

Supporting Information

A Bidirectional Bio-Inspired [FeFe]-Hydrogenase Model

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Experimental section.

Materials

Complex **1** was synthesized according to previously reported procedure.¹ Syntheses of all the complexes were performed either under anaerobic atmosphere or in an Ar Glove Box from MBRAUN. Complex **1** was synthesized using standard Schlenk techniques. 2-Ethylaniline and the solvents were used fresh after distillation, purchased from Merck. Thionyl chloride (SOCl_2) was purchased from Spectrochem Pvt. Ltd. (India). *p*-formaldehyde, superhydride ($\text{Li}[\text{HBET}_3]$, 1 M in THF), N,N-diisopropylethylamine, malonic acid and bis(cyclopentadienyl)cobalt(II) were purchased from Sigma-Aldrich chemicals Pvt. Ltd., and anhydrous Na_2SO_4 was purchased from Merck Specialities, Pvt. Ltd. (India). During electrochemistry the solvent (acetonitrile) was used after distillation with proper drying agent. Silica (60-120 mesh), for column chromatography, was purchased from SISCO Pvt. Ltd. (India). Edge Plane Graphite (EPG) discs were purchased from Pine Instruments. Glassy carbon plate (1 mm thick, type1) was purchased from Alfa Aesar. The FT-IR data are measured on the Perkin-Elmer FTIR Frontier instrument. The CaF_2 windows for FTIR spectroscopy

were purchased from Sigma Aldrich. The anaerobic setup for FTIR spectroscopy was purchased from PerkinElmer. All the NMR spectra were recorded on Bruker DPX-400 or DPX-500 spectrometers at room temperature. The mass spectra are recorded on an QTOF Micro YA263 instrument. UV-Vis absorption data were recorded in an Agilent technologies spectrophotometer model 8453 fitted with a diode-array detector. Mössbauer spectra were recorded in an alternating constant WissEl Mössbauer spectrometer, which consists of an MR 360 drive unit, an MVT 1000 velocity transducer, and an LND-45431 proportional counter mounted on an MB-600 Mössbauer bench with cryostat stand. The system was operated in a horizontal transmission geometry with source (^{57}Co in Rh-matrix), absorber and detector in a linear arrangement. The temperature was controlled and maintained using MBBC-N20106 Mössbauer cryostat for liquid nitrogen connected with Lake Shore-325 temperature controller unit. Measurements were performed at 90K. Data acquisition was performed using a 512 channel analyzer. Isomer shifts were referenced versus α -iron metal foil at the same temperature. The simulation of experimental data was performed using the Normos-A Mössbauer Fit programmes Site and Dist.

For **membrane-less fuel cell** measurements, commercial carbon black Vulcan VXC72 was obtained from Cabot and used as received. Gas diffusion layer (GDL) Sigracet 39-BC with hydrophobic treatment (5 wt % PTFE) and microporous layer was purchased from SGL Carbon GmbH (Germany). Platinum gas diffusion electrodes with $0.5 \text{ mg}_{\text{Pt}} \text{ cm}^{-2}$ (60% Pt on Vulcan carbon support) were purchased from FuelCellStore. Oxygen gas and hydrogen gas (Air Liquide ultrapure quality) were of 99.995% and 99.999% purity, respectively.

The Mechanism of **1H** Formation in Non-aqueous Media

Time-resolved FTIR spectra (Figure 4) reveal gradual conversion of complex **1** to its singly reduced and N-protonated form **1H**. These spectra combined with a number of additional stopped flow experiments have allowed us to make some conclusions on HER mechanism in non-aqueous media. Data from the additional stopped flow experiments have not been included in the SI for the purpose of conciseness, as the manuscript focuses on HER in aqueous media.

Two points must be considered before attempting to deduce the relevant reaction mechanism from time-resolved FTIR data. Firstly, the catalytic mechanism of HER in non-aqueous media need not be the same as the catalytic mechanism in the aqueous environment. Secondly, the observed rate of conversion from **1** to **1H** does not necessarily correspond to the rate of the reaction step(s) with which **1** undergoes proton-coupled electron transfer (PCET) to form **1H**.

With that in mind, we propose that the spectroscopically captured **1** and **1H** correspond to the species that are accumulated during the catalyst turnover, i.e. the intermediates preceding the rate determining step (RDS). Instead of being the result of a surprisingly slow single PCET from **1** to **1H**, the observed conversion from **1** to **1H** reflects a change in RDS. This change in RDS comes about as the reducing agent gets consumed, thus decreasing its reducing power and the rate of electron transfer. More than one catalytic pathway could exhibit such behaviour and additional experiments would be required to determine the exact catalytic mechanism at play in non-aqueous media.



Figure S1. Mössbauer sampling window.

Table S1. List of the amount of charge consumed, amount of H₂ oxidized and the faradaic yield.

BE potential (vs Fc ^{+/-})	Charge consumed (C)	Amount of Ammonium Detected (μmol)	FY (%)
-0.7 V	95.04	390	79.2
-0.7 V	59.27	250	81.4
-0.7 V	30.36	129	82.1
-0.7 V	20.1	86	82.6
-0.7 V	9.05	40	85.3

GDEs measurements

A detailed investigation of the catalytic activity has been carried out in 0.1 M KPF₆ (adjusted to pH 5.6 with HCl solution) aqueous solution using a previously described half-cell holder for gas diffusion electrodes setup.² Briefly, the GDEs (1.2 mm disc diameter, 1.13 cm cm²) were inserted in the sample holder. The middle of the GDEs (0.7 mm diameter, 0.384 cm² taken to calculate current densities) was then exposed to the electrolyte while the same surface area of the GDEs is fed with H₂ flow (1 atm). A gold grid provides the electrical contact. The electrochemical experiments were performed in a continuously degassed

electrolyte by nitrogen bubbling, in a three-electrode cell configuration and in a fuel cell configuration, respectively and using a SP300 Bio-Logic potentiostat.

