Pd-Functionalized β-Ketoenamine COF for Efficient Hydrogen Sensing Under Ambient Conditions

*Sujith Benarzee Nallamalla[a], Karreddula Raja[b], Balaji Rao Ravuri[c], Surendra Babu Manabolu Surya [a]**

[a]Department of Chemistry, School of Science, GITAM deemed to be University, Hyderabad campus, Hyderabad - 502329, Telangana, India.

[b]Department of Chemistry, Rajeev Gandhi Memorial College of Engineering and Technology (Autonomous), Nandyal, Andhra Pradesh-518501, India.

c Department of Physics and Astronomical Sciences, Central University of Jammu, Rahya-Suchani, Samba, Jammu & Kashmir 18114, India.

***Correspondence:** smanabol@gitam.edu (M. S. Surendra Babu).

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S1. EXPERIMENTAL SECTION

S1.1 Materials

The materials, Phloroglucinol (98%, AVRA Synthesis Ltd., Telangana, India), 4 – Amino benzonitrile (98%, Sd fine-Chem Ltd., Mumbai, India), Hexamethylenetetramine (99%, Sigma Aldrich), Tri - fluoro methane sulfonic acid (99%, AVRA Synthesis Ltd., Telangana, India), Na_2PdCl_4 (98%) are purchased from Sigma Aldrich. $NaBH_4$ (98%) is purchased from Merck Life Science Pvt. Ltd, Mesitylene (99%, AVRA Synthesis Ltd., Telangana, India), and 1,4 Dioxane (99%, SDFCL., Mumbai, India), Acetic acid (99.8% BLD Pharma Ltd., Telangana, India), Methanol, Acetone, Hexane, and anhydrous THF (99.8% BLD Pharma Ltd., Telangana, India), and Trifluoroacetic acid (TFA) (≥99%) is purchased from Sigma Aldrich.

S1.2 Synthesis of 2,4,6-Tris(4-aminophenyl) triazine (TAPT)

0.772g of 4-amino benzonitrile was taken in RBF at 0 ℃. Then 2ml of CF_3SO_3H was added dropwise for 20^0 min and maintained the temperature at 0 ℃. The resultant mixture was stirred for 24 hrs at room temperature in an inert atmosphere. After that 20 ml of distilled water was added to the mixture and it was neutralized by adding 2M NaOH solution until the pH reached 7. Initially with an increase in pH, the orange precipitate dissolved to give a bright orange solution which further increases in pH and gives a yellow precipitate. The resultant product was filtered and washed several times with distilled water [1].

S1.3 Synthesis of 1,3,5-triformylphloroglucinol (TFP)

The synthesis of 1,3,5-triformylphloroglucinol (TFP) involves the formylation of phloroglucinol using hexamethylenetetramine (HMTA) in the presence of trifluoroacetic acid (TFA) as both a solvent and catalyst. Initially, (108 mmol) of HMTA and (49 mmol) of dried phloroglucinol are dissolved in 90 mL of TFA under a nitrogen atmosphere to prevent oxidation [2]. The reaction mixture is then heated at 100 °C for 2.5 hours, allowing the formylation process to proceed, wherein the aldehyde (-CHO) groups are introduced at the C-2, C-4, and C-6 positions of phloroglucinol. Following this, 150 mL of 3M hydrochloric acid (HCl) is added, and the reaction is maintained at 100 °C for an additional hour to hydrolyze any intermediate species, ensuring complete formylation. After cooling to room temperature, the mixture is filtered through Celite to remove insoluble impurities and extracted using 350 mL of dichloromethane (DCM) to isolate the organic phase containing TFP. The product was filtered and washed with mesitylene, THF, and acetone to remove impurities.

S1.4 Synthesis of covalent organic framework (TAPT-COF)

The covalent organic frameworks (COF) were synthesized via Schiff base condensation reactions, following established protocols with slight modifications [3]. A mixture of 70 mg of 2,4,6-trihydroxy benzene-1,3,5-tricarbaldehyde, 56 mg of 2,4,6-Tris(4-aminophenyl) triazine, 1.5 mL of 1,4- dioxane, 2.0 mL of 1,3,5- trimethylbenzene, and 0.4 mL of 6M aqueous acetic acid was prepared. The solution was sonicated for 30 minutes under a nitrogen (N_2) atmosphere to ensure thorough mixing. The resulting mixture was then transferred into an autoclave and placed in a hot air oven, where it was heated at 160 ℃ for 3 days. After the reaction, the obtained product was sequentially washed with acetone, hexane, and anhydrous THF to remove unreacted precursors and by-products. Finally, the material was dried under vacuum at 100 ℃ for 24 hrs. The resulting mixture was then transferred into an autoclave and placed in a hot air oven, where it was heated at 160 ℃ for 3 days. After the reaction, the obtained product was sequentially washed with acetone, hexane, and anhydrous THF to remove unreacted precursors and by-products. Finally, the material was dried under vacuum at 100 ℃ for 24 hours.

S1.5 Synthesis of Pd@TAPT-COF

The Synthesis of Pd@COF was carried out following a previously reported procedure with modifications [4]. Activated COF (100 mg) was dispersed in 5 mL of methanol under ambient conditions. To this dispersion, a $PdCl_2$ (20 mg) solution in 2 mL methanol was added dropwise under vigorous stirring. Subsequently, 4 mL of methanol and 3 mL of $NaBH_4$ solution (Prepared in 2M methanol) were added while stirring vigorously. The reaction was maintained under continuous stirring for 12 hrs to ensure a complete reduction of Pd^{2+} to Pd^0. After completion, the product was centrifuged, and the residue was thoroughly washed with 5 x 50 mL to remove unreacted species or impurities. Finally, the obtained Pd@COF was dried in a vacuum oven at 50 °C. Although $PdCl_2$ is sparingly soluble in methanol, under continuous stirring and mild heating it forms a colloidal dispersion. This is sufficient for effective interaction with the TAPT-COF framework and subsequent reduction to Pd^0.

S1.6 Characterization techniques

S1.6.1 Solid-state ^{13}C CP/MAS NMR

Solid-state ^{13}C CP-MAS (Cross-Polarization with Magic Angle Spinning) spectra were recorded on a JEOL (model ECX-400 MHz) spectrometer to confirm the synthesized COFs, and the Samples were analyzed in their powder form.

S1.6.2 Powder X-ray diffraction studies

X-ray diffraction (XRD) was performed by using Rigaku Ultima IV powder XRD by Cu Kα radiation (15.4 nm) at 40 kV, 30 mA, and 5 deg/ min, and the scanning range was 5–70˚ and Samples were analyzed in their powder form.

S1.6.3 Optical spectroscopy studies

FTIR spectra are recorded with the Agilent ATR benchtop spectrometer 4500-400 cm-1 using KBr.

S1.6.4 Surface Analysis

The elemental electronic state of the adsorbent surface was confirmed by X-ray photoelectron spectroscopy (XPS) analysis of the composite using the AXIS Supra- Shimadzu model, Japan.

S1.6.5 Electron microscopy studies

Transmission electron microscopy (TEM) was performed using Talos F200 S (Thermo Fischer) operating at 200 kV. For HR -TEM imaging, COFs were diluted with a suitable solvent, sonicated for 10 min, and then 10 μL was drop-casted onto a carbon TEM grid. The The grid was dried under a hot air oven at 50 0 C for 30 min, then recorded the images, By the using Image J Software to generate FFT images

Field emission scanning electron microscopy (FESEM) data was collected using a ZEIS Evo SEM, EDAX Oxford instruments was used to analyze the morphology and particle

size and EDAX image.

Atomic force microscopy (AFM) is carried out using Agilent 5500 in tapping mode. Sample for AFM analysis is fabrication of thin films by drop casting onto undoped silicon wafers (0.5 cm x 0.5 cm)

S1.6.6 N_2-adsorption studies

Quanta Chrome and NOVA Win conducted a study on the adsorption-desorption of nitrogen and examined surface area, pore size, and pore volume.

