27.055905954
Cu	1.280818451	11.072394727	27.075009151
Cu	10.240771929	-0.010913440	27.074913303
Cu	8.978455868	2.183162414	27.052035405
Cu	7.693671049	4.419974366	27.184688901
Cu	6.423583329	6.676952720	27.048564115
Cu	5.131315442	8.889106066	27.026819730
Cu	3.846088363	11.074030705	27.078374907
Cu	12.793533751	-0.003557877	27.076791101
Cu	11.515666934	2.214957613	27.082175368
Cu	10.253748721	4.420572454	27.059577569
Cu	8.960714204	6.658300734	27.060626266
Cu	7.678239903	8.872388066	27.024461048
Cu	6.400645639	11.075651065	27.075578039
O	3.871023771	6.864200631	29.477476295
H	2.939459254	7.072961832	29.672780582
H	4.550299877	5.234345787	29.551802548
H	4.417158632	7.679207223	29.749001687
O	5.314451096	8.964389392	30.187556923
H	5.237854480	9.652286425	29.491240153
H	6.279315039	8.742528280	30.214415572
O	11.792686314	5.184578862	30.119523877
O	9.146639888	5.639163439	30.762588400
O	8.062310368	8.199139201	30.109029302
O	7.591473899	4.123885135	29.413448693
H	10.108676630	5.561001129	30.520350775
H	12.214094593	5.880324607	29.571523779
H	8.887806980	6.580897078	30.639924010
H	8.246789208	4.733868597	29.943715607
H	8.654720049	8.975798249	30.121957789
H	8.047982627	7.959268114	29.141638975
H	11.759059220	4.429411557	29.492118608
O	4.876905332	4.328574083	29.311136829
H	5.835544439	4.276497102	29.571644185
H	7.908168533	3.206959957	29.519314826
H	2.519825354	2.640923637	29.560689889
H	1.384216960	1.448276109	29.776442506

End final coordinates

NH_3-Cu111-Nafion

CELL_PARAMETERS (angstrom)

15.346059799	0.000000000	0.000000000
-7.673035145	13.290086719	0.000000000
0.000000000	0.000000000	50.000000000

ATOMIC_POSITIONS (angstrom)

Cu	-0.000007673	1.476683389	22.979020887	0	0	0
Cu	-1.278852374	3.691708473	22.979020887	0	0	0
Cu	-2.557700144	5.906735091	22.979020887	0	0	0
Cu	-3.836544845	8.121760175	22.979020887	0	0	0
Cu	-5.115392615	10.336788328	22.979020887	0	0	0
Cu	-6.394237316	12.551816481	22.979020887	0	0	0
Cu	2.557681729	1.476683389	22.979020887	0	0	0
Cu	1.278833959	3.691708473	22.979020887	0	0	0
Cu	-0.000009208	5.906735091	22.979020887	0	0	0
Cu	-1.278853909	8.121760175	22.979020887	0	0	0
Cu	-2.557701679	10.336788328	22.979020887	0	0	0
Cu	-3.836546380	12.551816481	22.979020887	0	0	0
Cu	5.115372665	1.476683389	22.979020887	0	0	0
Cu	3.836524895	3.691708473	22.979020887	0	0	0
Cu	2.557680194	5.906735091	22.979020887	0	0	0
Cu	1.278832424	8.121760175	22.979020887	0	0	0
Cu	-0.000012277	10.336788328	22.979020887	0	0	0
Cu	-1.278856978	12.551816481	22.979020887	0	0	0
Cu	7.673062067	1.476683389	22.979020887	0	0	0
Cu	6.394215831	3.691708473	22.979020887	0	0	0
Cu	5.115371131	5.906735091	22.979020887	0	0	0
Cu	3.836523360	8.121760175	22.979020887	0	0	0
Cu	2.557678660	10.336788328	22.979020887	0	0	0
Cu	1.278830889	12.551816481	22.979020887	0	0	0
Cu	10.230753003	1.476683389	22.979020887	0	0	0
Cu	8.951905233	3.691708473	22.979020887	0	0	0
Cu	7.673062067	5.906735091	22.979020887	0	0	0
Cu	6.394214297	8.121760175	22.979020887	0	0	0
Cu	5.115369596	10.336788328	22.979020887	0	0	0
Cu	3.836521826	12.551816481	22.979020887	0	0	0
Cu	12.788443940	1.476683389	22.979020887	0	0	0
Cu	11.509596170	3.691708473	22.979020887	0	0	0
Cu	10.230751469	5.906735091	22.979020887	0	0	0
Cu	8.951905233	8.121760175	22.979020887	0	0	0
Cu	7.673060532	10.336788328	22.979020887	0	0	0
Cu	6.394212762	12.551816481	22.979020887	0	0	0
N	1.482074750	2.486248122	29.357139388			
H	0.839597353	3.175108317	29.766747075			
Cu	1.281879293	0.775030542	25.070414844			
Cu	0.018458278	2.947844194	25.055297607			
Cu	-1.291099216	5.183902492	25.022461428			
Cu	-2.558553131	7.386973172	25.038200311			
Cu	-3.841877535	9.606744801	25.020747882			