In the conventional three-electrode cell setup, the counter electrode consisted of a graphite rod physically separated by the compartment containing the working electrode and the reference electrode was a Ag/AgCl,KCl (3 M) (denoted below Ag/AgCl). All potentials were converted against the Reversible Hydrogen Electrode (RHE) potential using the following equation: $E_{\text{vs RHE}} = E_{\text{vs Ag/AgCl}} - E_{\text{Ag/AgCl vs NHE}} + 0.059 \times \text{pH}$. The Ag/AgCl reference electrode was also calibrated with the $[\text{Fe}(\text{CN})_6]^{3-}/[\text{Fe}(\text{CN})_6]^{4-}$ couple in an external electrochemical setup. Calibration against the $[\text{Fe}(\text{CN})_6]^{3-}/[\text{Fe}(\text{CN})_6]^{4-}$ couple was performed with a glassy carbon electrode and a platinum wire as working and auxiliary electrodes, respectively, in 0.1 M potassium phosphate buffer (pH 7). The potential of the $[\text{Fe}(\text{CN})_6]^{3-}/[\text{Fe}(\text{CN})_6]^{4-}$ couple is denoted below as $E_{\text{Fe(III)/Fe(II) vs Ag/AgCl}}$ (0.22 V) and $E_{\text{Fe(III)/Fe(II) vs NHE}}$ (0.425 V) refers to the tabulated value of $E_{\text{Fe(III)/Fe(II)}}$ against the NHE potential.³ Thus, $E_{\text{Ag/AgCl vs NHE}}$ is 0.205 V. The working electrodes were those described above. Polarization curves were recorded between 0.8 V and –0.2 V vs RHE at a scan rate of 10 mV s⁻¹ and 25°C, under a back-flow of H₂ (1 atm).

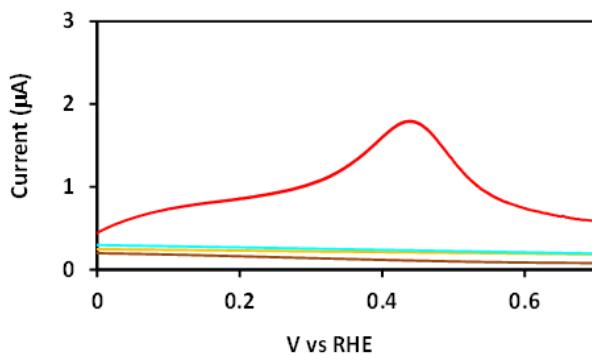


Figure S2. Overlay of linear sweep voltammetry of **2** physisorbed on EPG surface at different H₂ partial pressures in 0.1 M aq. KPF₆ solution (pH 5.5); 25% H₂ (yellow), 50% H₂ (sky blue), 100% H₂ (brown), and linear sweep voltammetry of **1** physiadsorbed on EPG surface in 0.1 M aq. KPF₆ solution at 50% H₂ (red) partial pressure, scan rate: 100 mVs⁻¹.

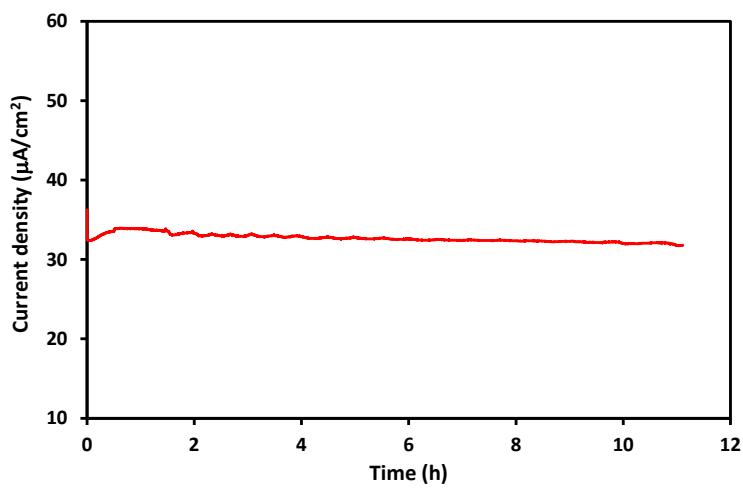


Figure S3. Chronoamperometric measurement of complex **1** physisorbed on EPG surface in H_2 saturated 0.1 M KPF₆ solution (pH 5.5) performed at 0.425 V vs RHE.

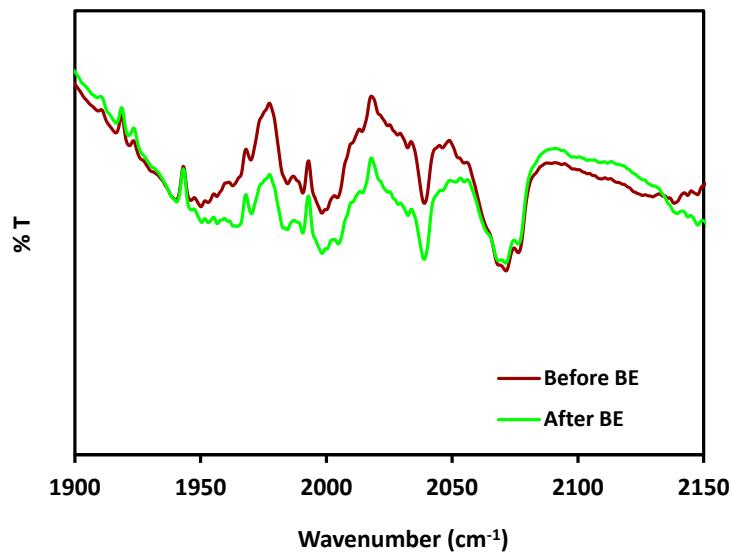


Figure S4. ATR-FTIR of complex **1** physisorbed on EPG surface before and after 3 hr of controlled potential electrolysis in H_2 saturated 0.1 M KPF₆ solution (pH 5.5).