S1.6.7 Thermal Analysis

TGA analyses were done on a Netzsch TG209F1 apparatus at 10 K min^{-1} under N_2 atmosphere.

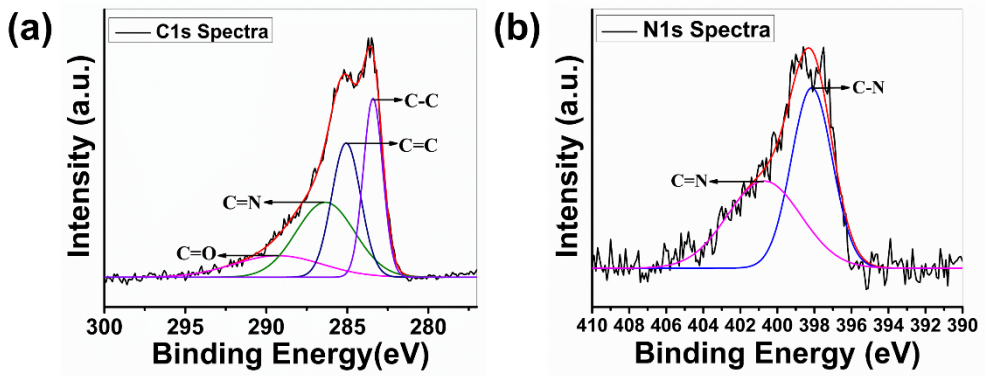


Figure S1. High-resolution XPS spectra of TAPT-COF (a) C 1s spectra, and (b) N 1s spectra.

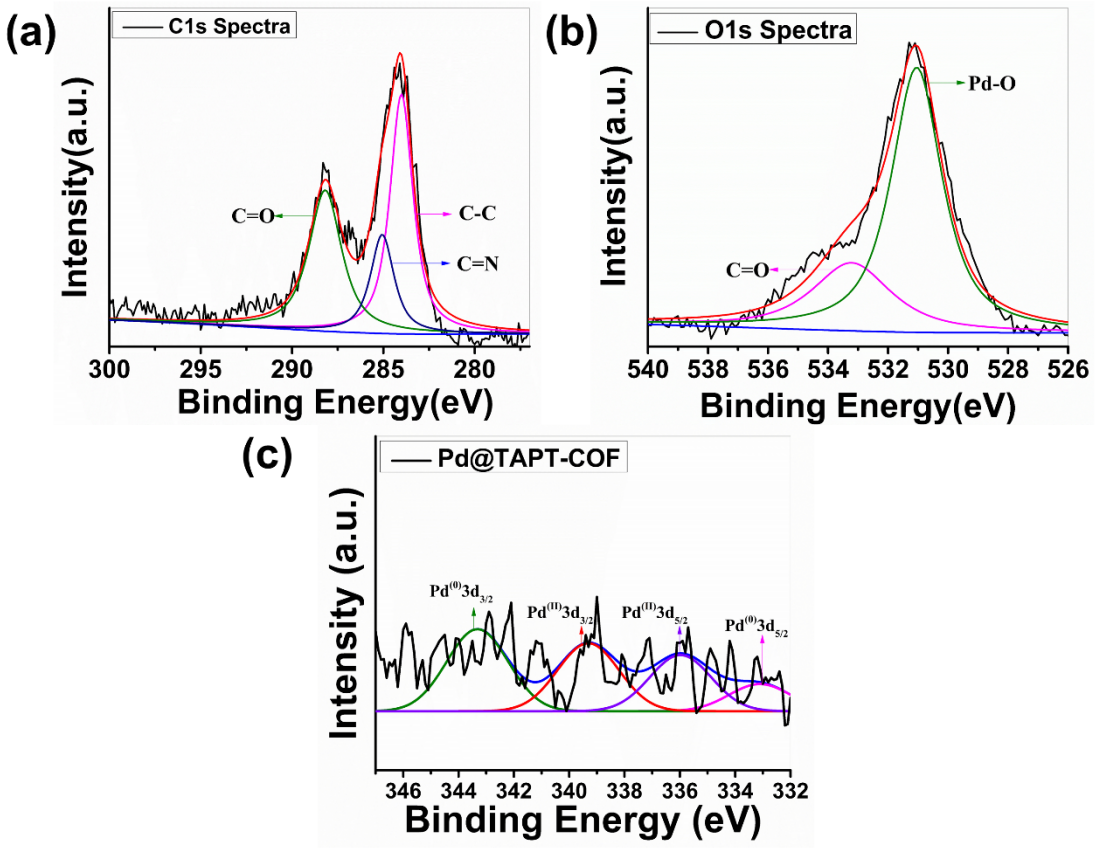
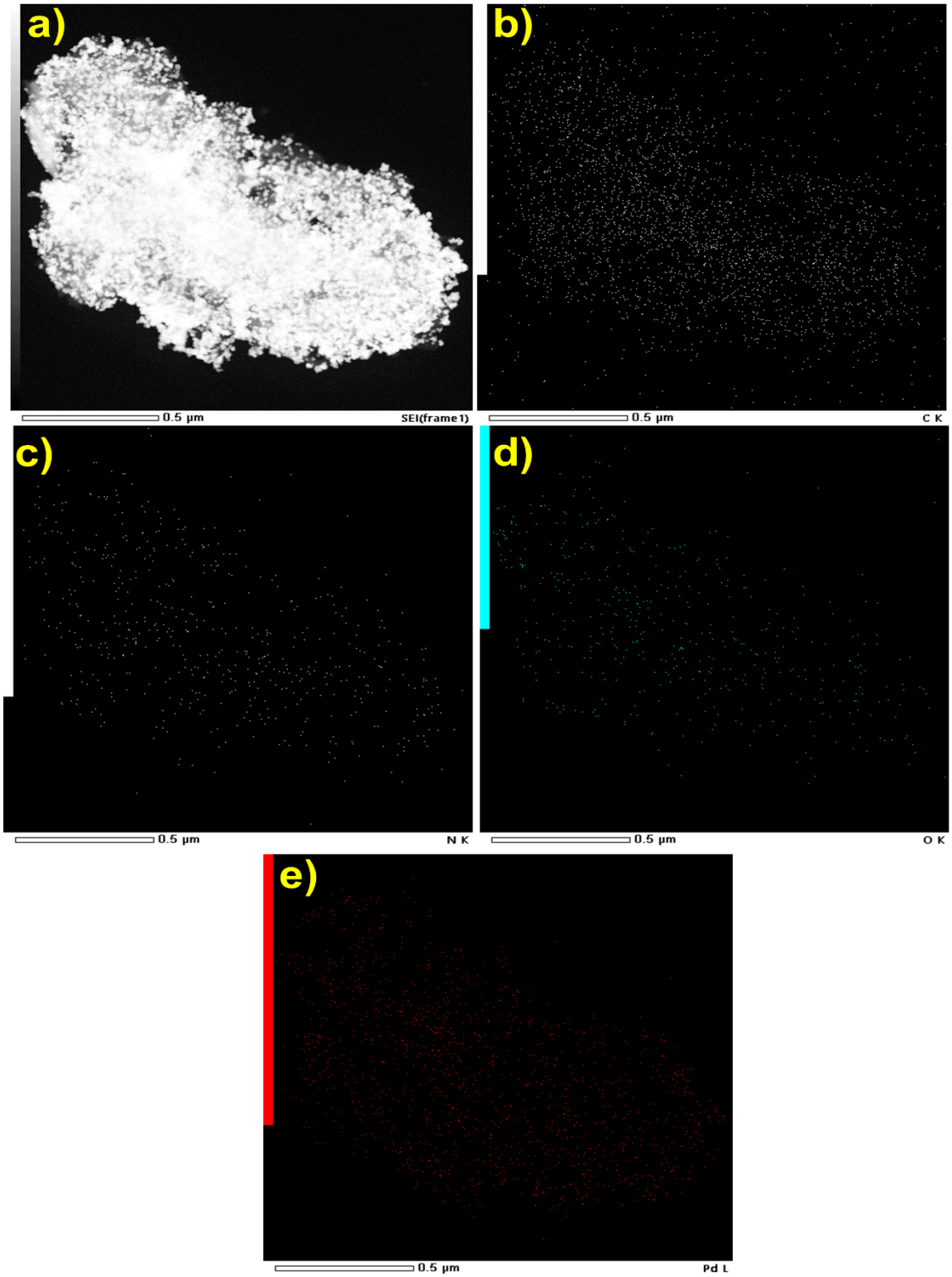
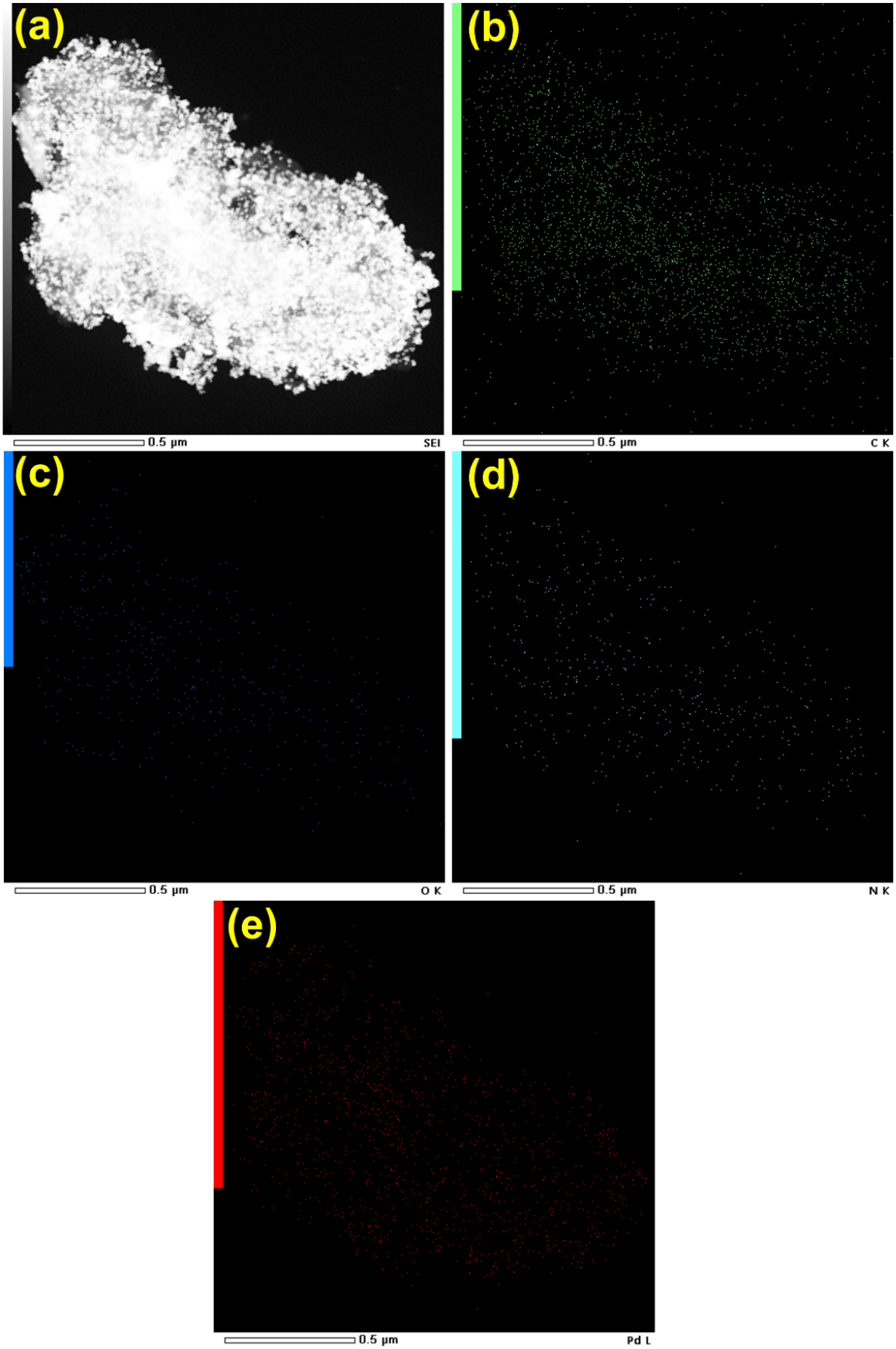


