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Supporting information

Electrochemical valorization of HCl for the production of chlorine *via* proton-filter functional covalent organic framework

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Chemicals required

4, 4',4''-(1,3,5-triazine-2,4,6-triyl)trianiline (Tta, TCI Chemicals), 2,6-diformylpyridine (Dfp, TCI Chemicals) 1,3,5-tris(4-aminophenyl)benzene (Tab, TCI Chemicals), 1, 4-dioxane (Sigma-Aldrich), mesitylene (Sigma-Aldrich), acetic acid (Merck), N, N-dimethylacetamide (DMA) (Sigma-Aldrich), acetone (Merck), methanol (Fisher Scientific), were used as received. All the reactions were carried out in oven-dried 35 ml heavy walled (HW) pressure glass vessel capped with Teflon screw cap with rubber internal thread under an air atmosphere unless otherwise mentioned. Rh_xS_y/C (30%) was obtained from De Nora; RuO_2 was obtained from Sigma-Aldrich

Physical characterization

For the preliminary analysis of the synthesized COFs, powder X-ray diffraction (P-XRD) measurements were performed on Rigaku Smart Lab II with Cu Kα (λ = 1.5405 Å) radiation source operating at 40 kV and 40 mA. The patterns were recorded with divergent slit of 1/16° over the 2θ range of 2–50° with step size = 0.02°. Fourier transform infrared (FT-IR) spectra were taken on a Bruker Optics ALPHA-E spectrometer with a universal Zn-Se ATR (attenuated total reflection) accessory in the 600- 4000 cm^{-1} region or using a Diamond ATR (Golden Gate) with 24 scan rate and 4 cm^{-1} resolution. Solid-state ^{13}C cross polarization-magic angle spinning (CP/MAS) NMR spectra of the COFs were recorded on a Bruker Avance 500 Wide Bore (500MHz) spectrometer at ambient temperature with a magic angle spinning rate of 18.0 kHz and the data were processed using Top Spin software. The BET and porosity analyses were performed on an Anton Paar Autosorb iQ combined physisorption and chemisorption instrument. For each measurement, 20 – 30 mg of COF samples were used and were activated at 80 °C for 16 hours in N_2 gas and utilised liquid N_2 bath (77 K) to collect full isotherms. Further, the surface areas were calculated using the multipoint Brunauer-Emmett-Teller (BET) model, and pore size distributions were evaluated/calculated using the non-local density functional theory (NLDFT). TGA analysis was performed using a PerkinElmer Simultaneous Thermal analyzer STA 6000 under N_2 environment at a heating rate of 15 °C min^{-1} and a temperature range of 30-900 °C.[1]

The morphological and elemental analyses was done by scanning electron microscopy (SEM, JEOL JSM-7610F FEG-SEM. The samples for SEM analyses were prepared by drop-casting 10 µL of material slurry on a silicon substrate (slurry prepared by dispersing it in isopropyl alcohol) and drying in air followed by Pt coating (nano-sized film) using the JEOL JEC-300FC Auto Fine instrument. Further, transmission electron microscopy (TEM) and high-resolution TEM (HR-TEM) were employed for the in-depth morphological analysis by FEI Tecnai TEM 20 kV. The TEM samples were prepared by drop casting the material slurry over carbon grids (TED PELLA, INC. 200 mesh) and then drying overnight in desiccators. X-ray photoelectron spectroscopy XPS measurements were performed using a Supra+ instrument (Kratos, Manchester, UK) equipped with an Al Kα excitation source and a monochromator. The charge neutralizer was on during the measurements. The take-off angle was 90°. XPS measurements and data processing were performed using ESCApe 1.5 software (Kratos). The powder samples were placed on a carbon tape attached to the silicon wafer. The area analysed was 300 by 700 microns. The measurements were performed at a pass energy of 20 eV. The base pressure in the main analysis chamber was 8 x 10^{-8} mbar. The binding energy scale was corrected based on the C-C/C-H peak at 284.8 eV in the C 1s spectrum.

Electrochemical investigation

The synthesized catalyst was meticulously homogenized in a mortar and pestle and 3.00 mg of it was added to 50 µl IPA followed by the addition of 945 µl of DI water and 5 µl of 0.25% Nafion solution. The mixture was ultrasonicated for an hour to obtain a uniform catalyst slurry. The carbon paper was cleansed in 5 M HNO3 to get rid of surface oxides before analysis, then it was ultrasonically processed for 15 minutes in water, followed by another 15 minutes in isopropyl alcohol (IPA). Following that, the 40 µl of catalytic ink was drop-casted on carbon paper and left to dry at room temperature. The electrochemical measurements were performed using Biologic VSP-300 potentiostat/galvanostat connected with EC-Lab software. The measurements were carried out using three-electrode assembly, which comprised of Ag/AgCl/3M KCl as reference electrode and graphite electrode was employed as counter electrode. The working electrode was prepared by drop-casting 20 µL of catalyst slurry followed by drying at room temperature.
The electrocatalytic activity w.r.t oxygen reduction reactions were analysed by linear sweep voltammetric (LSV) experiments were performed in O_2 and Ar saturated 0.4 M HCl at a scan rate of 10 mV s^{-1} across a potential range of 0.5 to -0.1 V vs. RHE. The hydrodynamic experiments viz, rotating disk electrode (RDE) using a glassy carbon disk electrode from Pine and experiments were performed using a speed controlling unit (AFMSRCE, Pine Research Instrument Inc., USA) at various rotation rate in the range of 100 to 1300 rpm. All the potential are converted to the RHE scale for uniformity unless detailed otherwise.

$$E_{RHE} = E_{Ag/AgCl} + E^{\circ}_{Ag/AgCl} + 0.059\ pH$$

The current density is calculated using the equation:

$$j = {}^{i}/_{A}$$

where i is the current in mA and A is the size of the electrode in cm^2.

Where E_{RHE} is the converted potential vs. RHE, $E_{Ag/AgCl}$ is the experimentally measured potential vs. Ag/AgCl (saturated KCl), and $E^{\circ}_{Ag/AgCl}$ is 0.1976 V at 25 °C.

Rotating disk electrode (RDE) analysis

The RDE measurements were performed for each variants by sweeping the potential from 0.5 V to -0.1 V in the oxygen saturated 0.4 M HCl solution at different rotation rates ranging from 0 to 1300 rpm. The measurements were recorded in Autolab 302 N modular potentiostat/galvanostat connected with Nova 1.11 software.

The mentioned K-L plots were extracted from RDE polarization curves using the following equation:

$$1/j = 1/j_k + 1/j_d$$

Where, 'j' stands for the measured current density, 'j_k' and 'j_d' represent kinetic and diffusion current densities, respectively. Furthermore, the slope of the K-L plot was computed by linearly fitting the graph between the inverse of the current density measured (y-axis) and inverse of square root of rotation rate (x-axis) to obtain the number of electrons transferred during the reaction. For calculating the kinetic parameters, the following equation was utilized;

$$j_d = 0.62nFD^{2/3}\upsilon^{-1/6}D_{O2}$$

Here, n depicts the number of electrons transferred during the ORR, F is the Faraday constant (96500 C mol^{-1}), D is the diffusion coefficient of dissolved oxygen ($1.43*10^{-5}$ cm^2 s^{-1}), υ is the kinematic viscosity ($1.13*10^{-2}$ cm^2 s^{-1}) and D_{O2} represents the concentration of dissolved oxygen (1.61 mol cm^{-3}) in 0.4 M HCl.

Electrochemical impedance spectroscopy (EIS)

EIS measurements were performed at 1.6 V vs. RHE under illumination over a frequency range from 7 MHz to 10 Hz. Further, to obtain charge transfer resistance (R_{ct}) the EIS curves were z fit using an appropriate equivalent circuit. Furthermore, the rate constant, k^0 was calculated from R_{ct} by using the formulae:

$$k^0 = \frac{RT}{n^2F^2ACR_{ct}}$$

Where R is gas constant, T is temperature in Kelvin, n is the no. of electrons involved in the reaction, F is the faraday constant, A is the area of the electrode, C is the concentration of the reacting species and R_{ct} is the charge transfer resistance.

Electrochemical surface area (ECSA)

The ECSA was estimated by electrochemical double-layer capacitance (C_{dl}) via CV plots obtained at different scan rates ranging from 20-300 mV s^{-1}, with a sweep potential ranging from 0.63 to 0.75 V vs. RHE. The C_{dl} can be calculated from the slope (k) of the current density against scan rate at 0.7 V vs. RHE.

Further, the ECSA was estimated according to the equation:

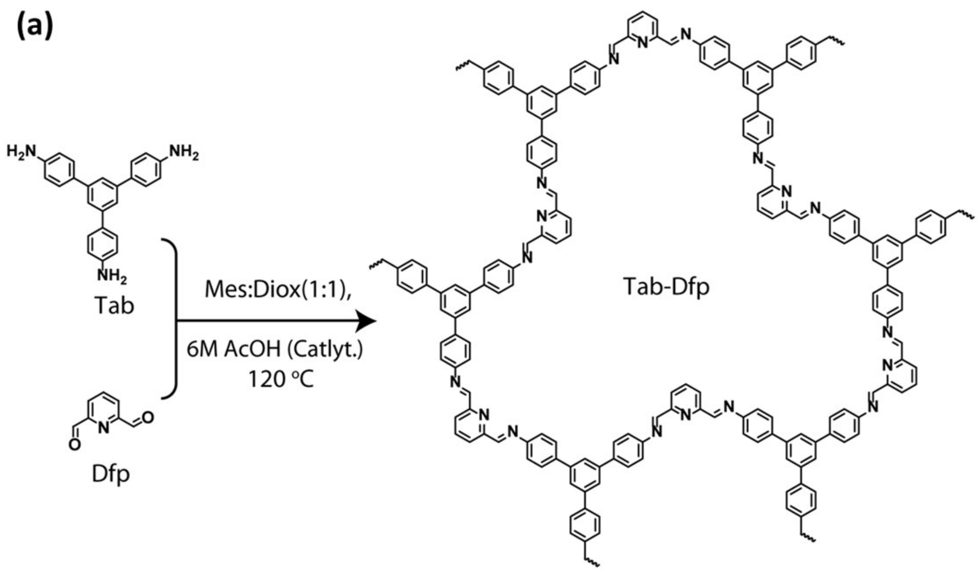
$$ECSA = \frac{C_{dl}}{C_s}$$

where C_s is a specific capacitance of 40 µF cm^{-2}
Additionally, specific surface area (SSA) has been calculated using the equation:

$$SSA = \frac{ECSA}{loading\ of\ the\ catalyst}$$

Scanning electrochemical microscopy (SECM) studies

The scanning electrochemical microscopic (SECM) approach was used to gain insight into the local electrocatalytic activity and distribution of active sites over the catalyst spot. Sensolytics Base SECM (Sensolytics, Bochum, Germany) with stepper-motor-driven x-y-z stages and an additional three-axis piezo-positioning system working in conjunction with the bi-potentiostat (Autolab 204, Metrohm) was utilized to record SECM analysis. To perform the SECM measurements, four electrodes assembly was used including Pt- micro-electrode (WE2) having diameter of 25 µm, Ag/AgCl/3M KCl as reference, Pt-coil as counter and glassy carbon plate containing catalyst spot as a working electrode (WE1) respectively in oxygen saturated 0.4 M HCl solution. The electrocatalytic ability of each spot vs. Pt-microelectrode towards oxygen reduction in 0.4 M HCl solution was measured using the redox competitive mode of SECM. The GC (WE1) electrode was polarized at different potentials (0.5, 0.2, 0.0 and -0.1 V) whereas, Pt- micro-electrode (WE2) was constantly polarized at 0.2 V vs. RHE. The array scan was performed in x-y using tilt-control mode and the data was analyzed using Gwyddion and Origin 8.5 software. Moreover, two distinct pulse potential profile was also employed in order to see the stability and durability of the catalysts.