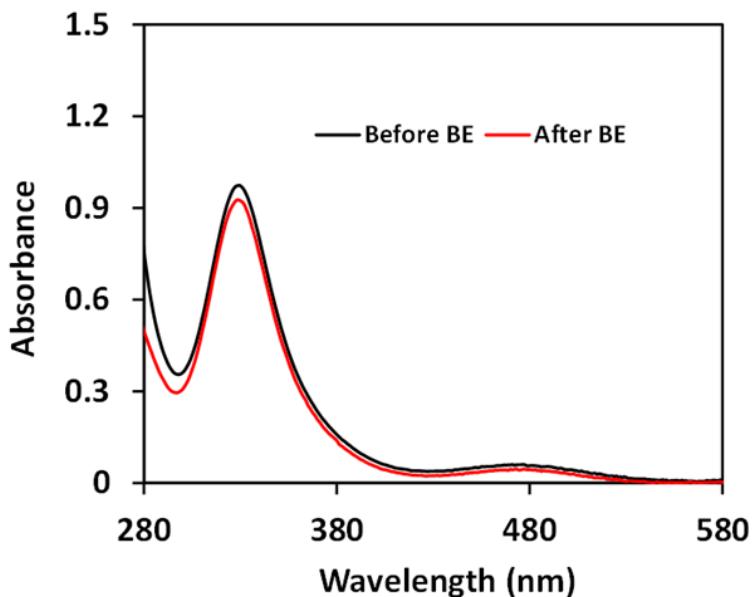


Figure S5. UV-vis spectra of complex **1** in H₂ saturated dry ACN in presence of 10 M *i*-Pr₂NEt and 100 mM Bu₄NClO₄ before (black line) and after (red line) 10 hr of controlled potential electrolysis at -0.7 V vs Fc^{+/-}. (d = 0.2 cm).

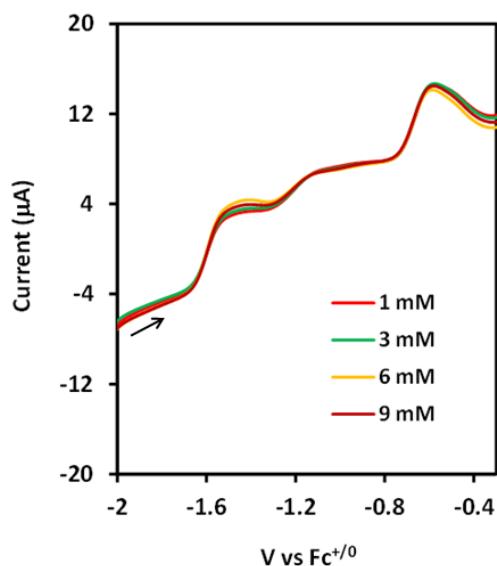


Figure S6. Linear sweep voltammetry of **2** in acetonitrile in the presence of different concentration of base, scan rate: 100 mVs⁻¹.

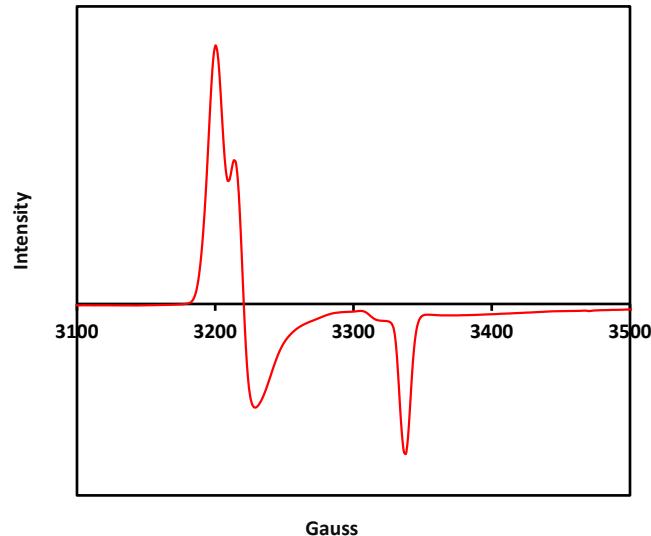


Figure S7. EPR spectra of **1H** recorded at 77 K.

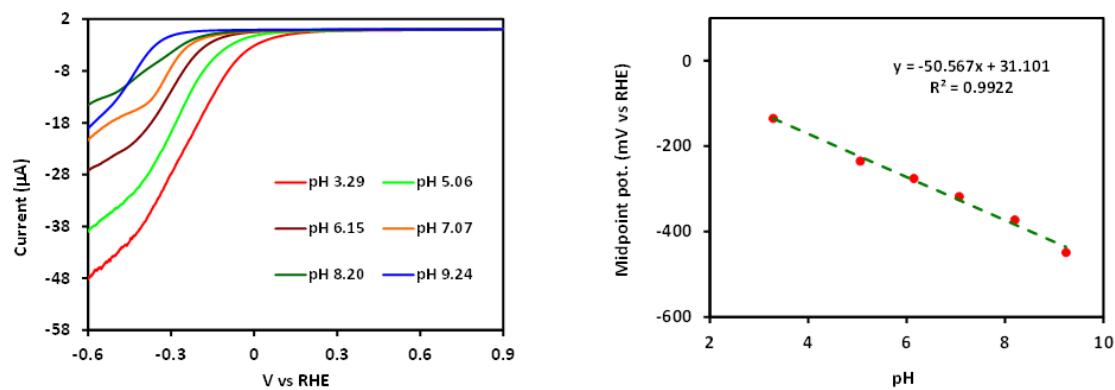


Figure S8. (left) Overlay of linear sweep voltammetry of **1** physisorbed on EPG surface at different pH. scan rate: 100 mVs^{-1} . (right) pH vs. midpoint of catalytic waves of HER plot.