Figure S2. High-resolution XPS spectra of Pd@TAPT-COF (a) C 1s spectra, (b) O 1s spectra, and (C) Pd in Pd@TAPT-COF.


a)
0.5 µm
SEI(frame1)
b)
0.5 µm
C K
c)
0.5 µm
N K
d)
0.5 µm
O K
e)
0.5 µm
Pd L



Fi

gure S3. (a-e) Elemental mapping of Pd@TAPT-COF, C, N, O, and Pd respectively

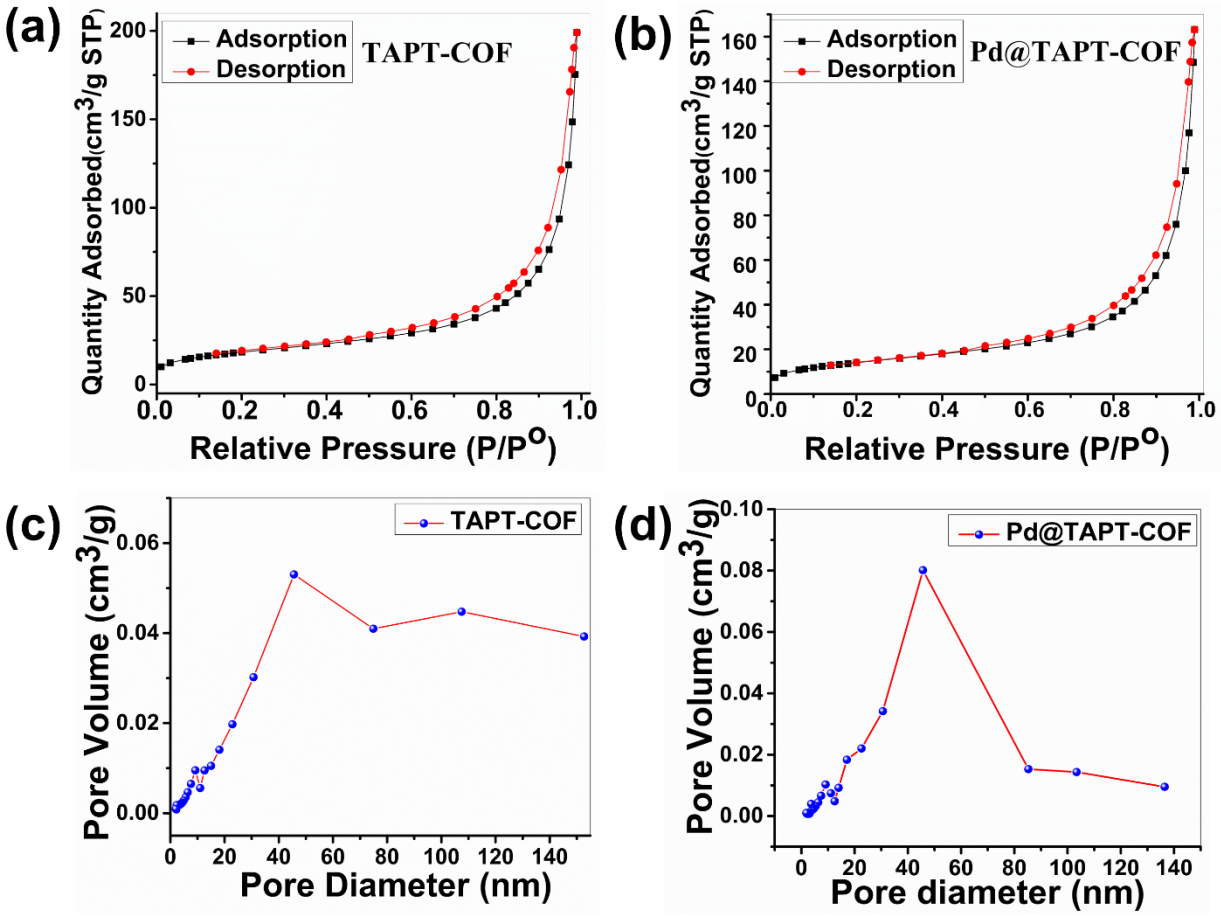


Figure S4. N_2 isotherms of COFs (a) TAPT-COF, (b) Pd@TAPT-COF, and BJH pore size distribution curves (c) TAPT-COF, and (d) Pd@TAPT-COF.