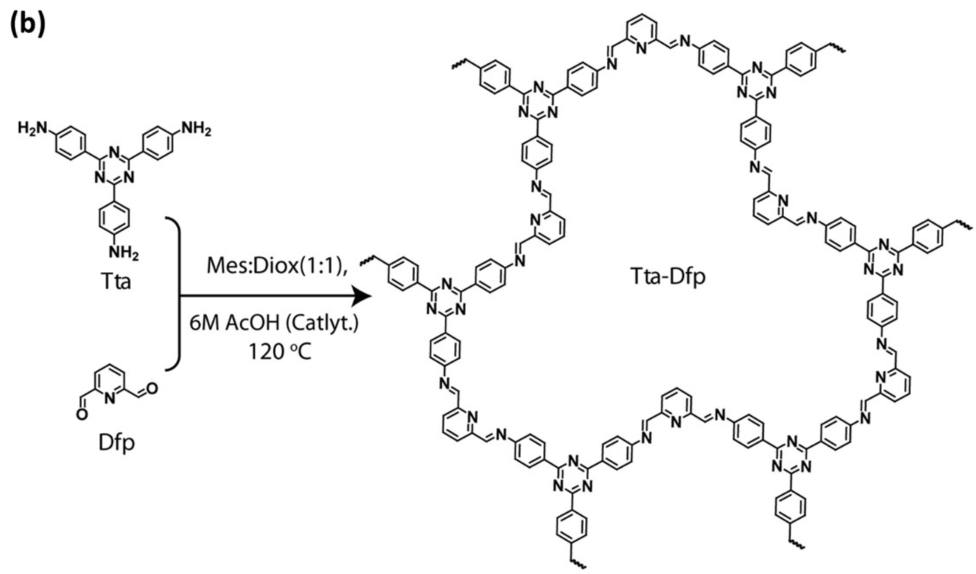


Fig. S1 Synthetic scheme of (a) **Tab-Dfp** and (b) **Tta-Dfp**.[1]

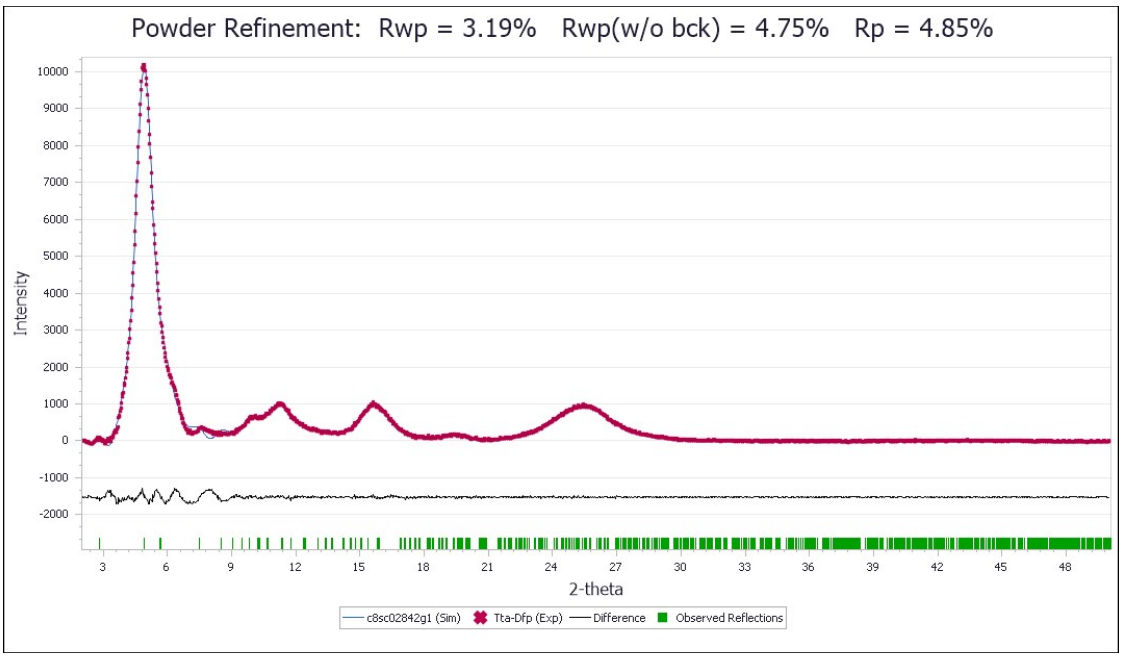


Fig. S2 Comparison of experimental P-XRD pattern of **Tta-Dfp** (-); with corresponding simulated, and Pawley refined difference; Background; inset shows Rp, Rwp, and Rwp (w/o bck) (lattice parameters: R, weighted profile R values: Rwp, Un-weighted profile R values Rp).

Table S1. Fractional atomic coordinates of unit cell and lattice parameters of **Tta-Dfp**.

Tta-Dfp (Space group P3)											
Unit cell parameters a = 35.92 Å, b = 35.92 Å, c = 9.75 Å; α = 90°, β = 90°, γ = 120°											
Atoms	x	y	z	**Atoms**	x	y	z	**Atoms**	x	y	z
H1	-0.87009	-1.07606	-0.03212	**C15**	-2.86932	-1.95742	-0.03478	**C45**	-0.61776	-1.95232	0.63011
H2	-0.94418	-1.07672	-0.03172	**C16**	-2.82751	-1.95827	-0.03486	**N46**	-0.60947	-1.98885	0.63271
H3	-0.86773	-0.92391	-0.03489	**C17**	-2.82686	-2.00033	-0.03397	**C47**	-0.64499	-2.03419	0.63486
H4	-0.79484	-0.92546	-0.03504	**C18**	-2.77232	-2.03094	-0.03072	**C48**	-0.63438	-2.07263	0.63705
H5	-0.7996	-1.06711	-0.02731	**N19**	-2.71311	-2.05533	-0.03125	**C49**	-0.70808	-2.24283	0.63533
H6	-0.6216	-1.07592	-0.04197	**C20**	-2.72317	-2.01999	-0.03202	**C50**	-0.70775	-2.20043	0.63383
H7	-0.75044	-1.28719	-0.03984	**C21**	-2.68642	-1.97343	-0.03434	**C51**	-0.66575	-2.1579	0.63909
H8	-0.75791	-1.21712	-0.04041	**C22**	-2.64043	-1.96401	-0.03613	**C52**	-0.62349	-2.15838	0.6468
H9	-0.60815	-1.1316	-0.00588	**C23**	-2.63112	-2.00065	-0.03583	**C53**	-0.62377	-2.20093	0.64821
H10	-0.60075	-1.20048	-0.00748	**C24**	-2.66821	-2.04682	-0.03313	**C54**	-0.6661	-2.24371	0.64221
C11	-0.95693	-0.99844	-0.03369	**C25**	-2.65777	-2.08524	-0.03348	**C55**	-0.66671	-2.28897	0.64316
C12	-0.86933	-1.04304	-0.0331	**C26**	-2.71915	-2.25334	-0.03246	**N56**	-0.37786	-1.67016	0.62749
C13	-0.91188	-1.0436	-0.03306	**C27**	-2.72353	-2.21334	-0.0329	**N57**	-0.66833	-2.11576	0.6372
C14	-0.91237	-0.99902	-0.034	**C28**	-2.68407	-2.16871	-0.02488	**N58**	-0.62611	-2.28996	0.64318
C15	-0.86932	-0.95742	-0.03478	**C29**	-2.63974	-2.1649	-0.01479	**H59**	-0.53273	-1.80838	0.66862
C16	-0.82751	-0.95827	-0.03486	**C30**	-2.63535	-2.20481	-0.01481	**H60**	-0.46416	-1.73173	0.66373
C17	-0.82686	-1.00033	-0.03397	**C31**	-2.67493	-2.24954	-0.02371	**H61**	-0.37789	-1.79335	0.59316
C18	-0.77232	-1.03094	-0.03072	**C32**	-2.66994	-2.29181	-0.02389	**H62**	-0.44769	-1.87115	0.5951
N19	-0.71311	-1.05533	-0.03125	**N33**	-2.99841	-2.03912	-0.03364	**H63**	-0.58842	-1.87658	0.61819
C20	-0.72317	-1.01999	-0.03202	**N34**	-2.78191	-1.99728	-0.0339	**C74**	-0.37331	-1.70883	0.62752
C21	-0.68642	-0.97343	-0.03434	**N35**	-2.69067	-2.1287	-0.02607	**C75**	-0.49961	-1.80619	0.64973
C22	-0.64043	-0.96401	-0.03613	**N36**	-2.62685	-2.28755	-0.02395	**C76**	-0.4599	-1.76176	0.6481
C23	-0.63112	-1.00065	-0.03583	**H109**	-2.69308	-1.94454	-0.03469	**C77**	-0.41539	-1.75619	0.62814
C24	-0.66821	-1.04682	-0.03313	**H110**	-2.61196	-1.92828	-0.038	**C78**	-0.4116	-1.7963	0.60936
C25	-0.65777	-1.08524	-0.03348	**H111**	-2.59524	-1.99301	-0.0376	**C79**	-0.45143	-1.84081	0.61021
C26	-0.71915	-1.25334	-0.03246	**H1**	-1.92394	-1.79403	-0.03212	**C80**	-0.49586	-1.84637	0.6296
C27	-0.72353	-1.21334	-0.0329	**H2**	-1.92328	-1.86746	-0.03172	**C81**	-0.57921	-1.90353	0.62681
C28	-0.68407	-1.16871	-0.02488	**H3**	-2.07609	-1.94382	-0.03489	**N104**	-0.53573	-1.89305	0.63087
C29	-0.63974	-1.1649	-0.01479	**H4**	-2.07454	-1.86938	-0.03504	**H112**	-0.72051	-2.07917	0.637
C30	-0.63535	-1.20481	-0.01481	**H5**	-1.93289	-1.73249	-0.02731	**H113**	-0.73632	-2.01406	0.63222
C31	-0.67493	-1.24954	-0.02371	**H6**	-1.92408	-1.54568	-0.04197	**H114**	-0.6713	-1.93278	0.62726
C32	-0.66994	-1.29181	-0.02389	**H7**	-1.71281	-1.46325	-0.03984	**N56**	-0.37786	-2.67016	0.62749
N33	-0.99841	-1.03912	-0.03364	**H8**	-1.78288	-1.54079	-0.04041	**N56**	0.62214	-1.67016	0.62749
N34	-0.78191	-0.99728	-0.0339	**H9**	-1.8684	-1.47655	-0.00588	**N56**	0.67016	-0.7077	0.62749
N35	-0.69067	-1.1287	-0.02607	**H10**	-1.79952	-1.40027	-0.00748	**N56**	-1.2923	-2.62214	0.62749
N36	-0.62685	-1.28755	-0.02395	**C11**	-2.00156	-1.95849	-0.03369	**N56**	-0.2923	-1.62214	0.62749
H109	-0.69308	-0.94454	-0.03469	**C12**	-1.95696	-1.82629	-0.0331	**C74**	-1.37331	-2.70883	0.62752
H110	-0.61196	-0.92828	-0.038	**C13**	-1.9564	-1.86828	-0.03306	**C74**	-0.29117	-2.66448	0.62752
H111	-0.59524	-0.99301	-0.0376	**C14**	-2.00098	-1.91335	-0.034	**C74**	0.70883	-1.66448	0.62752
H1	-0.92394	-1.79403	-0.03212	**C15**	-2.04258	-1.9119	-0.03478	**C74**	-0.33552	-1.62669	0.62752
H2	-0.92328	-1.86746	-0.03172	**C16**	-2.04173	-1.86924	-0.03486	**C74**	0.66448	-0.62669	0.62752
H3	-1.07609	-1.94382	-0.03489	**C17**	-1.99967	-1.82653	-0.03397	**H64**	-1.79169	-0.92087	0.29904
H4	-1.07454	-1.86938	-0.03504	**C18**	-1.96906	-1.74138	-0.03072	**H65**	-1.86551	-0.9213	0.2993
H5	-0.93289	-1.73249	-0.02731	**N19**	-1.94467	-1.65778	-0.03125	**H66**	-1.94028	-1.07214	0.30235
H6	-0.92408	-1.54568	-0.04197	**C20**	-1.98001	-1.70318	-0.03202	**H67**	-1.86607	-1.0714	0.30203
H7	-0.71281	-1.46325	-0.03984	**C21**	-2.02657	-1.71299	-0.03434	**H68**	-1.72941	-0.92907	0.29529
H8	-0.78288	-1.54079	-0.04041	**C22**	-2.03599	-1.67642	-0.03613	**H69**	-1.54183	-0.91917	0.30756
H9	-0.8684	-1.47655	-0.00588	**C23**	-1.99935	-1.63047	-0.03583	**H70**	-1.45865	-0.70855	0.33337
H10	-0.79952	-1.40027	-0.00748	**C24**	-1.95318	-1.62139	-0.03313	**H71**	-1.53643	-0.77838	0.33228
C11	-1.00156	-1.95849	-0.03369	**C25**	-1.91476	-1.57253	-0.03348	**H72**	-1.47361	-0.86339	0.2587
C12	-0.95696	-1.82629	-0.0331	**C26**	-1.74666	-1.46581	-0.03246	**H73**	-1.39701	-0.79478	0.2627
C13	-0.9564	-1.86828	-0.03306	**C27**	-1.78666	-1.51019	-0.0329	**C82**	-1.95428	-0.99733	0.30123
C14	-1.00098	-1.91335	-0.034	**C28**	-1.83129	-1.51536	-0.02488	**C83**	-1.82369	-0.95413	0.3002
C15	-1.04258	-1.9119	-0.03478	**C29**	-1.8351	-1.47484	-0.01479	**C84**	-1.86622	-0.95437	0.30043
C16	-1.04173	-1.86924	-0.03486	**C30**	-1.79519	-1.43054	-0.01481	**C85**	-1.90902	-0.99676	0.30142
C17	-0.99967	-1.82653	-0.03397	**C31**	-1.75046	-1.42539	-0.02371	**C86**	-1.90817	-1.03883	0.30215
C18	-0.96906	-1.74138	-0.03072	**C32**	-1.70819	-1.37813	-0.02389	**C87**	-1.86579	-1.03852	0.30198
N19	-0.94467	-1.65778	-0.03125	**N33**	-1.96088	-1.95929	-0.03364	**C88**	-1.82324	-0.99646	0.30093