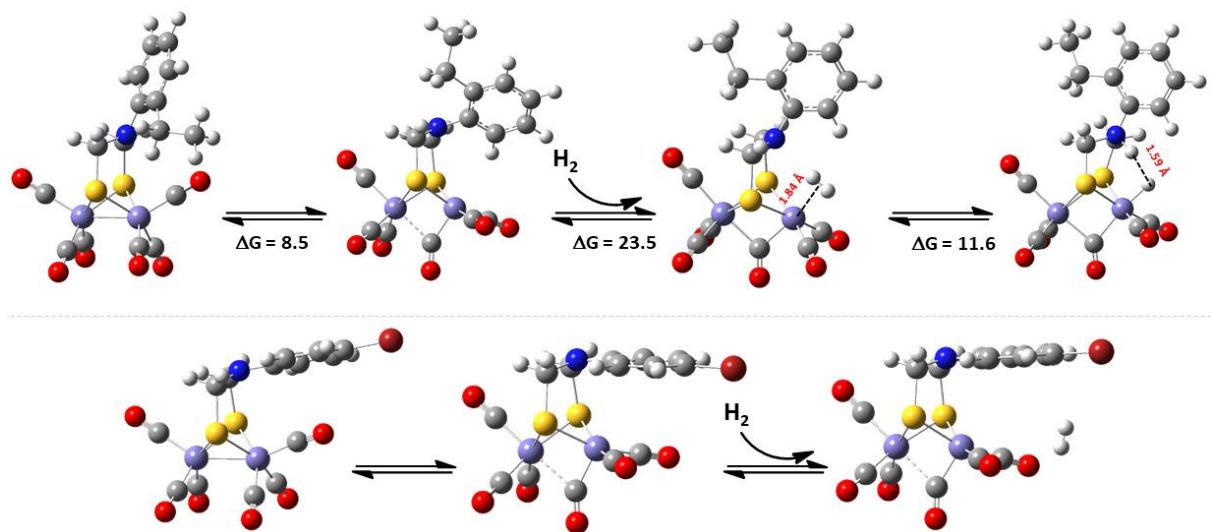


Figure S9. (Top) DFT calculated mechanism of H_2 oxidation by complex **1**. The energies are in kcal mol^{-1} and calculated using a PCM solvation model and acetonitrile as solvent. (bottom) DFT optimized structure of complex **2** before and after H_2 addition. The H_2 does not bind the Fe with the open co-ordination site due to the steric imposed by the aromatic ring flanking it.

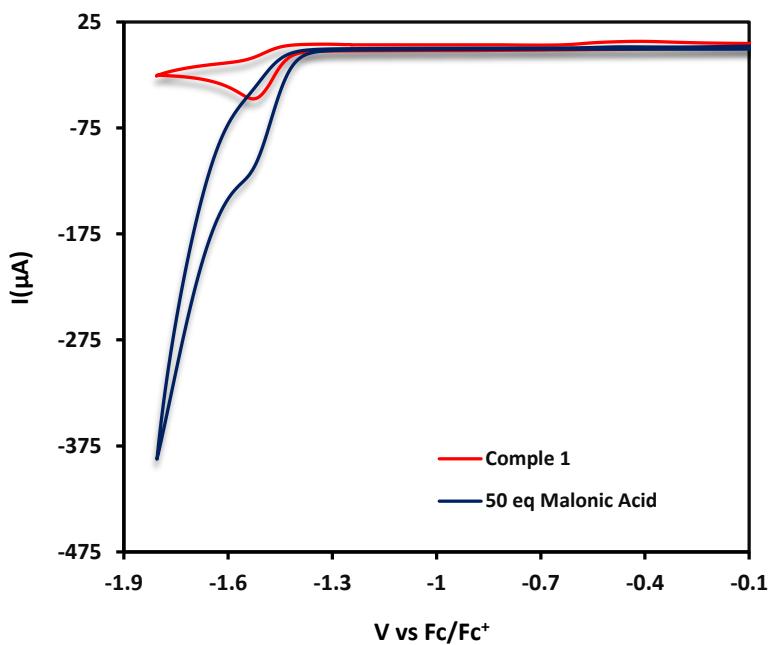


Figure S10. Overlay of cyclic voltammetry of **1** (red) and **1** in presence of 50 equivalent of malonic acid (blue) in acetonitrile medium under homogeneous condition. scan rate: 100 mVs^{-1} .