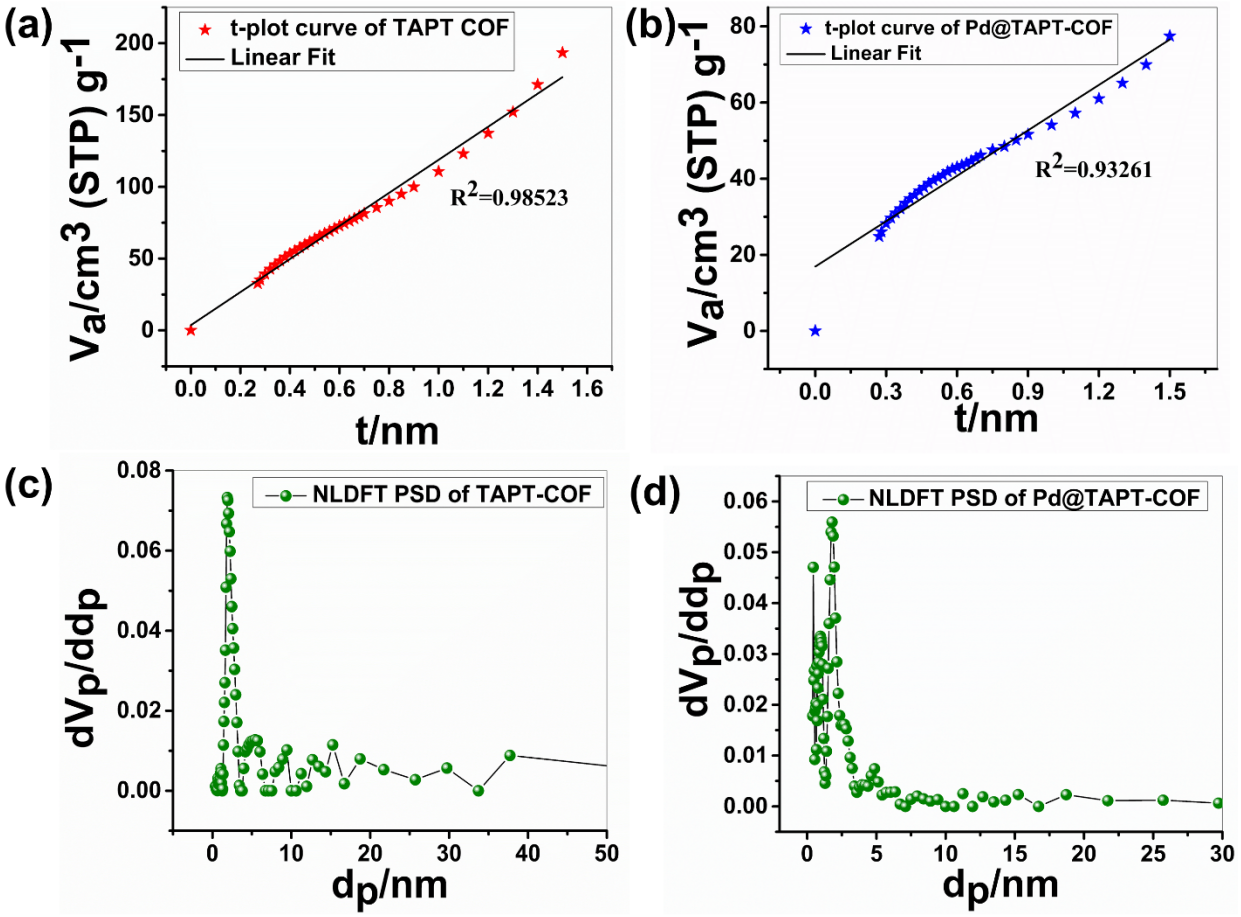


Figure S5. (a) and (b) t-plot curves of TAPT-COF and Pd@TAPT-COF with their respective linear fits, indicating microporous characteristics and the correlation coefficients ($R^2 = 0.98523$ and 0.93261). (c) and (d) NLDFT pore size distribution (PSD) plots of TAPT-COF and Pd@TAPT-COF showing dominant pore sizes in the microporous region, confirming the preservation of porosity after Pd incorporation.

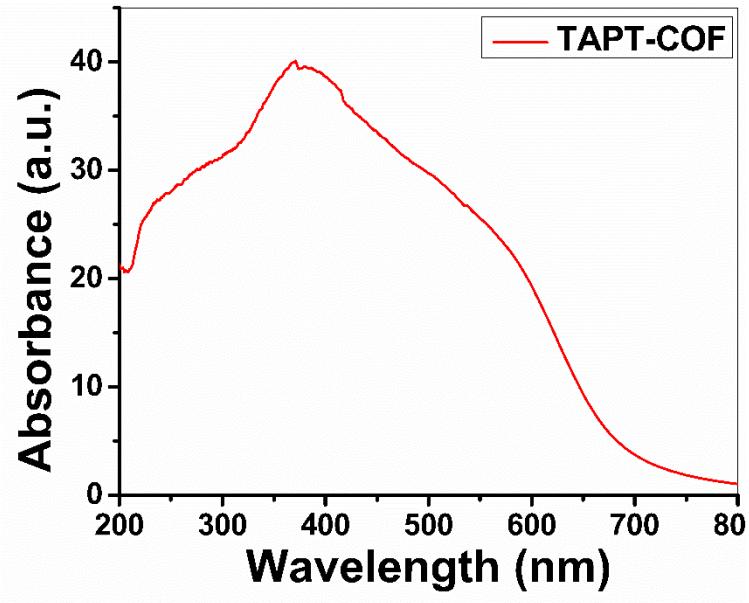


Figure S6. UV-Vis diffuse reflectance spectrum of TAPT-COF.

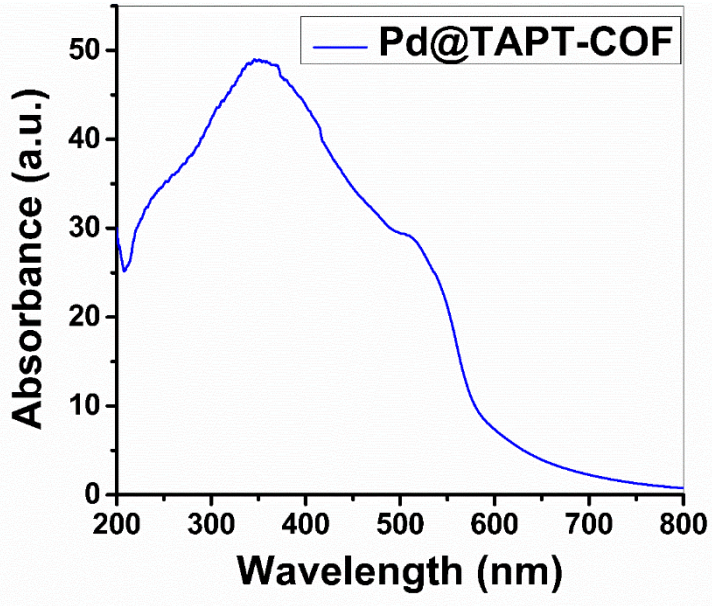


Figure S7. UV-Vis diffuse reflectance spectrum of Pd@TAPT-COF.