C20	-0.98001	-1.70318	-0.03202	**N34**	-2.00272	-1.78463	-0.0339	**C89**	-1.73797	-0.96515	0.29759
C21	-1.02657	-1.71299	-0.03434	**N35**	-1.8713	-1.56197	-0.02607	**N90**	-1.65416	-0.94021	0.29802
C22	-1.03599	-1.67642	-0.03613	**N36**	-1.71245	-1.3393	-0.02395	**C91**	-1.69951	-0.97575	0.29803
C23	-0.99935	-1.63047	-0.03583	**H109**	-2.05546	-1.74854	-0.03469	**C92**	-1.70903	-1.02222	0.29887
C24	-0.95318	-1.62139	-0.03313	**H110**	-2.07172	-1.68368	-0.038	**C93**	-1.67229	-1.03138	0.29994
C25	-0.91476	-1.57253	-0.03348	**H111**	-2.00699	-1.60223	-0.0376	**C94**	-1.62644	-0.99458	0.30033
C26	-0.74666	-1.46581	-0.03246	**C11**	-1.95693	-1.99844	-0.03369	**C95**	-1.61761	-0.94848	0.29916
C27	-0.78666	-1.51019	-0.0329	**C11**	-0.95693	-1.99844	-0.03369	**C96**	-1.56878	-0.90993	0.30061
C28	-0.83129	-1.51536	-0.02488	**C11**	-1.00156	-0.95849	-0.03369	**C97**	-1.46159	-0.74225	0.31726
C29	-0.8351	-1.47484	-0.01479	**C11**	-3.04151	-2.04307	-0.03369	**C98**	-1.50608	-0.78211	0.31688
C30	-0.79519	-1.43054	-0.01481	**C11**	-2.04151	-3.04307	-0.03369	**C99**	-1.51164	-0.82655	0.2977
C31	-0.75046	-1.42539	-0.02371	**C32**	-1.66994	-2.29181	-0.02389	**C100**	-1.47146	-0.83028	0.2773
C32	-0.70819	-1.37813	-0.02389	**C32**	-1.66994	-1.29181	-0.02389	**C101**	-1.42704	-0.79054	0.27846
N33	-0.96088	-1.95929	-0.03364	**C32**	-2.70819	-2.37813	-0.02389	**C102**	-1.42147	-0.74601	0.29826
N34	-1.00272	-1.78463	-0.0339	**C32**	-1.62187	-3.33006	-0.02389	**C103**	-1.37412	-0.70392	0.29867
N35	-0.8713	-1.56197	-0.02607	**C32**	-0.62187	-1.33006	-0.02389	**N105**	-1.95525	-0.95672	0.30118
N36	-0.71245	-1.3393	-0.02395	**N33**	-1.99841	-2.03912	-0.03364	**N106**	-1.78109	-0.99908	0.30031
H109	-1.05546	-1.74854	-0.03469	**N33**	-0.99841	-2.03912	-0.03364	**N107**	-1.55832	-0.86644	0.29734
H110	-1.07172	-1.68368	-0.038	**N33**	-2.96088	-1.95929	-0.03364	**N108**	-1.3689	-0.66046	0.29871
H111	-1.00699	-1.60223	-0.0376	**N33**	-0.96088	-0.95929	-0.03364	**H115**	-1.74449	-1.05126	0.29862
H1	-1.20597	-1.12991	-0.03212	**N33**	-2.04071	-3.00159	-0.03364	**H116**	-1.67936	-1.06706	0.30067
H2	-1.13254	-1.05582	-0.03172	**N36**	-1.62685	-2.28755	-0.02395	**H117**	-1.59806	-1.00203	0.30155
H3	-1.05618	-1.13227	-0.03489	**N36**	-1.62685	-1.28755	-0.02395	**H64**	-2.07913	-0.87082	0.29904
H4	-1.13062	-1.20516	-0.03504	**N36**	-2.71245	-2.3393	-0.02395	**H65**	-2.0787	-0.94421	0.2993
H5	-1.26751	-1.2004	-0.02731	**N36**	-1.71245	-3.3393	-0.02395	**H66**	-1.92786	-0.86814	0.30235
H6	-1.45432	-1.3784	-0.04197	**N36**	-0.6607	-1.37315	-0.02395	**H67**	-1.9286	-0.79467	0.30203
H7	-1.53675	-1.24956	-0.03984	**H37**	0.4017	-1.06409	0.63798	**H68**	-2.07093	-0.80034	0.29529
H8	-1.45921	-1.24209	-0.04041	**H38**	0.25863	-1.27491	0.63124	**H69**	-2.08083	-0.62266	0.30756
H9	-1.52345	-1.39185	-0.00588	**H39**	0.25941	-1.20069	0.62875	**H70**	-2.29145	-0.7501	0.33337
H10	-1.59973	-1.39925	-0.00748	**H40**	0.40971	-1.12641	0.65232	**H71**	-2.22162	-0.75805	0.33228
C11	-1.04151	-1.04307	-0.03369	**H41**	0.40924	-1.20026	0.65454	**H72**	-2.13661	-0.61022	0.2587
C12	-1.17371	-1.13067	-0.0331	**C42**	0.30852	-1.04372	0.63493	**H73**	-2.20522	-0.60223	0.2627
C13	-1.13172	-1.08812	-0.03306	**C43**	0.29935	-1.00698	0.63232	**C82**	-2.00267	-0.95695	0.30123
C14	-1.08665	-1.08763	-0.034	**C44**	0.33616	-0.96115	0.62961	**C83**	-2.04587	-0.86956	0.3002
C15	-1.0881	-1.13068	-0.03478	**C45**	0.38224	-0.95232	0.63011	**C84**	-2.04563	-0.91185	0.30043
C16	-1.13076	-1.17249	-0.03486	**N46**	0.39053	-0.98885	0.63271	**C85**	-2.00324	-0.91226	0.30142
C17	-1.17347	-1.17314	-0.03397	**C47**	0.35501	-1.03419	0.63486	**C86**	-1.96117	-0.86934	0.30215
C18	-1.25862	-1.22768	-0.03072	**C48**	0.36562	-1.07263	0.63705	**C87**	-1.96148	-0.82727	0.30198
N19	-1.34222	-1.28689	-0.03125	**C49**	0.29192	-1.24283	0.63533	**C88**	-2.00354	-0.82678	0.30093
C20	-1.29682	-1.27683	-0.03202	**C50**	0.29225	-1.20043	0.63383	**C89**	-2.03485	-0.77282	0.29759
C21	-1.28701	-1.31358	-0.03434	**C51**	0.33425	-1.1579	0.63909	**N90**	-2.05979	-0.71395	0.29802
C22	-1.32358	-1.35957	-0.03613	**C52**	0.37651	-1.15838	0.6468	**C91**	-2.02425	-0.72376	0.29803
C23	-1.36953	-1.36888	-0.03583	**C53**	0.37623	-1.20093	0.64821	**C92**	-1.97778	-0.68681	0.29887
C24	-1.37861	-1.33179	-0.03313	**C54**	0.3339	-1.24371	0.64221	**C93**	-1.96862	-0.64091	0.29994
C25	-1.42747	-1.34223	-0.03348	**C55**	0.33329	-1.28897	0.64316	**C94**	-2.00542	-0.63186	0.30033
C26	-1.53419	-1.28085	-0.03246	**N56**	0.62214	-0.67016	0.62749	**C95**	-2.05152	-0.66913	0.29916
C27	-1.48981	-1.27647	-0.0329	**N57**	0.33167	-1.11576	0.6372	**C96**	-2.09007	-0.65885	0.30061
C28	-1.48464	-1.31593	-0.02488	**N58**	0.37389	-1.28996	0.64318	**C97**	-2.25775	-0.71934	0.31726
C29	-1.52516	-1.36026	-0.01479	**H59**	0.46727	-0.80838	0.66862	**C98**	-2.21789	-0.72397	0.31688
C30	-1.56946	-1.36465	-0.01481	**H60**	0.53584	-0.73173	0.66373	**C99**	-2.17345	-0.68509	0.2977
C31	-1.57461	-1.32507	-0.02371	**H61**	0.62211	-0.79335	0.59316	**C100**	-2.16972	-0.64118	0.2773
C32	-1.62187	-1.33006	-0.02389	**H62**	0.55231	-0.87115	0.5951	**C101**	-2.20946	-0.6365	0.27846
N33	-1.04071	-1.00159	-0.03364	**H63**	0.41158	-0.87658	0.61819	**C102**	-2.25399	-0.67546	0.29826
N34	-1.21537	-1.21809	-0.0339	**C74**	0.62669	-0.70883	0.62752	**C103**	-2.29608	-0.6702	0.29867
N35	-1.43803	-1.30933	-0.02607	**C75**	0.50039	-0.80619	0.64973	**N105**	-2.04328	-0.99853	0.30118
N36	-1.6607	-1.37315	-0.02395	**C76**	0.5401	-0.76176	0.6481	**N106**	-2.00092	-0.78201	0.30031
H109	-1.25146	-1.30692	-0.03469	**C77**	0.58461	-0.75619	0.62814	**N107**	-2.13356	-0.69188	0.29734
H110	-1.31632	-1.38804	-0.038	**C78**	0.5884	-0.7963	0.60936	**N108**	-2.33954	-0.70844	0.29871
H111	-1.39777	-1.40476	-0.0376	**C79**	0.54857	-0.84081	0.61021	**H115**	-1.94874	-0.69323	0.29862
H1	-1.92394	-2.79403	-0.03212	**C80**	0.50414	-0.84637	0.6296	**H116**	-1.93294	-0.6123	0.30067
H2	-1.92328	-2.86746	-0.03172	**C81**	0.42079	-0.90353	0.62681	**H117**	-1.99797	-0.59603	0.30155
H3	-2.07609	-2.94382	-0.03489	**N104**	0.46427	-0.89305	0.63087	**H64**	-2.12918	-1.20831	0.29904
H4	-2.07454	-2.86938	-0.03504	**H112**	0.27949	-1.07917	0.637	**H65**	-2.05579	-1.13449	0.2993
H5	-1.93289	-2.73249	-0.02731	**H113**	0.26368	-1.01406	0.63222	**H66**	-2.13186	-1.05972	0.30235