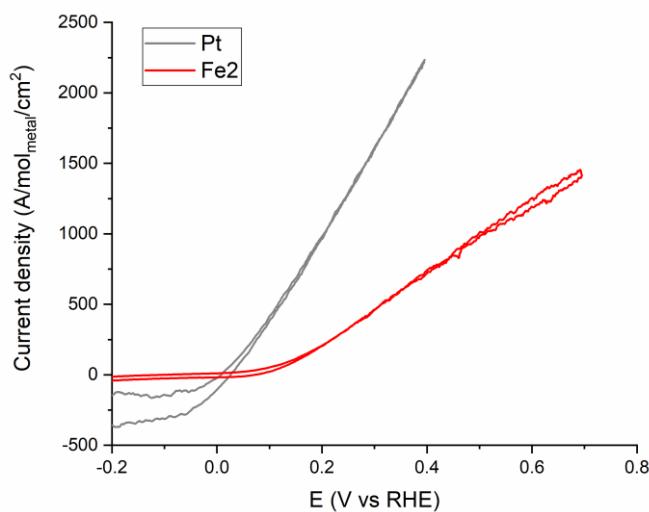


Figure S11. Specific current measured on a complex **1**/carbon black GDE (carbon black/complex **1** mass ratio of 2, $60 \text{ nmol}_{\text{complex } \mathbf{1}} \cdot \text{cm}^{-2}$) (red solid line) and a carbon black GDE (black solid line) of conventional Pt/C ($0.5 \text{ mg}_{\text{Pt}} \cdot \text{cm}^{-2}$) GDE (grey solid line) in 0.1 M aqueous KPF_6 $\text{pH} = 5.6$ adjusted with HCl under back-flow H_2 (1 atm H_2 , $S = 0.38 \text{ cm}^2$ & $v = 10 \text{ mV s}^{-1}$, 20°C).

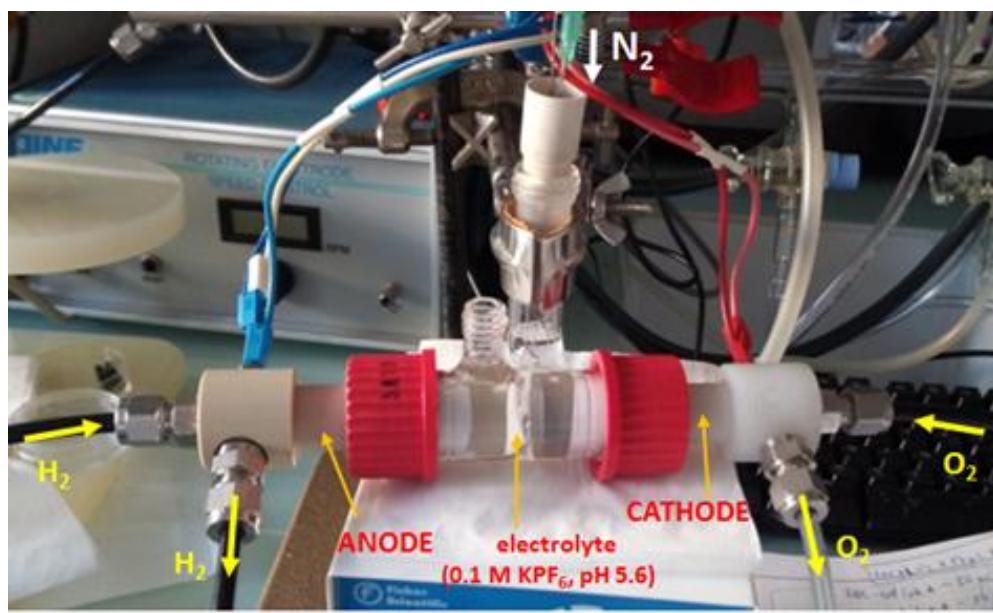


Figure S12. Membrane-less fuel cell experimental setup studied in this work.

References:

1. Ahmed, M.E., Dey, S., Daresbourg, M.Y. & Dey, A. Oxygen-Tolerant H₂ Production by [FeFe]-H₂ase Active Site Mimics Aided by Second Sphere Proton Shuttle. *Journal of the American Chemical Society* **140**, 12457-12468 (2018).
2. Le Goff, A. et al. From Hydrogenases to Noble Metal-Free Catalytic Nanomaterials for H₂ Production and Uptake. *Science* **326**, 1384-1387 (2009).
3. O'Reilly, J.E. Oxidation-reduction potential of the ferro-ferricyanide system in buffer solutions. *Biochimica et Biophysica Acta (BBA) - Bioenergetics* **292**, 509-515 (1973).

Coordinates of Optimized Geometry

1

Fe	3.24900300	3.06906100	2.88774200
Fe	1.10522900	2.18510900	2.04518100
S	1.25186400	3.46270700	3.95703100
S	2.68164300	0.82359000	3.02483300
O	-1.21472900	0.46519800	2.50221900
O	-0.25129400	4.47386100	0.81317200
O	4.90812600	3.79036500	5.18525100
O	2.11678700	1.21809400	-0.52630000
O	2.94646300	5.69073700	1.62907200
N	2.22770800	1.50047400	5.67379600
O	5.32789400	2.24195800	0.99743100
C	2.68759400	1.17712700	6.98932600
C	0.27646900	3.57879200	1.28711700
C	4.00667500	0.70859400	7.18740700
C	-0.31965300	1.15035300	2.31634200
C	4.51779300	2.57337900	1.73143000
C	2.09274800	0.41133900	4.73988500
H	1.05294800	0.07999200	4.64223200
H	2.69048200	-0.43637500	5.05979300
C	3.07723400	4.66908700	2.12625800