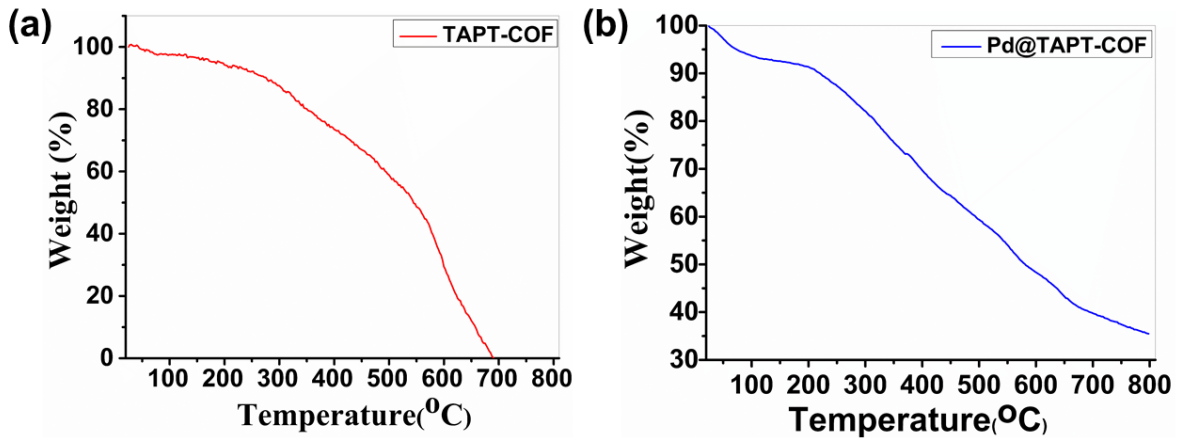


Figure S8. TGA curves of COFs (a) TAPT-COF and (b) Pd@TAPT-COF.

S2. CHEMIRESISTIVE GAS SENSING MEASUREMENTS

Firstly, TAPT-COF and Pd@TAPT-COF powders were synthesized and collected in dry form. Each COF sample (30 mg) was placed in an agate mortar, and a small amount of Polyvinylidene fluoride (PVDF, 10 mg) was added as a binder. A few drops of anhydrous ethanol (0.5 ml) were added to assist dispersion, and the mixture was thoroughly ground for 10 minutes to form a uniform slurry. The resulting slurry was drop-cast onto the pre-cleaned OHP sheet and allowed to air dry for 15 minutes, followed by vacuum drying at 60 °C for 6 hours to ensure good film formation and solvent removal. Gas sensing measurements were performed using a custom-designed gas sensing chamber. Each COF-coated substrate served as a chemiresistive sensor and was exposed to hydrogen gas at concentrations of 1, 5, 10, 25, and 50 ppm at room temperature. The sensor response was monitored by measuring the change in electrical resistance using a Keithley source meter.

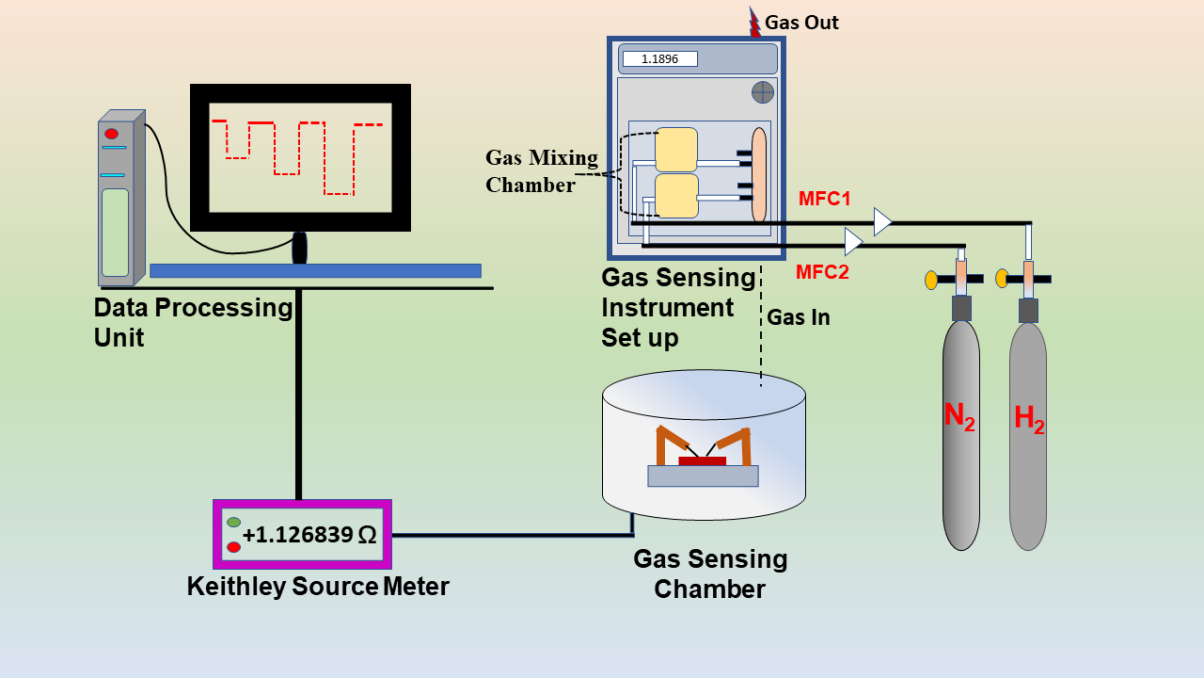


Figure S9. Schematic illustration of the Hydrogen gas sensing instrument setup.

S3. Gas Sensor Fabrication and Measurement

To establish the reproducibility of COF-based gas sensors, multiple independent sensors were fabricated and tested under identical conditions. The fabrication of COFs (TAPT-COF and Pd@TAPT-COF) was followed by their dispersion in an agate mortar, where polyvinylidene difluoride (PVDF) was added as a binding agent. To ensure uniform dispersion, a small amount of anhydrous ethanol was added dropwise while continuously grinding the mixture for 10 minutes. The obtained homogeneous paste was then carefully coated onto 1 cm X 2 cm OHP sheet substrates to form thin sensing films. The coated films were dried at room temperature for 30 minutes to remove residual solvent and enhance film adhesion. The fabricated COF-based sensors underwent an aging process for 72 hours using Winsen's TS-64B sensor gas-sensitive aging platform to enhance sensor stability and achieve a consistent response. This process is crucial for stabilizing the sensing material, ensuring minimal variations in response during subsequent measurements (**Figure S8**). Gas concentrations during the sensing experiments were controlled using a mass flow controller [AALBORG instruments, Model no GFC 17, USA], which allowed precise adjustment of the desired gas concentration. The flow rates were regulated to maintain consistent total flow and exposure conditions throughout the measurements.

Gas sensing tests were conducted at room temperature (25 ± 2 ^{o}C) under a controlled humidity of 0 -75% RH with a gas flow rate of 100 mL/min. Sensors were pre-exposed to dry air for 30 min before testing. H_2 concentrations ranged from 1 to 50 ppm, and the response was determined by the change in electrical resistance. Reproducibility was evaluated by performing multiple independent gas sensing measurements on identical COF-based sensors. The response (S) of the sensors was calculated using the equation:

$$S = R_a/R_g \quad (1)$$

Where R_a is the baseline resistance in air, and R_g is the resistance upon exposure to different concentrations of H_2 gas. To validate reproducibility, four consecutive sensing cycles were conducted at 1 ppm hydrogen concentration, and the response of each cycle was recorded. The results demonstrate minimal deviation between cycles, confirming the high reproducibility of the sensor's performance.

Additionally, the long-term stability of the fabricated sensors was assessed over 15 days by exposing the sensors to 1 ppm hydrogen at regular intervals. The response was monitored, and the results indicate that the sensors maintained a stable response with negligible fluctuations, highlighting the robustness and durability of COF-based materials for extended applications. Since environmental humidity can influence gas sensing performance, the impact of relative humidity (RH) on the sensing response was also examined. The sensors were tested at varying humidity levels ranging from 0 % to 75 % RH while maintaining a constant hydrogen gas concentration of 1 ppm.