H6	-1.92408	-2.54568	-0.04197	**H114**	0.3287	-0.93278	0.62726	**H67**	-2.20533	-1.13393	0.30203
H7	-1.71281	-2.46325	-0.03984	**H37**	0.06409	-1.53421	0.63798	**H68**	-2.19966	-1.27059	0.29529
H8	-1.78288	-2.54079	-0.04041	**H38**	0.27491	-1.46646	0.63124	**H69**	-2.37734	-1.45817	0.30756
H9	-1.8684	-2.47655	-0.00588	**H39**	0.20069	-1.5399	0.62875	**H70**	-2.2499	-1.54135	0.33337
H10	-1.79952	-2.40027	-0.00748	**H40**	0.12641	-1.46388	0.65232	**H71**	-2.24195	-1.46357	0.33228
C11	-2.00156	-2.95849	-0.03369	**H41**	0.20026	-1.3905	0.65454	**H72**	-2.38978	-1.52639	0.2587
C12	-1.95696	-2.82629	-0.0331	**C42**	0.04372	-1.64776	0.63493	**H73**	-2.39777	-1.60299	0.2627
C13	-1.9564	-2.86828	-0.03306	**C43**	0.00698	-1.69367	0.63232	**C82**	-2.04305	-1.04572	0.30123
C14	-2.00098	-2.91335	-0.034	**C44**	-0.03885	-1.70269	0.62961	**C83**	-2.13044	-1.17631	0.3002
C15	-2.04258	-2.9119	-0.03478	**C45**	-0.04768	-1.66544	0.63011	**C84**	-2.08815	-1.13378	0.30043
C16	-2.04173	-2.86924	-0.03486	**N46**	-0.01115	-1.62062	0.63271	**C85**	-2.08774	-1.09098	0.30142
C17	-1.99967	-2.82653	-0.03397	**C47**	0.03419	-1.6108	0.63486	**C86**	-2.13066	-1.09183	0.30215
C18	-1.96906	-2.74138	-0.03072	**C48**	0.07263	-1.56175	0.63705	**C87**	-2.17273	-1.13421	0.30198
N19	-1.94467	-2.65778	-0.03125	**C49**	0.24283	-1.46525	0.63533	**C88**	-2.17322	-1.17676	0.30093
C20	-1.98001	-2.70318	-0.03202	**C50**	0.20043	-1.50732	0.63383	**C89**	-2.22718	-1.26203	0.29759
C21	-2.02657	-2.71299	-0.03434	**C51**	0.1579	-1.50785	0.63909	**N90**	-2.28605	-1.34584	0.29802
C22	-2.03599	-2.67642	-0.03613	**C52**	0.15838	-1.46511	0.6468	**C91**	-2.27624	-1.30049	0.29803
C23	-1.99935	-2.63047	-0.03583	**C53**	0.20093	-1.42284	0.64821	**C92**	-2.31319	-1.29097	0.29887
C24	-1.95318	-2.62139	-0.03313	**C54**	0.24371	-1.42239	0.64221	**C93**	-2.35909	-1.32771	0.29994
C25	-1.91476	-2.57253	-0.03348	**C55**	0.28897	-1.37774	0.64316	**C94**	-2.36814	-1.37356	0.30033
C26	-1.74666	-2.46581	-0.03246	**N56**	-0.32984	-1.7077	0.62749	**C95**	-2.33087	-1.38239	0.29916
C27	-1.78666	-2.51019	-0.0329	**N57**	0.11576	-1.55257	0.6372	**C96**	-2.34115	-1.43122	0.30061
C28	-1.83129	-2.51536	-0.02488	**N58**	0.28996	-1.33615	0.64318	**C97**	-2.28066	-1.53841	0.31726
C29	-1.8351	-2.47484	-0.01479	**H59**	-0.19162	-1.72435	0.66862	**C98**	-2.27603	-1.49392	0.31688
C30	-1.79519	-2.43054	-0.01481	**H60**	-0.26827	-1.73243	0.66373	**C99**	-2.31491	-1.48836	0.2977
C31	-1.75046	-2.42539	-0.02371	**H61**	-0.20665	-1.58454	0.59316	**C100**	-2.35882	-1.52854	0.2773
C32	-1.70819	-2.37813	-0.02389	**H62**	-0.12885	-1.57654	0.5951	**C101**	-2.3635	-1.57296	0.27846
N33	-1.96088	-2.95929	-0.03364	**H63**	-0.12342	-1.71184	0.61819	**C102**	-2.32454	-1.57853	0.29826
N34	-2.00272	-2.78463	-0.0339	**C74**	-0.29117	-1.66448	0.62752	**C103**	-2.3298	-1.62588	0.29867
N35	-1.8713	-2.56197	-0.02607	**C75**	-0.19381	-1.69342	0.64973	**N105**	-2.00147	-1.04475	0.30118
N36	-1.71245	-2.3393	-0.02395	**C76**	-0.23824	-1.69814	0.6481	**N106**	-2.21799	-1.21891	0.30031
H109	-2.05546	-2.74854	-0.03469	**C77**	-0.24381	-1.6592	0.62814	**N107**	-2.30812	-1.44168	0.29734
H110	-2.07172	-2.68368	-0.038	**C78**	-0.2037	-1.6153	0.60936	**N108**	-2.29156	-1.6311	0.29871
H111	-2.00699	-2.60223	-0.0376	**C79**	-0.15919	-1.61062	0.61021	**H115**	-2.30677	-1.25551	0.29862
H1	-1.20597	-2.12991	-0.03212	**C80**	-0.15363	-1.64949	0.6296	**H116**	-2.3877	-1.32064	0.30067
H2	-1.13254	-2.05582	-0.03172	**C81**	-0.09647	-1.67568	0.62681	**H117**	-2.40397	-1.40194	0.30155
H3	-1.05618	-2.13227	-0.03489	**N104**	-0.10695	-1.64268	0.63087	**H64**	-3.07913	-1.87082	0.29904
H4	-1.13062	-2.20516	-0.03504	**H112**	0.07917	-1.64134	0.637	**H65**	-3.0787	-1.94421	0.2993
H5	-1.26751	-2.2004	-0.02731	**H113**	0.01406	-1.72226	0.63222	**H66**	-2.92786	-1.86814	0.30235
H6	-1.45432	-2.3784	-0.04197	**H114**	-0.06722	-1.73852	0.62726	**H67**	-2.9286	-1.79467	0.30203
H7	-1.53675	-2.24956	-0.03984	**H37**	0.53421	-1.4017	0.63798	**H68**	-3.07093	-1.80034	0.29529
H8	-1.45921	-2.24209	-0.04041	**H38**	0.46646	-1.25863	0.63124	**H69**	-3.08083	-1.62266	0.30756
H9	-1.52345	-2.39185	-0.00588	**H39**	0.5399	-1.25941	0.62875	**H70**	-3.29145	-1.7501	0.33337
H10	-1.59973	-2.39925	-0.00748	**H40**	0.46388	-1.40971	0.65232	**H71**	-3.22162	-1.75805	0.33228
C11	-1.04151	-2.04307	-0.03369	**H41**	0.3905	-1.40924	0.65454	**H72**	-3.13661	-1.61022	0.2587
C12	-1.17371	-2.13067	-0.0331	**C42**	0.64776	-1.30852	0.63493	**H73**	-3.20522	-1.60223	0.2627
C13	-1.13172	-2.08812	-0.03306	**C43**	0.69367	-1.29935	0.63232	**C82**	-3.00267	-1.95695	0.30123
C14	-1.08665	-2.08763	-0.034	**C44**	0.70269	-1.33616	0.62961	**C83**	-3.04587	-1.86956	0.3002
C15	-1.0881	-2.13068	-0.03478	**C45**	0.66544	-1.38224	0.63011	**C84**	-3.04563	-1.91185	0.30043
C16	-1.13076	-2.17249	-0.03486	**N46**	0.62062	-1.39053	0.63271	**C85**	-3.00324	-1.91226	0.30142
C17	-1.17347	-2.17314	-0.03397	**C47**	0.6108	-1.35501	0.63486	**C86**	-2.96117	-1.86934	0.30215
C18	-1.25862	-2.22768	-0.03072	**C48**	0.56175	-1.36562	0.63705	**C87**	-2.96148	-1.82727	0.30198
N19	-1.34222	-2.28689	-0.03125	**C49**	0.46525	-1.29192	0.63533	**C88**	-3.00354	-1.82678	0.30093
C20	-1.29682	-2.27683	-0.03202	**C50**	0.50732	-1.29225	0.63383	**C89**	-3.03485	-1.77282	0.29759
C21	-1.28701	-2.31358	-0.03434	**C51**	0.50785	-1.33425	0.63909	**N90**	-3.05979	-1.71395	0.29802
C22	-1.32358	-2.35957	-0.03613	**C52**	0.46511	-1.37651	0.6468	**C91**	-3.02425	-1.72376	0.29803
C23	-1.36953	-2.36888	-0.03583	**C53**	0.42284	-1.37623	0.64821	**C92**	-2.97778	-1.68681	0.29887
C24	-1.37861	-2.33179	-0.03313	**C54**	0.42239	-1.3339	0.64221	**C93**	-2.96862	-1.64091	0.29994
C25	-1.42747	-2.34223	-0.03348	**C55**	0.37774	-1.33329	0.64316	**C94**	-3.00542	-1.63186	0.30033
C26	-1.53419	-2.28085	-0.03246	**N56**	0.7077	-1.62214	0.62749	**C95**	-3.05152	-1.66913	0.29916
C27	-1.48981	-2.27647	-0.0329	**N57**	0.55257	-1.33167	0.6372	**C96**	-3.09007	-1.65885	0.30061
C28	-1.48464	-2.31593	-0.02488	**N58**	0.33615	-1.37389	0.64318	**C97**	-3.25775	-1.71934	0.31726
C29	-1.52516	-2.36026	-0.01479	**H59**	0.72435	-1.46727	0.66862	**C98**	-3.21789	-1.72397	0.31688
C30	-1.56946	-2.36465	-0.01481	**H60**	0.73243	-1.53584	0.66373	**C99**	-3.17345	-1.68509	0.2977