C	2.25881600	1.03915100	9.38027900
H	1.57811200	1.16914500	10.21514200
C	1.20055200	2.50022500	5.54526900
H	1.32971600	3.25510500	6.31717200
H	0.18265600	2.09451800	5.60706100
C	3.54968900	0.56103400	9.58497500
H	3.89536700	0.31726500	10.58407000
C	4.28080500	3.46031600	4.28924700
C	1.83002900	1.32857900	8.08863700
H	0.80975300	1.66006100	7.93427100
C	1.70209300	1.59262800	0.47066200
C	4.39915500	0.39615300	8.49382000
H	5.40354800	0.02437700	8.66538500
C	4.98566000	0.53511000	6.04115700
H	5.04781200	-0.52759300	5.77448800
H	4.59720900	1.03669000	5.15700600
C	6.39767600	1.06701300	6.31748800
H	6.90381600	0.51599600	7.11287900
H	7.01272800	0.98046600	5.41775500
H	6.36561000	2.12074600	6.60240000

1H

Fe	3.14790300	3.59649800	2.99881000
Fe	0.79997700	2.17468200	2.04953300
S	0.93865800	3.53530500	3.94329700
S	2.83270300	1.25058900	2.78056400
O	-1.09035900	0.14205700	3.13528100
O	-1.07898500	4.14013800	0.94653800
O	3.22422000	6.39003900	3.80538300
O	1.35861700	1.03904700	-0.59760500
O	3.31645800	4.10805800	0.12794600
N	2.37755300	1.74113900	5.51199300

O	5.89449900	3.16913300	3.84563200
C	2.63224300	1.27420100	6.89744800
C	-0.33764600	3.37482600	1.36595800
C	3.66267800	1.86886600	7.63865000
C	-0.36900900	0.91348400	2.69437900
C	4.77657400	3.33576100	3.58432500
C	2.60318200	0.64313500	4.49184500
H	1.75894800	-0.03960300	4.54176900
H	3.51118300	0.12978700	4.79694100
C	3.14160800	3.87058200	1.24627600
C	2.02296200	-0.18110200	8.70560700
H	1.39314700	-0.96454300	9.11007900
C	1.03352700	2.43054300	5.39288800
H	0.91480900	3.02846200	6.29234400
H	0.26575800	1.66190000	5.35542200
C	3.03745900	0.38520400	9.47128300
H	3.20710700	0.04395600	10.48645100
C	3.20498100	5.29093000	3.46573200
C	1.81728600	0.26907000	7.40546000
H	1.02672100	-0.16250500	6.80390900
C	1.13869400	1.48930500	0.43189200
C	3.84049900	1.39370400	8.94226600
H	4.62115200	1.81777500	9.56047400
C	4.53172100	2.96063900	7.04165600
H	5.04259200	2.56373300	6.15947600
H	3.89426200	3.77341600	6.67373800
H	3.06593000	2.47553000	5.25698400
C	5.58569100	3.56405200	7.96916400
H	6.30633600	2.81475500	8.30535400
H	6.13973800	4.33825600	7.43481500
H	5.13490700	4.02527700	8.85128600

1H- μ H

Fe	0.37872000	1.62932200	4.31060700
Fe	2.79772300	-0.16193100	2.67280700
S	0.49164900	0.33087400	2.31860200
S	2.62078300	2.08159100	3.60833800
C	-1.07426600	0.72469800	4.81011500
O	-1.95668100	0.07486600	5.11745900
C	0.79661600	2.25311000	5.92755900
O	1.13214800	2.59388200	6.96043100
C	4.51159100	-0.17931700	3.04002200
O	5.63748800	-0.14454200	3.29655500
C	2.43742300	-1.55495700	3.68862900
O	2.25172600	-2.57538500	4.21214900
C	3.09941300	-0.46940100	0.98301900
O	3.28848400	-0.82449200	-0.11294500
N	1.21848100	2.88158900	1.26964300
C	0.58363500	1.52454200	0.94938600
H	1.14530400	1.07324200	0.14130400
H	-0.41727700	1.77682600	0.60452600
C	2.55264400	2.95630600	2.00625700
H	2.72111400	4.02336100	2.13879700
H	3.31373000	2.52517300	1.37302700
O	-1.17378900	4.04811800	3.60675800
H	0.56752400	3.29608100	1.93478400
C	1.16957600	3.78335000	0.08013700
C	0.22734000	4.80977400	0.15652800
C	1.99031400	3.60100600	-1.03925400
C	0.08073300	5.69735400	-0.90047000
C	1.80951800	4.51365800	-2.08961700
C	0.87917400	5.54361500	-2.03196500
H	-0.65119100	6.49377500	-0.83857000
H	2.42200200	4.39862500	-2.97777400

H	0.77419100	6.22291000	-2.87041400
H	1.02907200	0.40183600	4.90766400
C	-0.52754200	3.12278500	3.78481100
H	-0.39582500	4.91704200	1.03877000
C	3.05845200	2.53870300	-1.20744600
H	2.95123600	1.72303100	-0.49691600
H	2.92706200	2.08026500	-2.19171800
C	4.48303600	3.10894700	-1.10558500
H	5.21793400	2.31107600	-1.23440400
H	4.66263600	3.86305700	-1.87485100
H	4.66073000	3.57980900	-0.13546500

1H-tH

Fe	0.82744800	1.71338600	4.05946700
Fe	2.45878000	-0.50767000	3.53145900
S	0.63110100	0.45317800	2.02827600
S	3.06648000	2.25136600	3.44657600
C	1.34625800	0.13028500	5.11797300
O	1.12827700	-0.30627300	6.17929000
C	-0.90243200	1.42857000	4.32900300
O	-2.02930100	1.30083700	4.46487500
C	1.05264200	2.77323100	5.46188400
O	1.19998100	3.49998900	6.33058400
C	3.84082400	-0.63484300	4.71960100
O	4.70717200	-0.81462200	5.44823700
C	1.66606600	-2.15929500	3.70627900
O	1.21959900	-3.20392800	3.85092600
C	3.47465100	-0.93023600	2.05811500
O	4.07921800	-1.12682600	1.10791100
N	1.58588900	2.92203900	1.16718000
C	1.51087100	1.45907300	0.77562700
H	2.52275800	1.10268300	0.61465400