S3.1 Calculations of gas sensing parameters

i) Sensor Response (S):

The sensor response is defined as the ratio of the resistance of the sensor in air (R_a) to the resistance of the sensor in the presence of the target gas (R_g).

$$S = R_a/R_g$$

Where,

R_a-Resistance in air

R_g-Resistance in the presence of H_2 gas

ii) Response Time (T_{res}):

The response time is the time required for the sensor to achieve 90 % of the total resistance change after exposure to the target gas.

$$T_{res} = T_2\text{-}T_1$$

Where,

T_{res} – Sensor response time

T_2 - The total time required to achieve a 90 % response upon exposure to the target gas.

T_1 – The starting time is taken from the baseline in the presence of balance gas.

iii) Recovery Time (T_{rec}):

The recovery time is the time taken for the sensor to return to 10 % of its original baseline resistance after the removal of the target gas.

$T_{rec} = T_4 - T_3$

Where,

T_{rec} – Sensor recovery time

T_4 - The total time required to achieve a 90 % recovery upon exposure to the target gas.

T_3 – The amount of time required to stabilize the baseline resistance with an analyte gas.

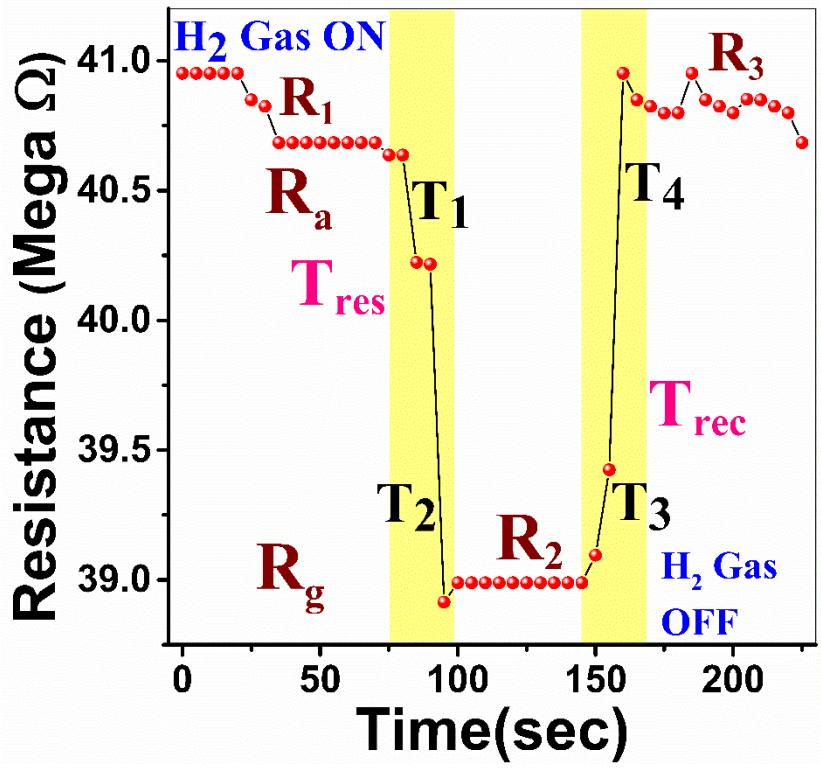


Figure S10. The dynamic resistance curve of the TAPT-COF and Pd@TAPT-COF based sensor shows response time and recovery time upon H_2 exposure and removal at room temperature.

S3. After Hydrogen Sensing Characterization

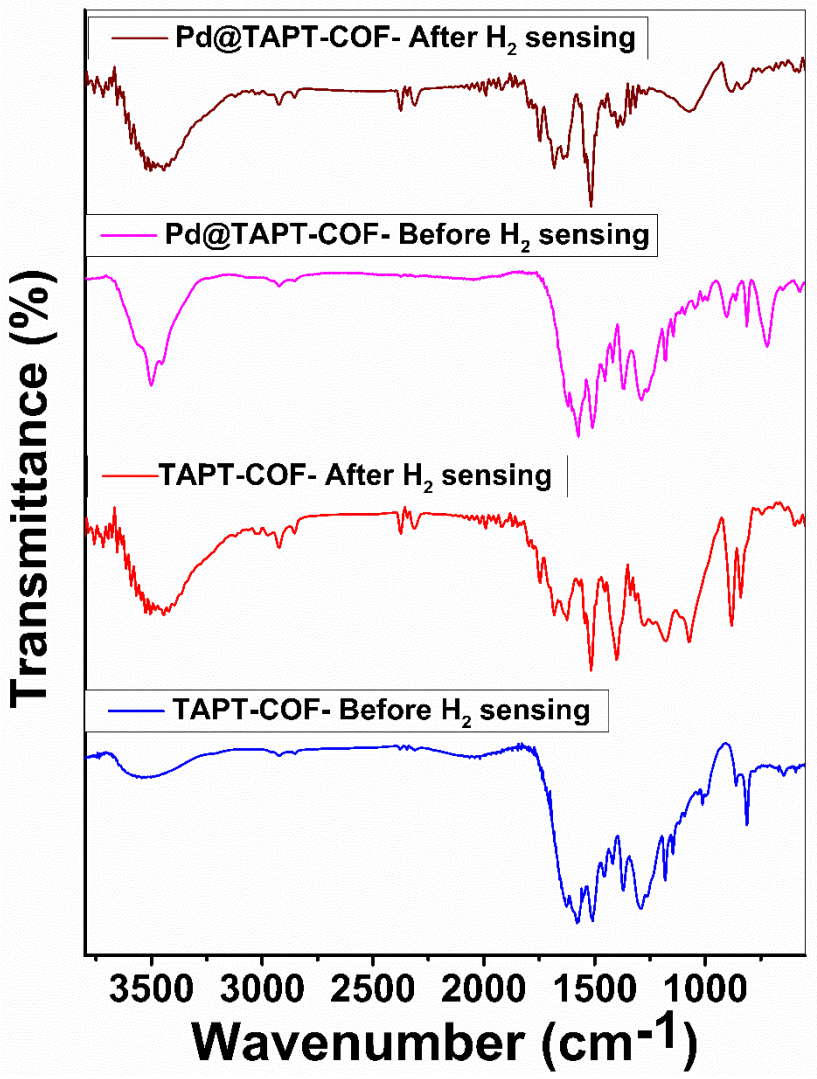


Figure S11. Fourier transform infrared spectroscopy (FTIR) comparison spectra of COFs after H_2 sensing, respectively.

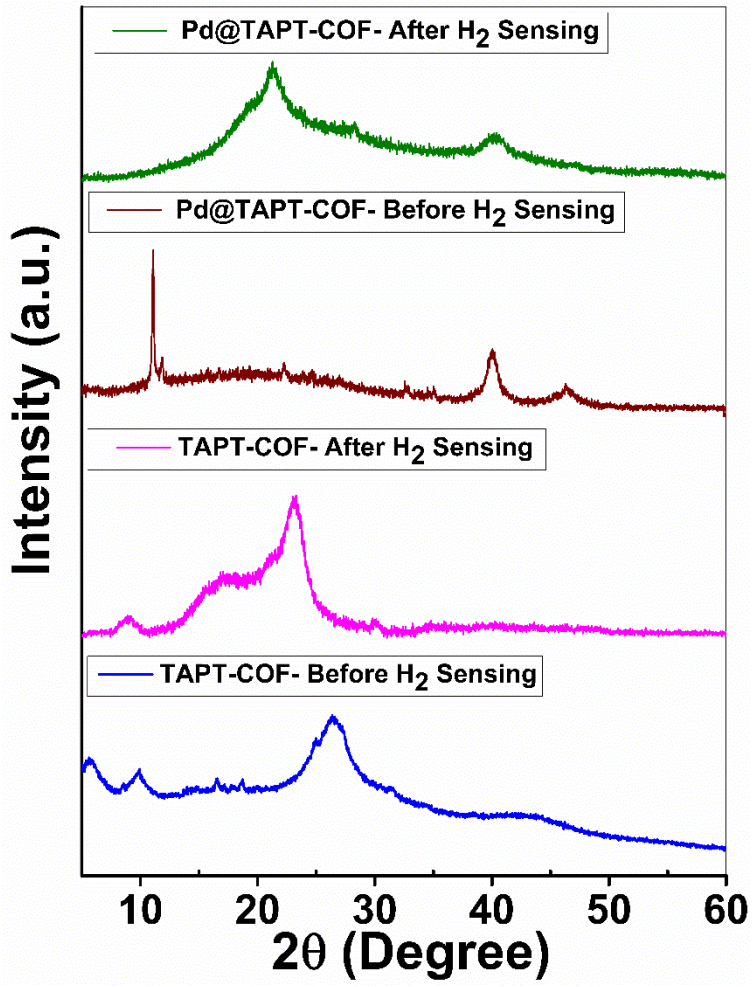


Figure S12. Powder X-ray diffraction (PXRD) patterns of COFs after H_2 sensing, respectively.