Cu -5.118576885 11.824679989 25.020532239
Cu 3.838690472 0.740005099 25.014229898
Cu 2.545388297 2.953030814 25.045722545
Cu 1.272022862 5.191012396 25.025014342
Cu -0.009167566 7.383379770 25.055539259
Cu -1.288233843 9.602342112 25.020506520
Cu -2.561151027 11.816372820 25.024286415
Cu 6.393192029 0.737986397 25.019788830
Cu 5.121146423 2.977119345 25.040524447
Cu 3.862062344 5.185820881 25.068325822
Cu 2.561934906 7.377283439 25.066350814
Cu 1.273949447 9.598191026 25.016346498
Cu -0.002318412 11.813189556 25.023022834
Cu 8.952699094 0.736620355 25.023140744
Cu 7.675915473 2.949287436 25.009124341
Cu 6.381782587 5.167701147 25.041628618
Cu 5.105483036 7.383584287 25.042261003
Cu 3.836983439 9.606361961 25.011057401
Cu 2.558577201 11.813764640 25.023865944
Cu 11.510827759 0.741280145 25.028753003
Cu 10.230753879 2.950153628 25.018277456
Cu 8.953973346 5.173402269 24.999359601
Cu 7.673048521 7.390913719 24.999116737
Cu 6.399931674 9.614271187 25.002163110
Cu 5.118177088 11.822273045 25.024867973
Cu 14.069718157 0.744045217 25.026265975
Cu 12.788118183 2.951714017 25.010599453
Cu 11.498493548 5.173018442 25.010276309
Cu 10.227192653 7.395647094 25.010066672
Cu 8.955982728 9.613793313 25.011755533
Cu 7.677968698 11.828406079 25.023930929
Cu -0.006515099 0.006945322 27.070095825
Cu -1.303670954 2.222203471 27.061891558
Cu -2.585413755 4.419183840 27.028752345
Cu -3.874059678 6.645067133 27.051368178
Cu -5.126818305 8.867677585 27.067217713
Cu -6.394581220 11.086620596 27.073728588
Cu 2.570538273 -0.004650780 27.063874039
Cu 1.283766457 2.251836399 27.251809052
Cu -0.033609311 4.452228059 27.025428155
Cu -1.328265943 6.655074657 27.120071374
Cu -2.580765776 8.879530489 27.065513215
Cu -3.844758763 11.082407449 27.074735636
Cu 5.120472096 0.002758759 27.071999041
Cu 3.862709601 2.195700330 27.025192551
Cu 2.545166101 4.464988587 27.006111172
Cu 1.256966520 6.664378033 27.112493133
Cu -0.014556126 8.900632892 27.051659133
Cu -1.287689559 11.084744290 27.072558733
Cu 7.677823655 -0.002151145 27.071440250
Cu 6.429427551 2.199240700 27.059747969
Cu 5.135494545 4.413618452 27.167936416
Cu 3.857373434 6.692946551 27.161591543
Cu 2.558843904 8.913854974 27.044227115
Cu 1.277575064 11.089377518 27.072572993
Cu 10.232049869 0.004093107 27.069450088
Cu 8.954418241 2.218000023 27.074271322
Cu 7.698485901 4.432363710 27.020078715
Cu 6.437531578 6.668417121 27.047154163
Cu 5.137091321 8.901172333 27.024880858
Cu 3.846720921 11.089573270 27.077060838
Cu 12.789459365 0.009148525 27.077315370
Cu 11.499753052 2.220915375 27.080597195
Cu 10.218832659 4.428021290 27.062799008
Cu 8.949578564 6.647067306 27.042857152
Cu 7.676537059 8.880588206 27.029602787
Cu 6.401292731 11.090100905 27.077086120
O 0.168293313 5.269067100 31.033447202
S -0.038590597 6.501793143 30.282166633
C -0.174990922 7.941120901 31.518212655
C -1.321188386 7.838401208 32.576958769
O -1.065277656 6.739675041 33.380494340
C -1.709953146 6.595416301 34.603518864
F -1.179314459 7.405406862 35.543734822
F -3.035614772 6.849878025 34.526594822
F -1.525986607 5.321048639 34.977000930
F -1.367327119 8.998302185 33.293604276
F -2.526290516 7.718732989 31.941879497
F -0.389978863 9.071567987 30.793465206
F 1.011622993 8.056947683 32.173641038
O -1.324721179 6.590997587 29.531453523
O 1.121015431 6.948099780 29.456826406
O 3.861641873 6.793391608 29.410213900
H 2.909653971 6.908055357 29.652348701
H 4.608936132 5.251715146 29.575622702
H 4.380798033 7.597261675 29.725130722
O 5.385063564 8.858889638 30.203575254
H 5.350137393 9.548474779 29.504859918
H 6.329078146 8.586104341 30.227064428
O 11.740054646 5.169015413 30.135451674
O 9.504863893 5.778272322 30.945417867
O 8.265331210 7.927685863 30.051665918
O 7.884243843 3.837623983 30.160586560
H 10.527771449 5.595073030 30.560041137
H 12.522017555 5.781040620 30.061682518
H 9.091671269 6.642316825 30.597998146
H 8.899637083 5.010537914 30.666054357
H 8.829991883 8.723648253 29.962219338
H 8.102484867 7.687381024 29.091132233
H 11.642091492 4.800729416 29.218935528
H 8.083679020 3.665880047 29.194883297
O 4.957117036 4.338360473 29.374667106
H 5.860626614 4.273227629 29.750935879
H 7.972309715 2.963105825 30.584672979
H 2.434567322 2.788778235 29.587433412
H 1.322176140 1.587103974 29.820606716
End final coordinates