H	0.94709300	1.40237300	-0.14971200
C	2.82497100	3.28955900	1.96893700
H	2.67808600	4.32994500	2.25186400
H	3.68963800	3.20702500	1.31816900
H	0.83605400	3.03362100	1.87863400
C	1.28742400	3.89622200	0.08800000
C	0.25673500	4.78653100	0.37798800
C	2.00017700	3.93431700	-1.12155700
C	-0.09858000	5.76336500	-0.54477000
C	1.61611800	4.93275800	-2.02580400
C	0.58972500	5.83331500	-1.75096800
H	-0.90120100	6.45547500	-0.31880100
H	2.13223400	5.01201000	-2.97356500
H	0.33040300	6.58853300	-2.48463000
H	0.30200100	3.01270900	3.38033300
H	-0.26608500	4.71807500	1.32641800
C	3.09454900	2.94166300	-1.47987700
H	3.70752700	2.72872200	-0.60251100
H	2.62647600	1.98798100	-1.74670200
C	4.02963900	3.36167500	-2.61666000
H	4.82891000	2.62526200	-2.72160600
H	3.51314200	3.41836800	-3.57703200
H	4.49025100	4.33288000	-2.41910100

1H₂

Fe	0.36822300	1.82804000	3.81233800
Fe	2.53330200	0.06069800	3.30248000
S	0.58873600	0.38612700	1.93245800
S	2.63859100	2.45628700	3.39147200
C	1.18202500	0.39069800	4.75198200
O	0.98218900	-0.12885000	5.80071500
C	-1.25445200	1.17307200	4.10572200

O	-2.28286300	0.71625900	4.29957400
C	0.37149300	2.86823000	5.25018000
O	0.40019600	3.52278600	6.18533000
C	3.79249100	0.00940600	4.56672600
O	4.57858700	0.00266000	5.39224400
C	2.11995000	-1.67358100	3.38970300
O	1.82184900	-2.77215300	3.45236500
C	3.70751700	-0.10768300	1.87632900
O	4.47656400	-0.30339700	1.05949000
N	1.52483100	2.79769200	0.84793600
C	1.18616200	1.43845700	0.50752600
H	2.02220600	0.88026700	0.07599000
H	0.36486400	1.44843300	-0.20479300
C	2.73700100	2.99185100	1.60801400
H	2.96735200	4.05376800	1.63370300
H	3.59331500	2.45860900	1.17886000
C	1.18869000	3.84315700	-0.09097500
C	0.45360400	4.92830100	0.39369700
C	1.60839800	3.81603800	-1.43892200
C	0.09217300	5.98198400	-0.44043500
C	1.21067500	4.87470900	-2.26474900
C	0.46090200	5.94506300	-1.78152000
H	-0.47930000	6.81511700	-0.04541600
H	1.51003800	4.88002700	-3.30585100
H	0.17852000	6.75093900	-2.45100000
H	0.05486400	3.07479100	2.45082900
H	-0.50870100	3.19788600	2.96888500
C	2.48508500	2.69435000	-1.97011000
H	3.20627700	2.42033100	-1.19519200
H	1.87449400	1.79891700	-2.13167000
C	3.25134900	2.99853500	-3.25990500
H	3.92525100	2.17119000	-3.49415900

H	2.58486100	3.12567500	-4.11625500
H	3.85354600	3.90613700	-3.16428300
H	0.16764200	4.94505000	1.43762300

1-μCO

Fe	0.46565700	1.86921000	3.27162000
Fe	2.39651300	0.14267600	3.58113800
S	1.07148200	0.33126200	1.62478600
S	2.72604700	2.47861400	3.35008400
C	0.55380000	0.71196100	4.63191700
O	0.06742400	0.29500000	5.61131700
C	-1.22046300	1.61330800	2.83506700
O	-2.31316100	1.45020800	2.52931300
C	0.07627400	3.30707000	4.20828700
O	-0.16316100	4.26080800	4.79808000
C	3.16410200	0.23620300	5.20702000
O	3.65293100	0.31259400	6.23117500
C	1.79613600	-1.54382100	3.76650300
O	1.40631600	-2.60777700	3.86493500
C	3.90217600	-0.29902500	2.68620400
O	4.85749000	-0.60088600	2.14528000
N	2.51808300	2.50456100	0.50049500
C	2.16305200	1.13357600	0.30794300
H	3.05924700	0.51566500	0.24000800
H	1.58066000	1.00994100	-0.59729500
C	3.39033700	2.76693800	1.59592200
H	3.69309700	3.81073400	1.59224800
H	4.27816400	2.13806800	1.51890800
C	1.66617700	3.53363600	-0.00671300
C	1.08982300	4.47447500	0.85654300
C	1.45547300	3.64048100	-1.40206800
C	0.26953000	5.48808700	0.37202100

C	0.59917100	4.64958900	-1.85680000
C	0.00242500	5.56313500	-0.99098300
H	-0.16653300	6.20161600	1.06320900
H	0.41375000	4.74475600	-2.92046200
H	-0.64899700	6.33672600	-1.38375800
H	1.27846000	4.41313800	1.91862700
C	2.17338300	2.73639000	-2.38890700
H	3.08381500	2.36269900	-1.91294800
H	1.56259800	1.84923300	-2.59905900
C	2.54929800	3.39603900	-3.72124900
H	3.16844900	2.71619200	-4.31186400
H	1.67458300	3.64353300	-4.32659800
H	3.11709700	4.31643500	-3.56009200