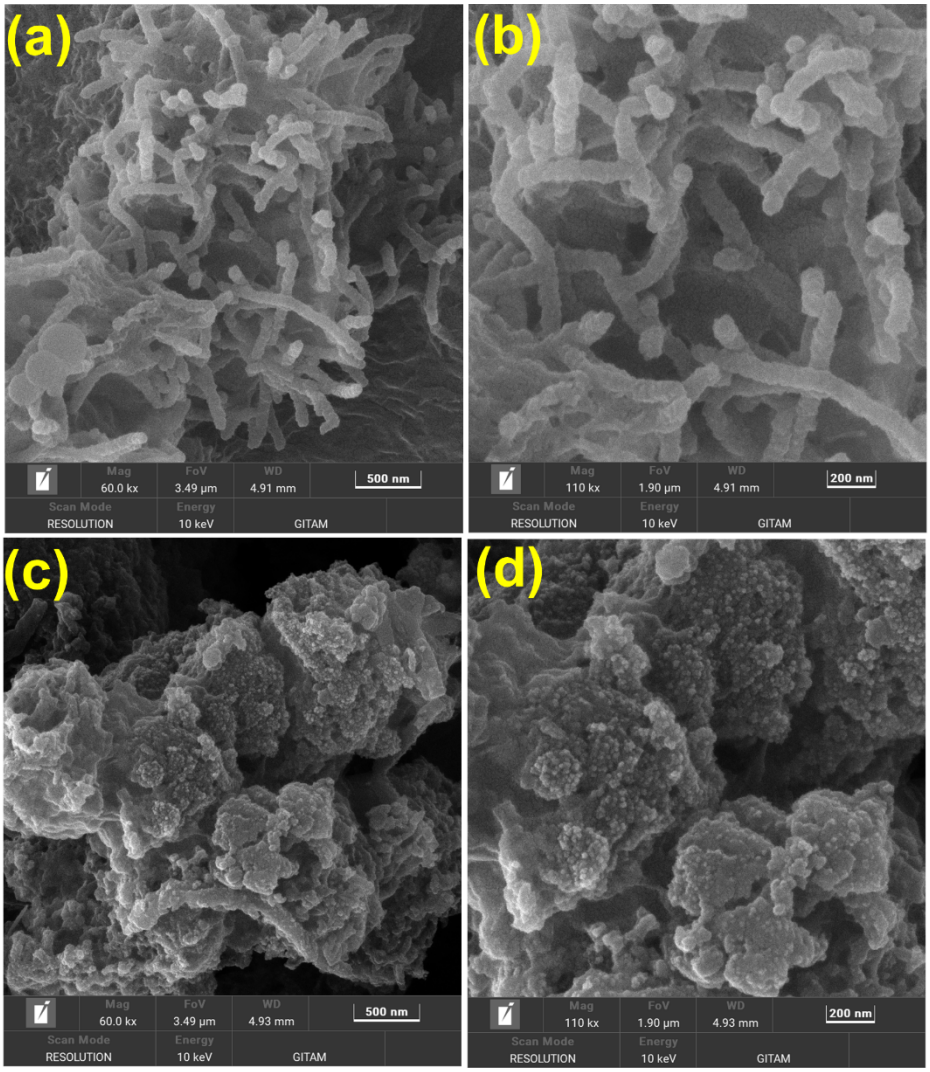


Figure S13. FESEM images of COFs after H_2 sensing, (a, b) TAPT-COF and (c, d) Pd@TAPT-COF, respectively.

S4. THEORETICAL STUDIES AND RESULTS

DFT calculations have been performed using the Gaussian 16 quantum chemical software [5]. To optimize the geometry of Covalent Organic Frameworks (COFs) and perform energy calculations both with and without the hydrogen molecule (H_2), we used the B3LYP functional level along with the 6-311+g(d)* [6] and empirical dispersion=gd3bj basis set [7]. For HOMO-LUMO studies, we used the VMD software, and for PDOS and RDG studies [6], we used the Multiwfn application [8]. The following equation can be utilized to determine the hydrogen adsorption energy and binding energy on TAPT-COF and Pd@TAPT-COF, respectively.

$$E_{ads\,(COF)} = E_{H_2/COF} - (E_{COFs} + E_{H_2}) \qquad \text{---------- (1)}$$

Equation (1) gives the adsorption energy of TAPT-COF and Pd@TAPT-COF when H_2 is present. The energies of the COF complexes are characterized as $E_{H_2/COF}$, where E_{H_2} signifies the energy of a single "H_2" molecule and "E" represents the total energy of the TAPT-COF and Pd@TAPT-COF. The Gaussian 16W software for electronic structure was utilized for all calculations following the construction of the fundamental structure with ChemDraw.

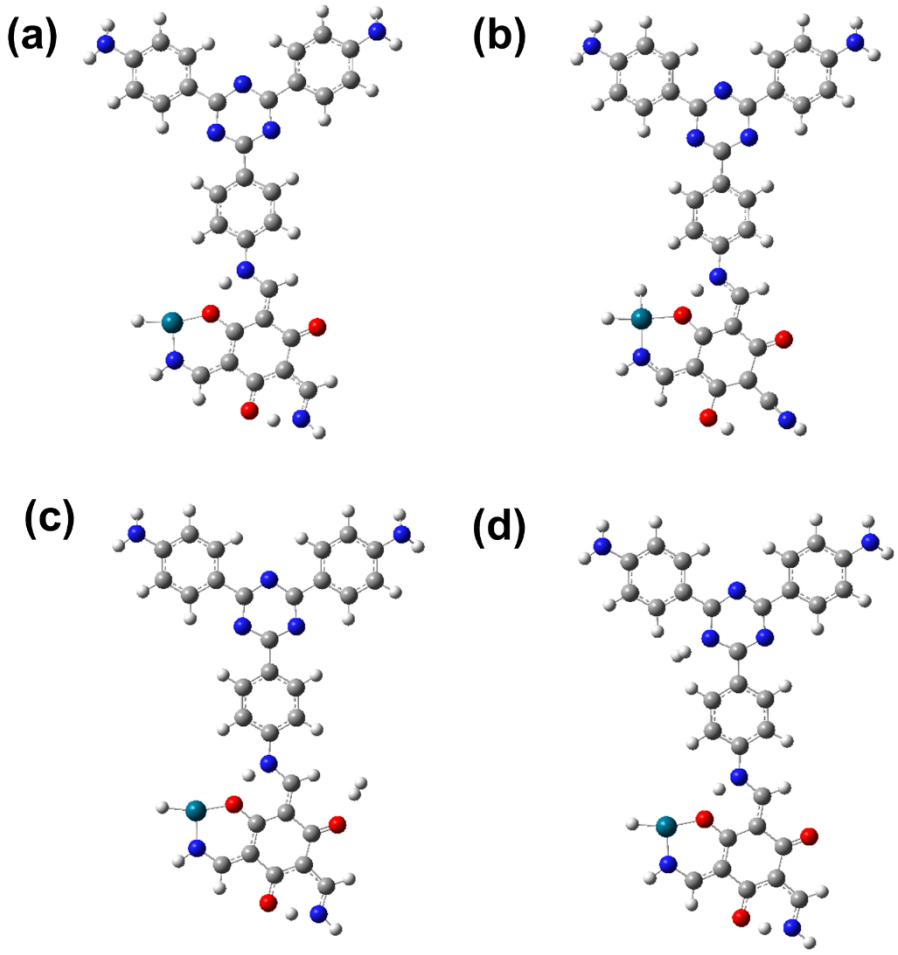


Figure S14. Geometrical optimized structure of (a) Pd@TAPT-COF, (b) Pd@TAPT-COF-H_2 site -1, (c) Pd@TAPT-COF-H_2 site -2, and (d) Pd@TAPT-COF-H_2 site -3.