C31	-1.57461	-2.32507	-0.02371	**H61**	0.58454	-1.62211	0.59316	**C100**	-3.16972	-1.64118	0.2773
C32	-1.62187	-2.33006	-0.02389	**H62**	0.57654	-1.55231	0.5951	**C101**	-3.20946	-1.6365	0.27846
N33	-1.04071	-2.00159	-0.03364	**H63**	0.71184	-1.41158	0.61819	**C102**	-3.25399	-1.67546	0.29826
N34	-1.21537	-2.21809	-0.0339	**C74**	0.66448	-1.62669	0.62752	**C103**	-3.29608	-1.6702	0.29867
N35	-1.43803	-2.30933	-0.02607	**C75**	0.69342	-1.50039	0.64973	**N105**	-3.04328	-1.99853	0.30118
N36	-1.6607	-2.37315	-0.02395	**C76**	0.69814	-1.5401	0.6481	**N106**	-3.00092	-1.78201	0.30031
H109	-1.25146	-2.30692	-0.03469	**C77**	0.6592	-1.58461	0.62814	**N107**	-3.13356	-1.69188	0.29734
H110	-1.31632	-2.38804	-0.038	**C78**	0.6153	-1.5884	0.60936	**N108**	-3.33954	-1.70844	0.29871
H111	-1.39777	-2.40476	-0.0376	**C79**	0.61062	-1.54857	0.61021	**H115**	-2.94874	-1.69323	0.29862
H1	-1.87009	-3.07606	-0.03212	**C80**	0.64949	-1.50414	0.6296	**H116**	-2.93294	-1.6123	0.30067
H2	-1.94418	-3.07672	-0.03172	**C81**	0.67568	-1.42079	0.62681	**H117**	-2.99797	-1.59603	0.30155
H3	-1.86773	-2.92391	-0.03489	**N104**	0.64268	-1.46427	0.63087	**H64**	-3.12918	-2.20831	0.29904
H4	-1.79484	-2.92546	-0.03504	**H112**	0.64134	-1.27949	0.637	**H65**	-3.05579	-2.13449	0.2993
H5	-1.7996	-3.06711	-0.02731	**H113**	0.72226	-1.26368	0.63222	**H66**	-3.13186	-2.05972	0.30235
H6	-1.6216	-3.07592	-0.04197	**H114**	0.73852	-1.3287	0.62726	**H67**	-3.20533	-2.13393	0.30203
H7	-1.75044	-3.28719	-0.03984	**H37**	-0.93591	-2.53421	0.63798	**H68**	-3.19966	-2.27059	0.29529
H8	-1.75791	-3.21712	-0.04041	**H38**	-0.72509	-2.46646	0.63124	**H69**	-3.37734	-2.45817	0.30756
H9	-1.60815	-3.1316	-0.00588	**H39**	-0.79931	-2.5399	0.62875	**H70**	-3.2499	-2.54135	0.33337
H10	-1.60075	-3.20048	-0.00748	**H40**	-0.87359	-2.46388	0.65232	**H71**	-3.24195	-2.46357	0.33228
C11	-1.95693	-2.99844	-0.03369	**H41**	-0.79974	-2.3905	0.65454	**H72**	-3.38978	-2.52639	0.2587
C12	-1.86933	-3.04304	-0.0331	**C42**	-0.95628	-2.64776	0.63493	**H73**	-3.39777	-2.60299	0.2627
C13	-1.91188	-3.0436	-0.03306	**C43**	-0.99302	-2.69367	0.63232	**C82**	-3.04305	-2.04572	0.30123
C14	-1.91237	-2.99902	-0.034	**C44**	-1.03885	-2.70269	0.62961	**C83**	-3.13044	-2.17631	0.3002
C15	-1.86932	-2.95742	-0.03478	**C45**	-1.04768	-2.66544	0.63011	**C84**	-3.08815	-2.13378	0.30043
C16	-1.82751	-2.95827	-0.03486	**N46**	-1.01115	-2.62062	0.63271	**C85**	-3.08774	-2.09098	0.30142
C17	-1.82686	-3.00033	-0.03397	**C47**	-0.96581	-2.6108	0.63486	**C86**	-3.13066	-2.09183	0.30215
C18	-1.77232	-3.03094	-0.03072	**C48**	-0.92737	-2.56175	0.63705	**C87**	-3.17273	-2.13421	0.30198
N19	-1.71311	-3.05533	-0.03125	**C49**	-0.75717	-2.46525	0.63533	**C88**	-3.17322	-2.17676	0.30093
C20	-1.72317	-3.01999	-0.03202	**C50**	-0.79957	-2.50732	0.63383	**C89**	-3.22718	-2.26203	0.29759
C21	-1.68642	-2.97343	-0.03434	**C51**	-0.8421	-2.50785	0.63909	**N90**	-3.28605	-2.34584	0.29802
C22	-1.64043	-2.96401	-0.03613	**C52**	-0.84162	-2.46511	0.6468	**C91**	-3.27624	-2.30049	0.29803
C23	-1.63112	-3.00065	-0.03583	**C53**	-0.79907	-2.42284	0.64821	**C92**	-3.31319	-2.29097	0.29887
C24	-1.66821	-3.04682	-0.03313	**C54**	-0.75629	-2.42239	0.64221	**C93**	-3.35909	-2.32771	0.29994
C25	-1.65777	-3.08524	-0.03348	**C55**	-0.71103	-2.37774	0.64316	**C94**	-3.36814	-2.37356	0.30033
C26	-1.71915	-3.25334	-0.03246	**N56**	-1.32984	-2.7077	0.62749	**C95**	-3.33087	-2.38239	0.29916
C27	-1.72353	-3.21334	-0.0329	**N57**	-0.88424	-2.55257	0.6372	**C96**	-3.34115	-2.43122	0.30061
C28	-1.68407	-3.16871	-0.02488	**N58**	-0.71004	-2.33615	0.64318	**C97**	-3.28066	-2.53841	0.31726
C29	-1.63974	-3.1649	-0.01479	**H59**	-1.19162	-2.72435	0.66862	**C98**	-3.27603	-2.49392	0.31688
C30	-1.63535	-3.20481	-0.01481	**H60**	-1.26827	-2.73243	0.66373	**C99**	-3.31491	-2.48836	0.2977
C31	-1.67493	-3.24954	-0.02371	**H61**	-1.20665	-2.58454	0.59316	**C100**	-3.35882	-2.52854	0.2773
C32	-1.66994	-3.29181	-0.02389	**H62**	-1.12885	-2.57654	0.5951	**C101**	-3.3635	-2.57296	0.27846
N33	-1.99841	-3.03912	-0.03364	**H63**	-1.12342	-2.71184	0.61819	**C102**	-3.32454	-2.57853	0.29826
N34	-1.78191	-2.99728	-0.0339	**C74**	-1.29117	-2.66448	0.62752	**C103**	-3.3298	-2.62588	0.29867
N35	-1.69067	-3.1287	-0.02607	**C75**	-1.19381	-2.69342	0.64973	**N105**	-3.00147	-2.04475	0.30118
N36	-1.62685	-3.28755	-0.02395	**C76**	-1.23824	-2.69814	0.6481	**N106**	-3.21799	-2.21891	0.30031
H109	-1.69308	-2.94454	-0.03469	**C77**	-1.24381	-2.6592	0.62814	**N107**	-3.30812	-2.44168	0.29734
H110	-1.61196	-2.92828	-0.038	**C78**	-1.2037	-2.6153	0.60936	**N108**	-3.29156	-2.6311	0.29871
H111	-1.59524	-2.99301	-0.0376	**C79**	-1.15919	-2.61062	0.61021	**H115**	-3.30677	-2.25551	0.29862
H1	-2.20597	-2.12991	-0.03212	**C80**	-1.15363	-2.64949	0.6296	**H116**	-3.3877	-2.32064	0.30067
H2	-2.13254	-2.05582	-0.03172	**C81**	-1.09647	-2.67568	0.62681	**H117**	-3.40397	-2.40194	0.30155
H3	-2.05618	-2.13227	-0.03489	**N104**	-1.10695	-2.64268	0.63087	**H64**	-2.79169	-1.92087	0.29904
H4	-2.13062	-2.20516	-0.03504	**H112**	-0.92083	-2.64134	0.637	**H65**	-2.86551	-1.9213	0.2993
H5	-2.26751	-2.2004	-0.02731	**H113**	-0.98594	-2.72226	0.63222	**H66**	-2.94028	-2.07214	0.30235
H6	-2.45432	-2.3784	-0.04197	**H114**	-1.06722	-2.73852	0.62726	**H67**	-2.86607	-2.0714	0.30203
H7	-2.53675	-2.24956	-0.03984	**H37**	-0.46579	-2.4017	0.63798	**H68**	-2.72941	-1.92907	0.29529
H8	-2.45921	-2.24209	-0.04041	**H38**	-0.53354	-2.25863	0.63124	**H69**	-2.54183	-1.91917	0.30756
H9	-2.52345	-2.39185	-0.00588	**H39**	-0.4601	-2.25941	0.62875	**H70**	-2.45865	-1.70855	0.33337
H10	-2.59973	-2.39925	-0.00748	**H40**	-0.53612	-2.40971	0.65232	**H71**	-2.53643	-1.77838	0.33228
C11	-2.04151	-2.04307	-0.03369	**H41**	-0.6095	-2.40924	0.65454	**H72**	-2.47361	-1.86339	0.2587
C12	-2.17371	-2.13067	-0.0331	**C42**	-0.35224	-2.30852	0.63493	**H73**	-2.39701	-1.79478	0.2627
C13	-2.13172	-2.08812	-0.03306	**C43**	-0.30633	-2.29935	0.63232	**C82**	-2.95428	-1.99733	0.30123
C14	-2.08665	-2.08763	-0.034	**C44**	-0.29731	-2.33616	0.62961	**C83**	-2.82369	-1.95413	0.3002
C15	-2.0881	-2.13068	-0.03478	**C45**	-0.33456	-2.38224	0.63011	**C84**	-2.86622	-1.95437	0.30043
C16	-2.13076	-2.17249	-0.03486	**N46**	-0.37938	-2.39053	0.63271	**C85**	-2.90902	-1.99676	0.30142

C17	-2.17347	-2.17314	-0.03397	**C47**	-0.3892	-2.35501	0.63486	**C86**	-2.90817	-2.03883	0.30215
C18	-2.25862	-2.22768	-0.03072	**C48**	-0.43825	-2.36562	0.63705	**C87**	-2.86579	-2.03852	0.30198
N19	-2.34222	-2.28689	-0.03125	**C49**	-0.53475	-2.29192	0.63533	**C88**	-2.82324	-1.99646	0.30093
C20	-2.29682	-2.27683	-0.03202	**C50**	-0.49268	-2.29225	0.63383	**C89**	-2.73797	-1.96515	0.29759
C21	-2.28701	-2.31358	-0.03434	**C51**	-0.49215	-2.33425	0.63909	**N90**	-2.65416	-1.94021	0.29802
C22	-2.32358	-2.35957	-0.03613	**C52**	-0.53489	-2.37651	0.6468	**C91**	-2.69951	-1.97575	0.29803
C23	-2.36953	-2.36888	-0.03583	**C53**	-0.57716	-2.37623	0.64821	**C92**	-2.70903	-2.02222	0.29887
C24	-2.37861	-2.33179	-0.03313	**C54**	-0.57761	-2.3339	0.64221	**C93**	-2.67229	-2.03138	0.29994
C25	-2.42747	-2.34223	-0.03348	**C55**	-0.62226	-2.33329	0.64316	**C94**	-2.62644	-1.99458	0.30033
C26	-2.53419	-2.28085	-0.03246	**N56**	-0.2923	-2.62214	0.62749	**C95**	-2.61761	-1.94848	0.29916
C27	-2.48981	-2.27647	-0.0329	**N57**	-0.44743	-2.33167	0.6372	**C96**	-2.56878	-1.90993	0.30061
C28	-2.48464	-2.31593	-0.02488	**N58**	-0.66385	-2.37389	0.64318	**C97**	-2.46159	-1.74225	0.31726
C29	-2.52516	-2.36026	-0.01479	**H59**	-0.27565	-2.46727	0.66862	**C98**	-2.50608	-1.78211	0.31688
C30	-2.56946	-2.36465	-0.01481	**H60**	-0.26757	-2.53584	0.66373	**C99**	-2.51164	-1.82655	0.2977
C31	-2.57461	-2.32507	-0.02371	**H61**	-0.41546	-2.62211	0.59316	**C100**	-2.47146	-1.83028	0.2773
C32	-2.62187	-2.33006	-0.02389	**H62**	-0.42346	-2.55231	0.5951	**C101**	-2.42704	-1.79054	0.27846
N33	-2.04071	-2.00159	-0.03364	**H63**	-0.28816	-2.41158	0.61819	**C102**	-2.42147	-1.74601	0.29826
N34	-2.21537	-2.21809	-0.0339	**C74**	-0.33552	-2.62669	0.62752	**C103**	-2.37412	-1.70392	0.29867
N35	-2.43803	-2.30933	-0.02607	**C75**	-0.30658	-2.50039	0.64973	**N105**	-2.95525	-1.95672	0.30118
N36	-2.6607	-2.37315	-0.02395	**C76**	-0.30186	-2.5401	0.6481	**N106**	-2.78109	-1.99908	0.30031
H109	-2.25146	-2.30692	-0.03469	**C77**	-0.3408	-2.58461	0.62814	**N107**	-2.55832	-1.86644	0.29734
H110	-2.31632	-2.38804	-0.038	**C78**	-0.3847	-2.5884	0.60936	**N108**	-2.3689	-1.66046	0.29871
H111	-2.39777	-2.40476	-0.0376	**C79**	-0.38938	-2.54857	0.61021	**H115**	-2.74449	-2.05126	0.29862
H1	-2.87009	-2.07606	-0.03212	**C80**	-0.35051	-2.50414	0.6296	**H116**	-2.67936	-2.06706	0.30067
H2	-2.94418	-2.07672	-0.03172	**C81**	-0.32432	-2.42079	0.62681	**H117**	-2.59806	-2.00203	0.30155
H3	-2.86773	-1.92391	-0.03489	**N104**	-0.35732	-2.46427	0.63087	**C103**	-3.37412	-1.70392	0.29867
H4	-2.79484	-1.92546	-0.03504	**H112**	-0.35866	-2.27949	0.637	**C103**	-2.37412	-0.70392	0.29867
H5	-2.7996	-2.06711	-0.02731	**H113**	-0.27774	-2.26368	0.63222	**C103**	-3.29608	-2.6702	0.29867
H6	-2.6216	-2.07592	-0.04197	**H114**	-0.26148	-2.3287	0.62726	**C103**	-2.29608	-1.6702	0.29867
H7	-2.75044	-2.28719	-0.03984	**H37**	-0.5983	-2.06409	0.63798	**C103**	-1.3298	-0.62588	0.29867
H8	-2.75791	-2.21712	-0.04041	**H38**	-0.74137	-2.27491	0.63124	**N108**	-3.3689	-2.66046	0.29871
H9	-2.60815	-2.1316	-0.00588	**H39**	-0.74059	-2.20069	0.62875	**N108**	-2.33954	-1.70844	0.29871
H10	-2.60075	-2.20048	-0.00748	**H40**	-0.59029	-2.12641	0.65232	**N108**	-1.33954	-0.70844	0.29871
C11	-2.95693	-1.99844	-0.03369	**H41**	-0.59076	-2.20026	0.65454	**N108**	-3.29156	-1.6311	0.29871
C12	-2.86933	-2.04304	-0.0331	**C42**	-0.69148	-2.04372	0.63493	**N108**	-2.29156	-0.6311	0.29871
C13	-2.91188	-2.0436	-0.03306	**C43**	-0.70065	-2.00698	0.63232				
C14	-2.91237	-1.99902	-0.034	**C44**	-0.66384	-1.96115	0.62961				