H₂

H	-1.62831300	1.20370400	0.00000000
H	-2.37045300	1.20370400	0.00000000

2

Fe	0.79063000	1.17162400	3.97475100
Fe	2.89014200	0.16306400	3.19455000
S	1.06010500	0.41884100	1.79518500
S	2.70827900	2.44131600	3.59901200
Br	-3.42809100	6.61340700	2.32612500
C	0.36014000	3.91235800	1.44842800
C	-0.66903200	2.20382000	3.85741900
O	-1.65763800	2.77351200	3.85640300
C	1.10556700	1.44874200	5.70915700
O	1.32599500	1.63210900	6.81450700
C	-0.00429800	-0.38670500	4.29812000
O	-0.49698100	-1.39900400	4.49606100
C	3.75115400	0.04500300	4.75531600

O	4.28583100	-0.01375900	5.76338600
C	2.56958300	-1.59659000	3.15682900
O	2.35727200	-2.71828000	3.12404400
C	4.25503100	0.20789300	2.05109300
O	5.12837600	0.26535200	1.31655200
N	1.49683800	3.13099300	1.16238900
C	-0.84197200	3.73591800	0.73931800
H	-0.93551800	2.97709500	-0.02509600
C	-1.95246000	4.53058900	0.99192700
H	-2.86473400	4.36602700	0.43183800
C	-1.88388700	5.52582200	1.96047900
C	-0.71078100	5.72758900	2.67493500
H	-0.65347100	6.49051200	3.44148700
C	0.39673900	4.92518100	2.42454600
H	1.27489000	5.08683300	3.03330300
C	1.37491000	1.82415700	0.58823500
H	2.29935400	1.56566500	0.07337300
H	0.56588900	1.76848700	-0.13001300
C	2.69240300	3.29864200	1.92833500
H	2.89827500	4.34665100	2.12248000
H	3.53415600	2.88923900	1.37332600

2- μ CO

Fe	0.47162900	1.95453600	3.17881800
Fe	2.40631300	0.21825500	3.30127600
S	0.98850100	0.47659100	1.41976700
S	2.74621000	2.56245500	3.22024500
C	0.57512800	0.74098200	4.48157400
O	0.13966400	0.26545500	5.45589100
C	-1.22377800	1.77813100	2.74651000
O	-2.32081300	1.68115100	2.42880000
C	0.13465400	3.38849800	4.13938600

O	-0.07268900	4.34628300	4.73391800
C	3.24124300	0.21516500	4.89748700
O	3.77391400	0.22898600	5.90201500
C	1.81566800	-1.47835800	3.43411400
O	1.43605300	-2.54805500	3.50225500
C	3.86621600	-0.15220700	2.30826800
O	4.78764400	-0.38478400	1.68183500
N	2.17151000	2.84194000	0.49109000
C	1.93993200	1.46946400	0.13635600
H	2.89577700	0.97686900	-0.02609300
H	1.36342800	1.38095700	-0.77888900
C	3.22630000	2.99531900	1.45387200
H	3.58656200	4.01815500	1.49747500
H	4.06347700	2.36165700	1.17031700
C	1.07419100	3.73363000	0.53003200
C	1.15728400	4.96406800	1.20676700
C	-0.13379900	3.43343100	-0.12526700
C	0.08237200	5.84435000	1.24171100
C	-1.21146500	4.31042100	-0.09305100
H	-0.27065900	2.49856300	-0.64932100
C	-1.10227400	5.51265900	0.59538000
H	0.17370500	6.77530300	1.78725400
H	-2.13319400	4.04017000	-0.59305000
H	2.04944900	5.24903300	1.74541700
Br	-2.60272900	6.71279900	0.67064100

2H₂

Fe	0.61319100	1.77548600	3.22743300
Fe	2.59524800	0.15491700	3.28674200
S	1.17444500	0.39315500	1.43883900
S	2.83367200	2.48490300	3.24858200
C	0.80589700	0.52906300	4.46573300

O	0.39411100	0.00795200	5.42441900
C	-1.07884000	1.52409900	2.84641600
O	-2.17301700	1.36597200	2.57074400
C	0.22978300	3.12579700	4.27914900
O	-0.00094400	4.01940100	4.94671400
C	3.45063400	0.15233900	4.87335000
O	3.98348800	0.17590900	5.86856000
C	2.08740500	-1.57197300	3.37722800
O	1.74924200	-2.64844100	3.41884400
C	4.06326900	-0.13378500	2.27740900
O	4.97819100	-0.30742400	1.63696500
N	2.29336600	2.77297100	0.53957600
C	2.08941600	1.40310000	0.17828700
H	3.05657800	0.93587300	0.00852200
H	1.52439900	1.31250900	-0.74292300
C	3.32335200	2.94528900	1.51914800
H	3.66115500	3.97447100	1.56880800
H	4.18174000	2.34053700	1.23660900
C	1.21035000	3.66808400	0.50683300
C	1.28553900	4.92194200	1.12719000
C	0.03275600	3.36043700	-0.18705600
C	0.24913300	5.83513900	1.03257300
C	-1.00525800	4.27201500	-0.28373800
H	-0.10539700	2.39825600	-0.65749500
C	-0.89254900	5.51200500	0.31986100
H	0.33864500	6.79526000	1.52447600
H	-1.90258200	4.00149800	-0.82541400
H	2.15090800	5.21017400	1.70536000
Br	-2.32521100	6.76426300	0.19965800
H	-2.17875500	4.74414500	2.62616100
H	-2.43314700	4.26533300	3.13550200