First protonation on Zn(111) surfaces

NO-Eigen-Zn111
CELL_PARAMETERS (angstrom)
15.967919350 0.000000000 0.000000000
-7.983965199 13.828620613 0.000000000
0.000000000 0.000000000 39.353633881

ATOMIC_POSITIONS (angstrom)
Zn 1.099035447 0.588204010 22.686877592 0 0 0
Zn -0.231625908 2.892974167 22.686877592 0 0 0
Zn -1.562287263 5.197744323 22.686877592 0 0 0
Zn -2.892948618 7.502516077 22.686877592 0 0 0
Zn -4.223609973 9.807286233 22.686877592 0 0 0
Zn -5.554269732 12.112056390 22.686877592 0 0 0
Zn 3.760356561 0.588204010 22.686877592 0 0 0
Zn 2.429695206 2.892974167 22.686877592 0 0 0
Zn 1.099033851 5.197744323 22.686877592 0 0 0
Zn -0.231627505 7.502516077 22.686877592 0 0 0
Zn -1.562288860 9.807286233 22.686877592 0 0 0
Zn -2.892950215 12.112056390 22.686877592 0 0 0
Zn 6.421677675 0.588204010 22.686877592 0 0 0
Zn 5.091016320 2.892974167 22.686877592 0 0 0

Zn 3.760354964 5.197744323 22.686877592 0 0 0
Zn 2.429693609 7.502516077 22.686877592 0 0 0
Zn 1.099032254 9.807286233 22.686877592 0 0 0
Zn -0.231629101 12.112056390 22.686877592 0 0 0
Zn 9.082997192 0.588204010 22.686877592 0 0 0
Zn 7.752335837 2.892974167 22.686877592 0 0 0
Zn 6.421674481 5.197744323 22.686877592 0 0 0
Zn 5.091013126 7.502516077 22.686877592 0 0 0
Zn 3.760351771 9.807286233 22.686877592 0 0 0
Zn 2.429690416 12.112056390 22.686877592 0 0 0
Zn 11.744318305 0.588204010 22.686877592 0 0 0
Zn 10.413656950 2.892974167 22.686877592 0 0 0
Zn 9.082995595 5.197744323 22.686877592 0 0 0
Zn 7.752334240 7.502516077 22.686877592 0 0 0
Zn 6.421672885 9.807286233 22.686877592 0 0 0
Zn 5.091011529 12.112056390 22.686877592 0 0 0
Zn 14.405637822 0.588204010 22.686877592 0 0 0
Zn 13.074978064 2.892974167 22.686877592 0 0 0
Zn 11.744316709 5.197744323 22.686877592 0 0 0
Zn 10.413655353 7.502516077 22.686877592 0 0 0
Zn 9.082993998 9.807286233 22.686877592 0 0 0
Zn 7.752332643 12.112056390 22.686877592 0 0 0
Zn -0.258265705 1.319772147 25.678271638
Zn -1.595465512 3.629237772 25.351834162
Zn -2.897149252 5.946776730 25.316443398
Zn -4.225020925 8.250421108 25.295965200
Zn -5.553270854 10.558006401 25.330972316
Zn -6.906936060 12.853470665 25.380987009
Zn 2.402352568 1.321211404 25.604930580
Zn 1.067533470 3.620216800 25.575664960
Zn -0.259401993 5.919826392 25.308716398
Zn -1.571004582 8.250868991 25.310225087
Zn -2.904086903 10.554409212 25.325488017
Zn -4.255135448 12.856243554 25.362134956
Zn 5.065504311 1.332207874 25.318511461
Zn 3.748224606 3.628937548 25.312516774
Zn 2.406278644 5.922906840 25.304430455
Zn 1.077445284 8.232386577 25.361234383
Zn -0.249672013 10.553138344 25.365394819
Zn -1.593005782 12.861320595 25.367706032
Zn 7.740981088 1.314075219 25.314720834
Zn 6.416039562 3.605253748 25.309051117
Zn 5.059050922 5.952182251 25.282373527
Zn 3.727557191 8.266196206 25.296770936
Zn 2.415635356 10.553197201 25.376938876
Zn 1.082183306 12.851294899 25.369774781
Zn 10.398920904 1.311980056 25.326343333
Zn 9.072355325 3.612998385 25.299379071
Zn 7.734457903 5.934533387 25.281894086
Zn 6.391265072 8.258836799 25.283564824
Zn 5.056318898 10.561002622 25.332453238
Zn 3.752173817 12.862372462 25.439077284
Zn 13.062027180 1.330644633 25.347946591
Zn 11.722373122 3.607052147 25.338654210
Zn 10.409170791 5.931971874 25.309067259
Zn 9.066723566 8.254442874 25.311351158
Zn 7.714618633 10.562576645 25.345308731
Zn 6.411208399 12.861784083 25.383127859
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0.000000000 0.000000000 39.353633881