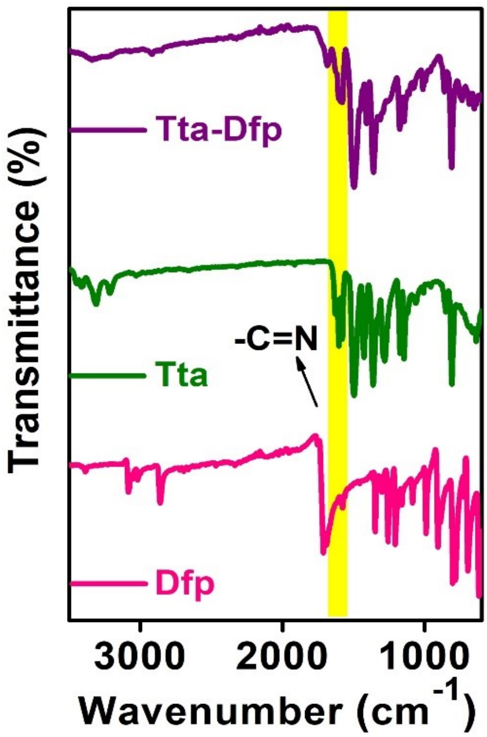


Fig. S3 FT-IR spectra of **Tta, Dfp** and **Tta-Dfp**.[1]

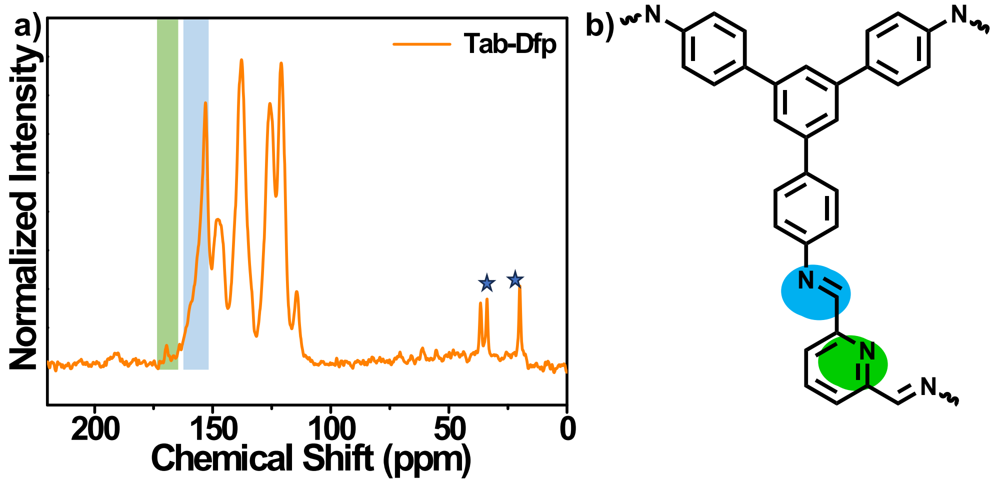


Fig. S4 a) ^{13}C CPMAS NMR spectrum of **Tab-Dfp** b) Structural building unit of **Tab-Dfp**; asterisks denote spinning sidebands or trapped trace of washing solvent (DMAc) due to the microporous network.[1]

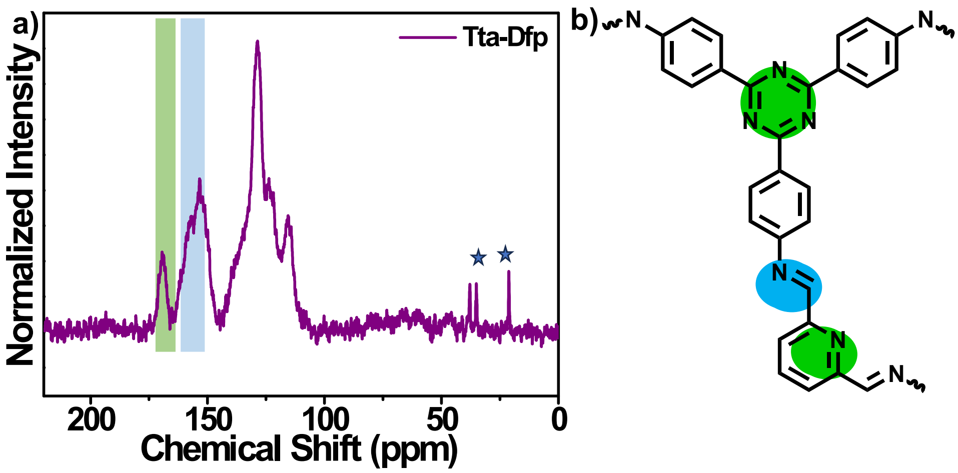


Fig. S5 a) ^{13}C CPMAS NMR spectrum of **Tta-Dfp** b) Structural building unit of **Tta-Dfp**; asterisks denote spinning sidebands or trapped trace of washing solvent (DMAc) due to the microporous network.[1]

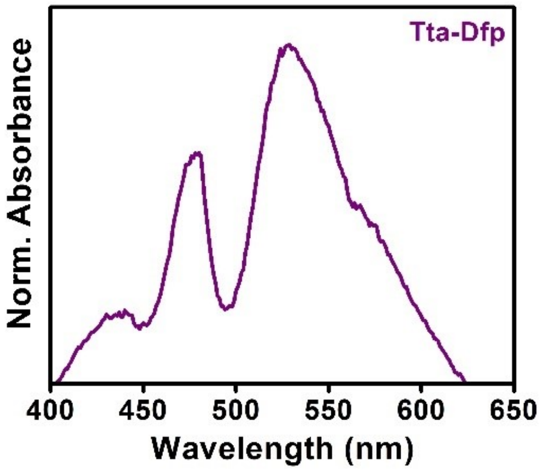


Fig. S6 UV-Vis spectra of **Tta- Dfp.**[1]

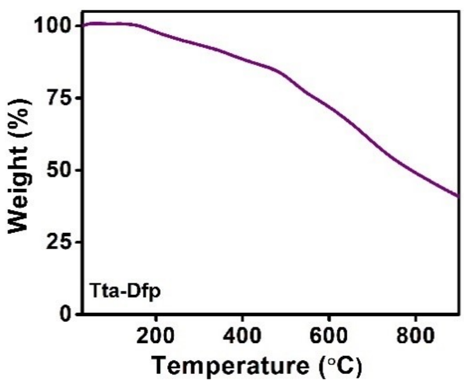


Fig. S7 TGA of **Tta- Dfp.**[1]

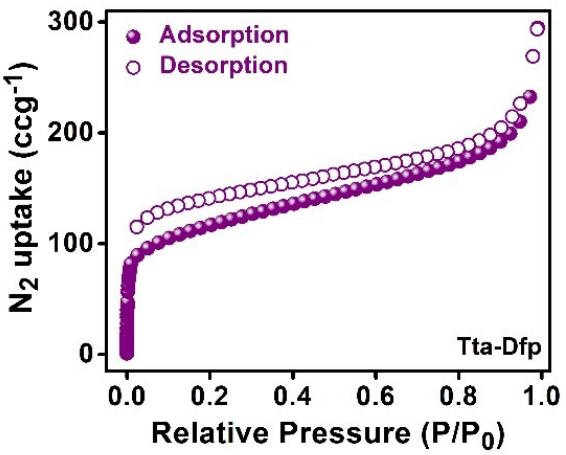


Fig. S8 BET N_2 adsorption/desorption of **Tta-Dfp.**[1]

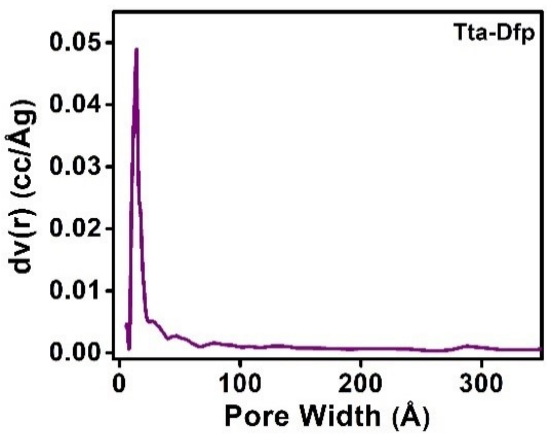


Fig. S9 Pore-size distribution profile of **Tta-Dfp.**[1]

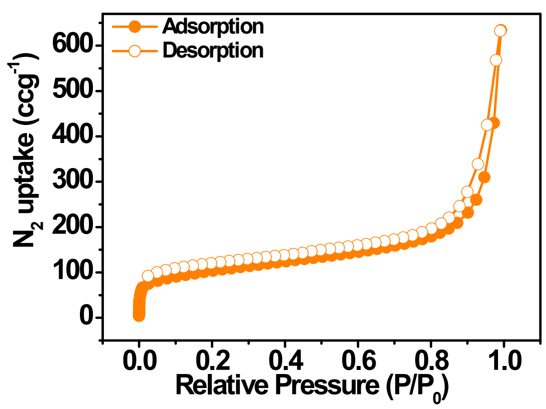


Fig. S10 BET N_2 adsorption/desorption of **Tab-Dfp.**[1]

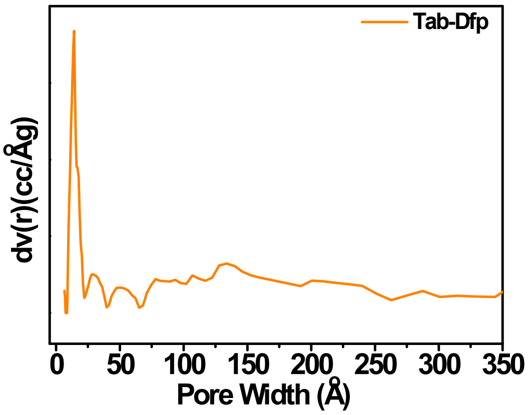


Fig. S11 Pore-size distribution profile of **Tab-Dfp.**[1]

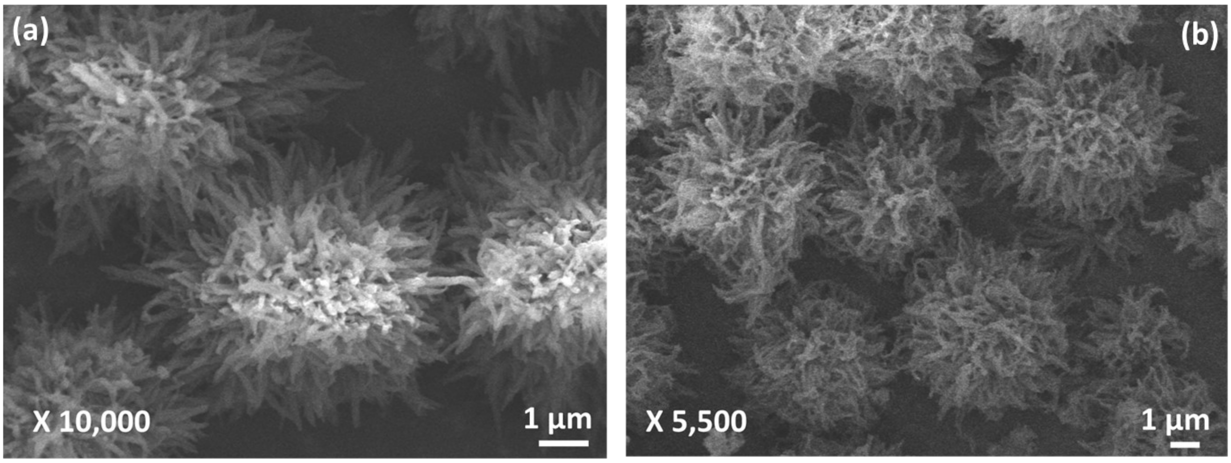


Fig. S12 FE-SEM images for (a) **Tta-Dfp** and (b) **Tab-Dfp**.

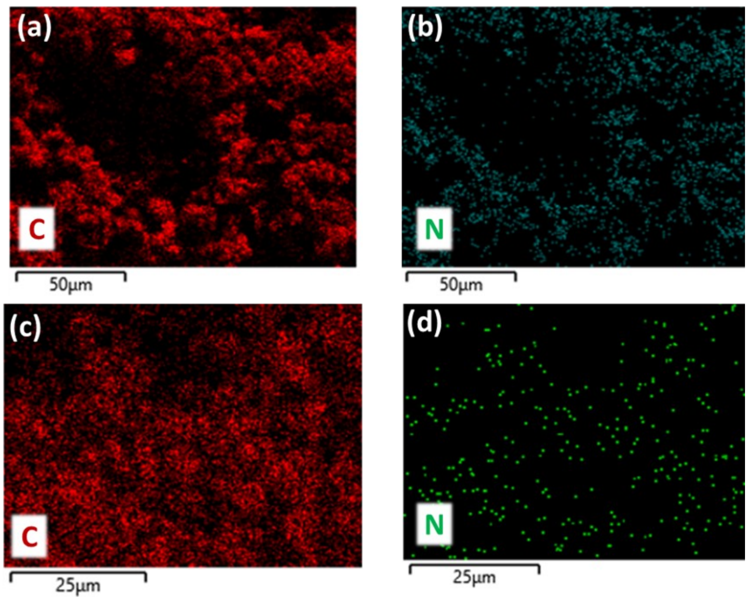


Fig. S13 Elemental dot mapping images for (a) C, (b) N in **Tta-Dfp** and (c) C, (d) N in **Tab-Dfp**.

Table S2. Elemental composition (weight percentage) analysis of all the elements.

Elements	EDS		CHN-O	
	Tta-Dfp	Tab-Dfp	Tta-Dfp	Tab-Dfp
C	81	90.9	82.5	89.5
N	19	9.1	17.5	10.5

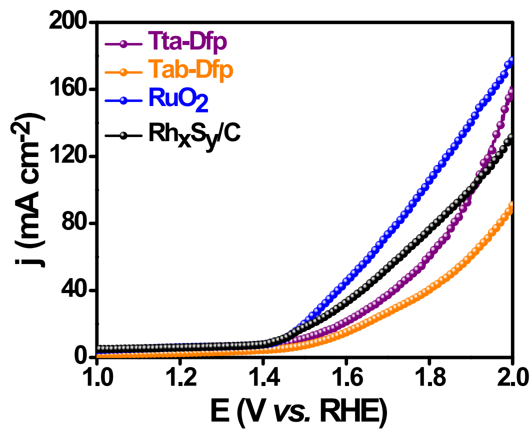


Fig. S14A LSV curves for the comparison of **Tta-Dfp** and **Tab-Dfp** with the benchmark CER electrocatalysts (RuO_2 and Rh_xS_y/C)

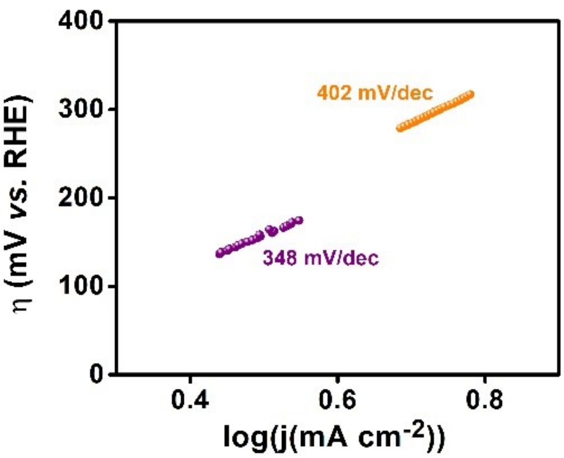


Fig. S14B Tafel slopes extracted from Fig. 2a for **Tta-Dfp** and **Tab-Dfp**.

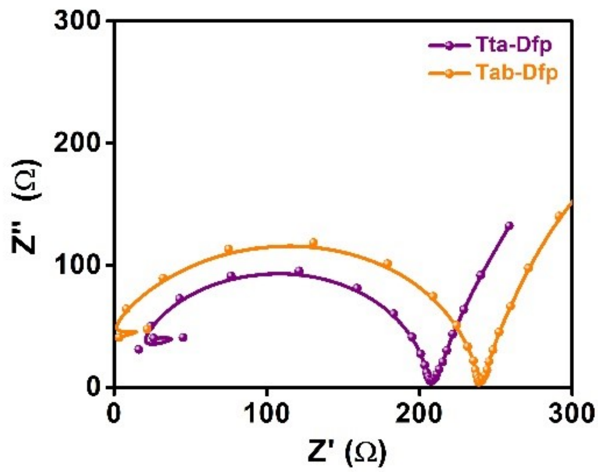


Fig. S15 Nyquists plot for **Tta-Dfp** and **Tab-Dfp.**

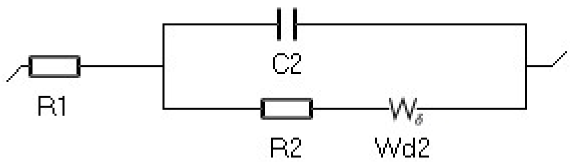


Fig. S16 Equivalent circuit obtained after fitting Nyquist plots of **Tta-Dfp**.

Table S3. EIS analysis (R_{ct} and rate constant) of Tta-Dfp and Tab-Dfp during CER in 0.4 M HCl**.**

Catalyst	R_s **(Ω, Solution resistance)**	R_p **(Ω, Polarization resistance)**	R_{ct} **(Ω, Charge-transfer resistance)**	**Rate constant, k (x 10^{-5} cm s^{-1})**
Tta-Dfp	13.70	203.9	190.20	1.40
Tab-Dfp	0.91	235.91	235.00	1.13

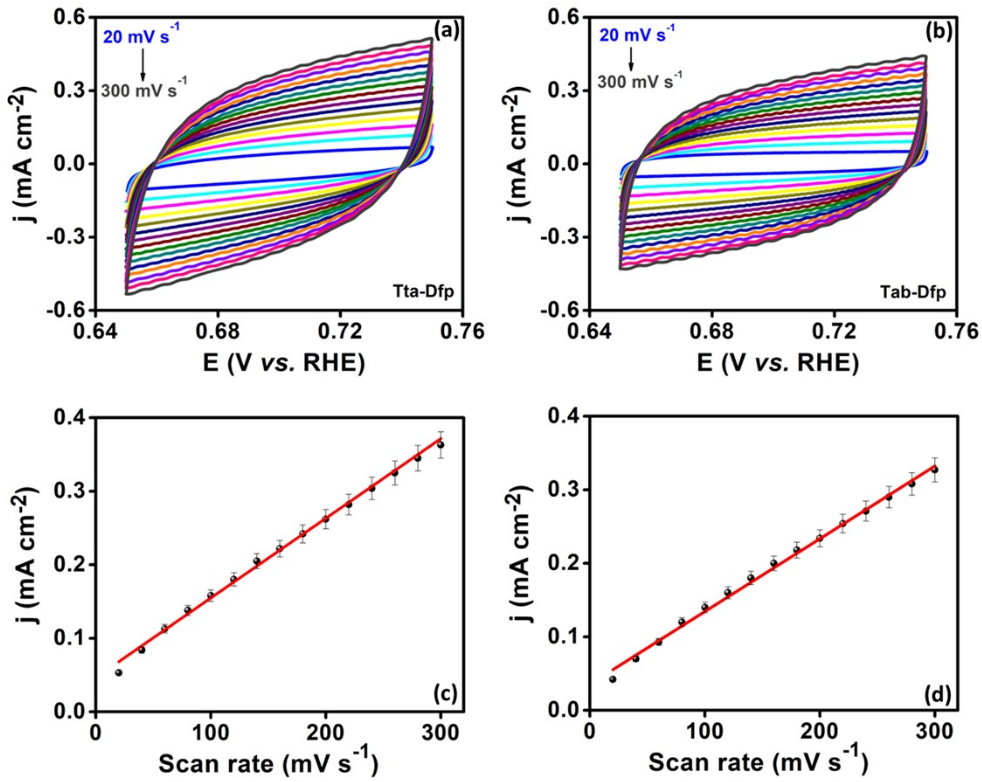


Fig. S17 (a), (b) Cyclic voltammograms in the non-faradaic region for CER at different scan rates (20 mV s^{-1} to 300 mV s^{-1}) and (c), (d) corresponding current density *vs.* scan rate curves for the measurement of C_{dl}, ECSA and SSA.

Table S4. $C_{dl,}$ ECSA and SSA of **Tta-Dfp** and **Tab-Dfp** in 0.4 M HCl.

Catalyst	**C_{dl} * (µF) at 0.7 V *vs.* RHE**	**ECSA (mm^2)**	**SSA (mm^2/mg)**
Tta-Dfp	1.08	2.70	22.5
Tab-Dfp	0.989	2.47	20.5

Quantification of chlorine gas: Iodometric titration

The amount of chlorine (Cl_2) gas evolved was estimated by performing the chronoamperometry for 60 s at 1.5 V *vs.* RHE in 0.4 M HCl. Further, the obtained Cl_2 was trapped by the immediate addition of an excess amount of potassium iodide (KI), and the solution was kept to attain equilibrium. The obtained amount was determined by performing Iodometric titration versus 0.1 M $Na_2S_2O_3$ and the following reactions will take place.

$Cl_2 + KI \rightarrow I_3^- + Cl^-$ (Equation 1)

$I_3^- + 2\ S_2O_3^{2-} \rightarrow 3I^- + S_4O_6^{2-}$ (Equation 2)

Calculation

Total volume of 0.1 M $Na_2S_2O_3$ consumed during titration = 2.1mL

Volume taken in the flask (0.4 M HCl and excess KI) = 30 mL

On applying the molarity equation:

$$M_1 * V_1 = M_2 * V_2$$

$$0.1\ M * 2.1\ mL = M_2 * 30\ mL$$

$$M_2 = 0.007\ M\ (I_3^-)$$

As can be seen in the stoichiometric equation two thio molecules are required for one (I_3^-), therefore the concentration of thio would be equal to = 0.0035 M or mol/l.

Further, the amount of evolved chlorine was used to calculate the Faradaic efficiency as:

$$Q_{theo} = \frac{i * t}{nF}$$

$$Q_{theo} = \frac{22\ mA.s}{2 * 96500\ C/mol} = 1.1 * 10^{-7}\ mol$$

Upon converting the obtained value in mol/l considering the 30 ml of volume taken to evolve the chlorine: 0.0038* 10^{-3} mol/l

$$F.E.(\%) = \frac{Q_{exp}}{Q_{theo}}$$

$$F.E.(\%) = \frac{0.0035\ mol/l}{0.0038\ mol\ l} = 92\%$$

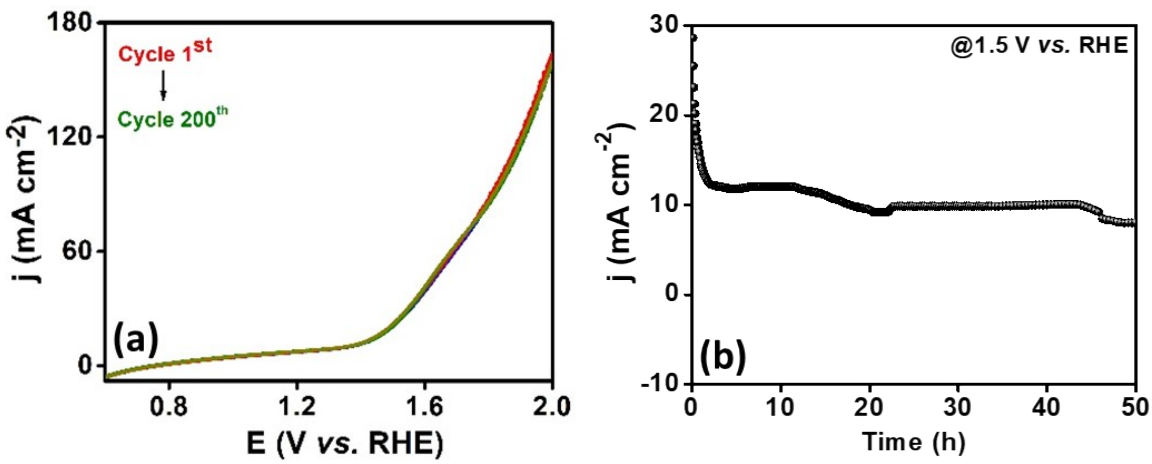


Fig. S18 (a) LSV curves recorded CER of **Tta-Dfp** for 200 cycles at a scan rate of 50 mV s^{-1} in 0.4 HCl and (b) chronoamperometry curve in 0.4 HCl at 1.5 V *vs.* RHE for 50 h.