ATOMIC_POSITIONS (angstrom)
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Zn	2.429693609	7.502516077	22.686877592	0	0	0
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End final coordinates

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ATOMIC_POSITIONS (angstrom)
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End final coordinates

NOH-Zn111-Nafion
CELL_PARAMETERS (angstrom)
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-7.983965199 13.828620613 0.000000000
0.000000000 0.000000000 39.353633881

ATOMIC_POSITIONS (angstrom)
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End final coordinates

Supplementary references

1. Z. Y.Wu, M. Karamad, X. Yong, Q. Huang, D. A. Cullen, P. Zhu, C. Xia, Q. Xiao, M. Shakouri, F. Y. Chen, J. Y. Kim, Y. Xia, K. Heck, Y. Hu, M. S. Wong, Q. Li, I. Gates and S. Siahrostami, *Nat. Commun.*, 2021, **12**, 2870–2879.
2. G. F. Chen, Y. Yuan, H. Jiang, S. Y. Ren, L. X. Ding, L. Ma, T. Wu, J. Lu and H. Wang, *Nat. Energy*., 2020, **5**, 605–613.
3. B. P. Chaplin, J. R. Shapley and C. J. Werth, *Catal. Lett.*, 2009, **130**, 56–62.
4. M. Machida, K. Sato, I. Ishibashi, M. A. Hasnat and K. Ikeue, *Chem. Commun.*, 2006, **7**, 732–734.
5. M. A. Hasnat, M. R. Karim and M. Machida, *Catal. Commun.*, 2009, **10**, 1975–1979.
6. P. Gayen, J. Spataro, S. Avasarala, A. M. Ali, J. M. Cerrato and B. P. Chaplin, *Environ. Sci. Technol.*, 2018, **52**, 9370–9379.
7. X. Deng, Y. Yang, L. Wang, X. Z. Fu and J. L. Luo, *Adv. Sci.*, 2021, **8**, 2004523–2004531.
8. C. Wang, Z. Liu, T. Hu, J. Li, L. Dong, F. Du, C. Li and C. Guo, *ChemSusChem.*, 2021, **14**, 1825–1829.
9. Y. Wang, A. Xu, Z. Wang, L. Huang, J. Li, F. Li, J. Wicks, M. Luo, D. H. Nam, C. S. Tan, Y. Ding, J. Wu, Y. Lum, C. T. Dinh, D. Sinton, G. Zheng and E. H. Sargent, *J. Am. Chem. Soc.*, 2020, **142**, 5702–5708.
10. Y. Yu, C. Wang, Y. Yu, Y. Wang and B. Zhang, *Sci. China Chem.*, 2020, **63**, 1469–1476.
11. Y. Wang, C. Liu, B. Zhang and Y. Yu, *Sci. China Mater.*, 2020, **63**, 2530–2538.
12. M. S. El-Deab, *Electrochimica Acta.*, 2004, **49**, 1639–1645.
13. L. Su, K. Li, H. Zhang, M. Fan, D. Ying, T. Sun, Y. Wang and J. Jia, *Water Res.* 2017, **120**, 1–11.

14. J. Y. Zhu, Q. Xue, Y. Y. Xue, Y. Ding, F. M. Li, P. Jin, P. Chen and Y. Chen, *ACS Appl. Mater. Interfaces*, 2020, **12**, 14064–14070.