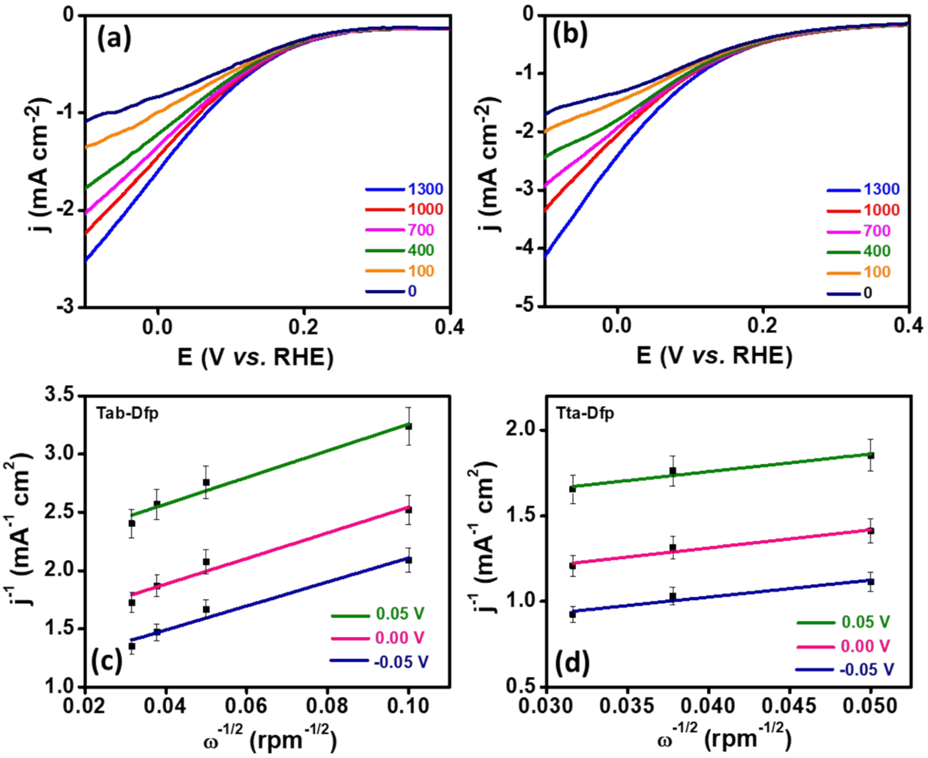


Fig. S19A RDE polarization curve (a) **Tab-Dfp**, (b) **Tta-Dfp** and K-L plots derived for (c) **Tab-Dfp**, (d) **Tta-Dfp** catalysts from respective RDE polarization curves at various rotation rates at different potentials (0.05 V, 0.00 V and -0.05 V *vs.* RHE).

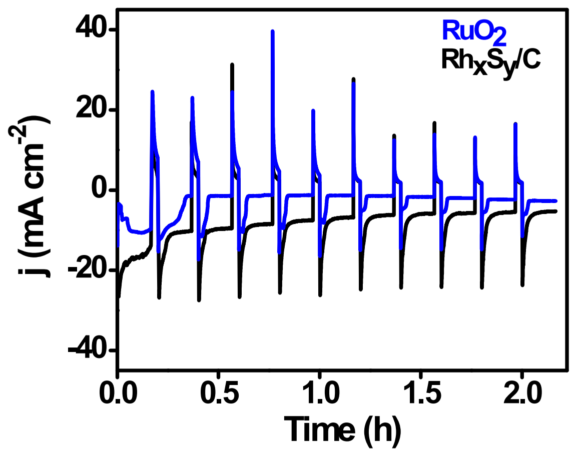


Fig. S19B Chronoamperometry analysis performed for 10 minutes of operation @0 V and 2 minutes of shutdown (i.e. system off) for RuO_2 and Rh_xS_y/C.

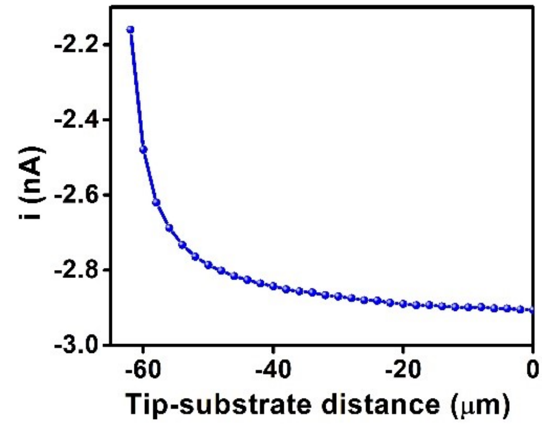


Fig. S20 Approach curve (I vs. tip substrate distance) for tip positioning.

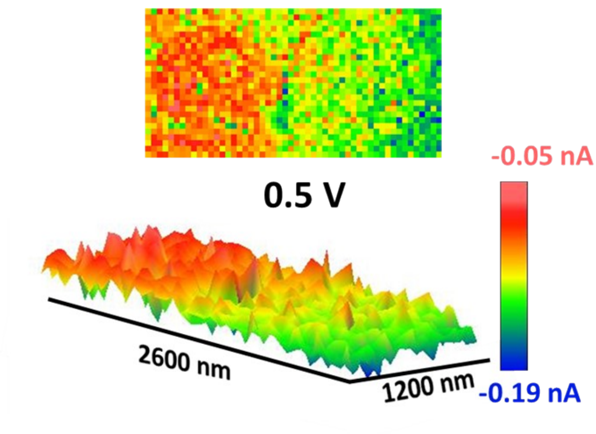


Fig. S21 2D SECM images of **Tta-Dfp** and **Tab-Dfp** catalyst spot at a reduction potential of 0.5 *vs.* RHE

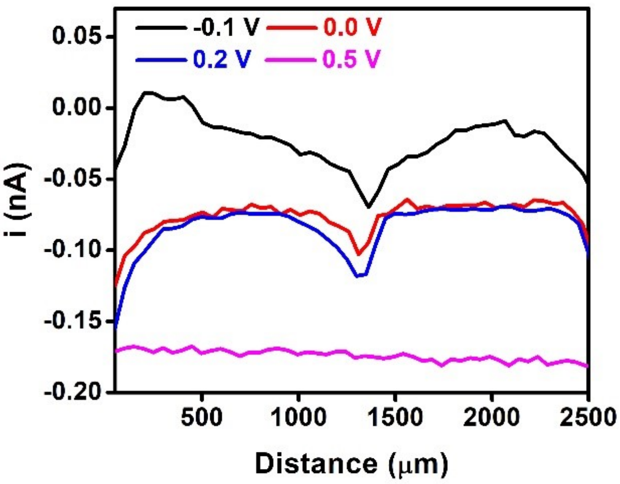


Fig. S22 RC-SECM x-line scan of the catalyst's spots polarized at different potentials (-0.1, 0.0, 0.2 and 0.5 V *vs*. RHE).

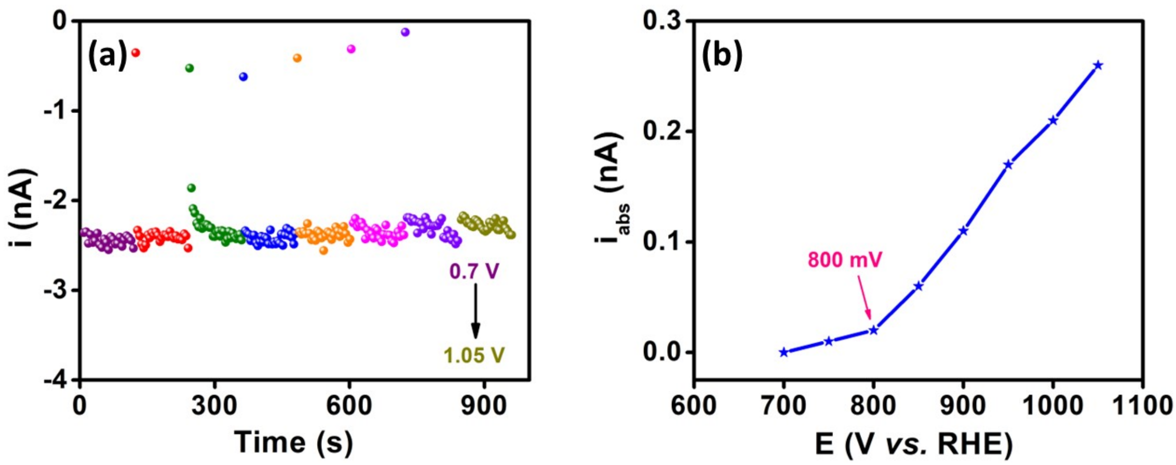


Fig. S23 (a) Sequential chronoamperometric curves at Pt tip in 0.4 M HCl in the potential range of 0.15 V to 0.50 V *vs.* Ag/AgCl/3 M KCl with an interval of 50 mV and (b) Absolute current difference *vs.* applied potential obtained from Figure S23a.

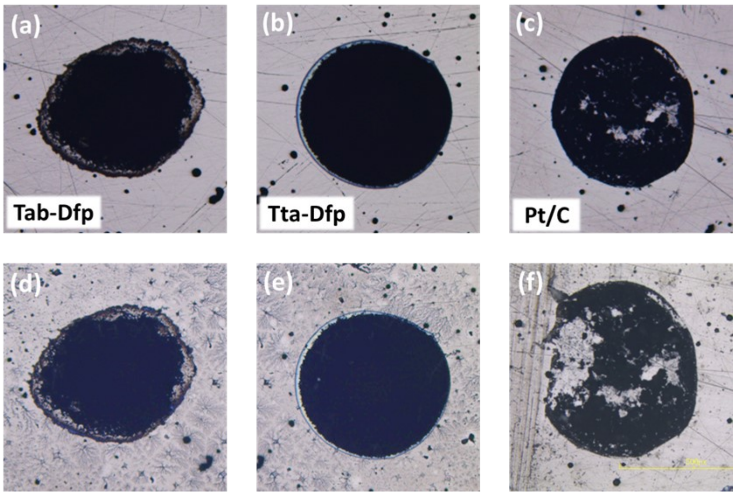


Fig. S24 Optical microscopic images before SECM analysis (a) **Tab-Dfp**, (b) **Tta-Dfp,** (c) Pt/C (20%) and after SECM analysis (a) **Tab-Dfp,** (b) **Tta-Dfp**, (c) Pt/C (20%).

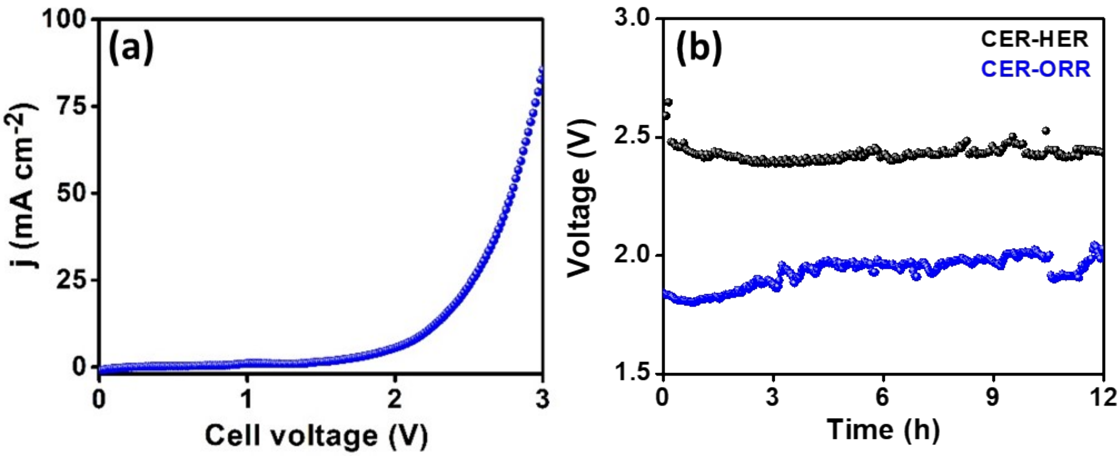


Fig. S25 (a) LSV under full cell conditions (CER-ODC) with **Tta-Dfp** employed at both anode and cathode, (b) chronopotentiometry curves for CER-HER and CER-ODC cells at 10 mA cm^{-2} for 12 h each.

References

1. K. C. Ranjeesh, S. Kaur, A. K. Mohammed, S. Gaber, D. Gupta, K. Badawy, M. Aslam, N. Singh, T. Skorjanc, M. Finšgar, J. Raya, T. C. Nagaiah and D. Shetty, *Advanced Energy Materials*, **n/a**, 2303068.