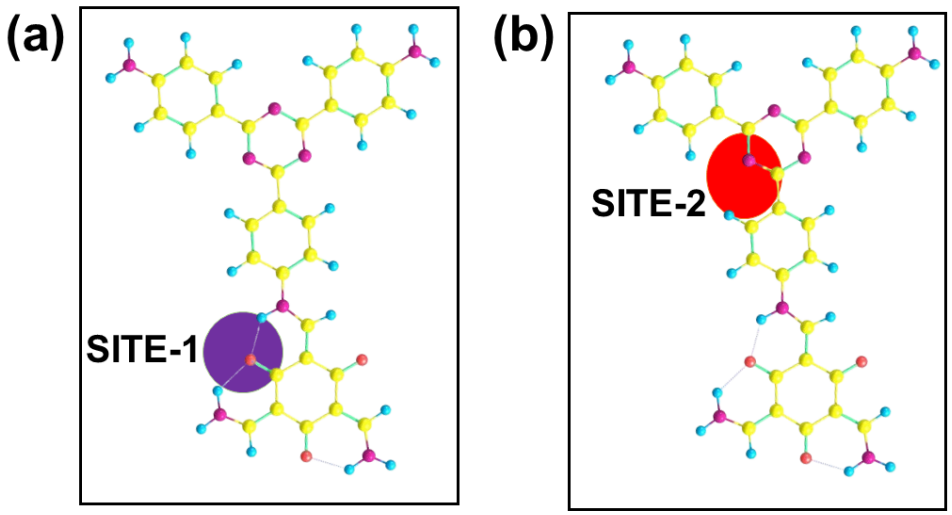


Figure S15. DFT -computed binding energies of the gas molecules with the active adsorption sites in TAPT-COF.

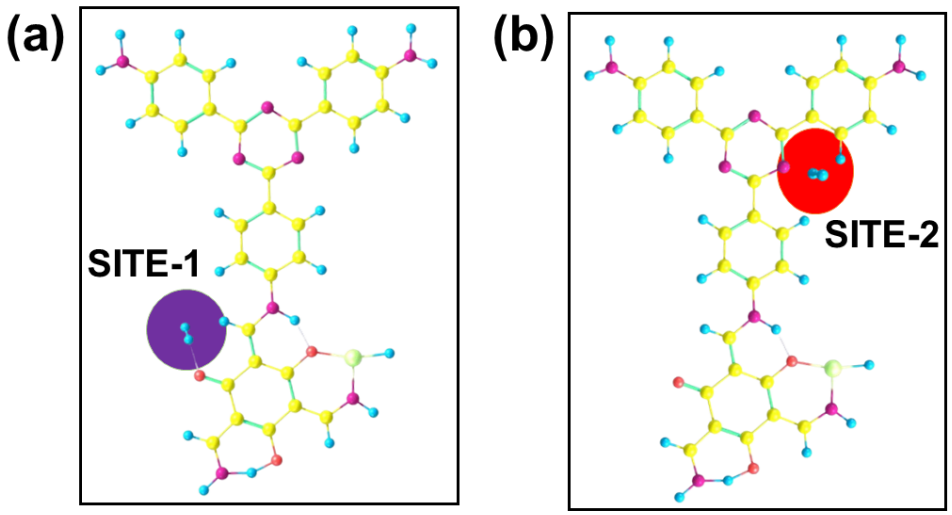


Figure S16. DFT -computed binding energies of the gas molecules with the active adsorption sites in Pd@TAPT-COF.

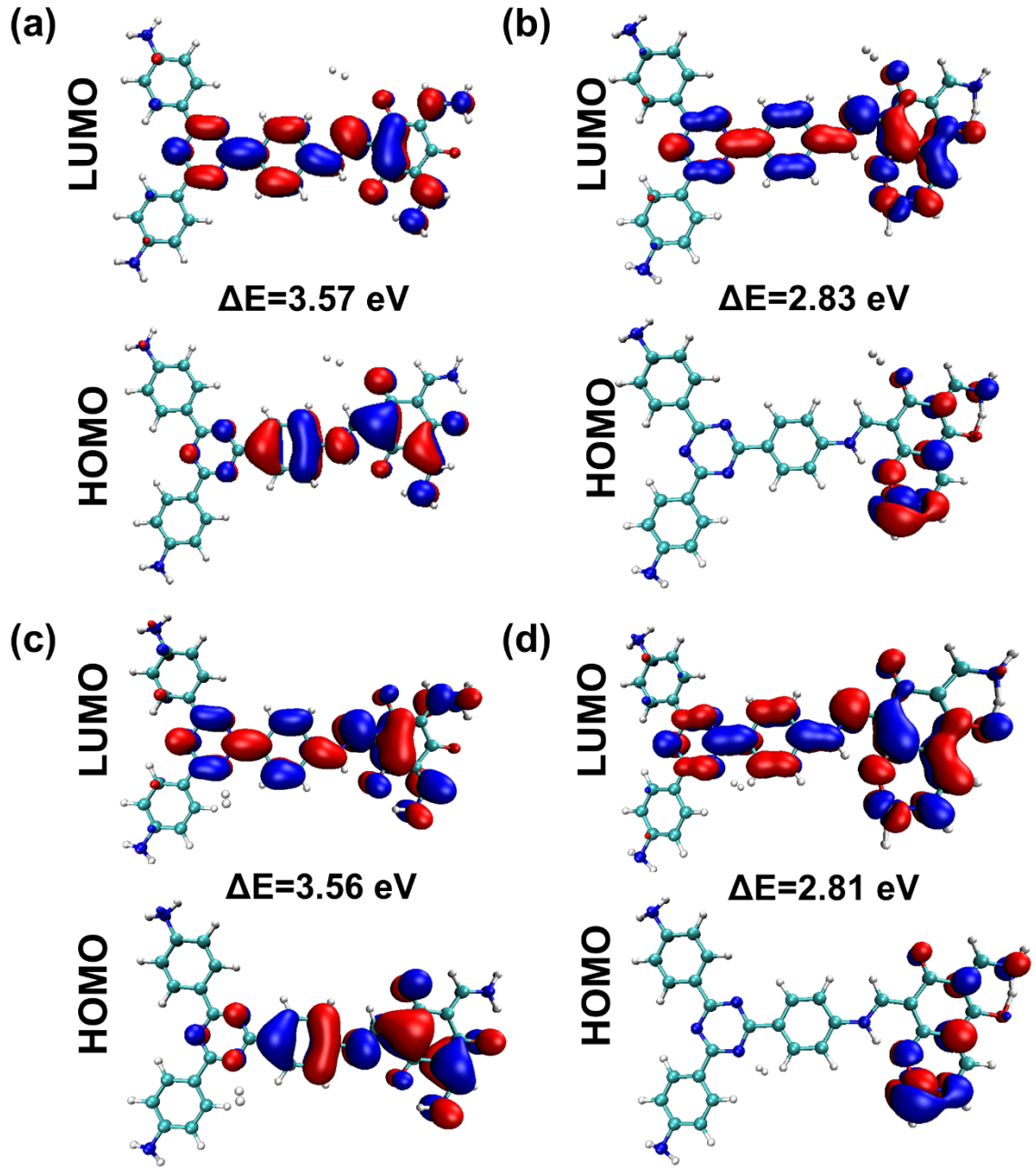


Figure S17. HOMO and LUMO plots of site-1 (a) TAPT-COF-H_2 (b) Pd@TAPT-COF-H_2, and site-2 (c) TAPT-COF-H_2 (d) Pd@TAPT-COF-H_2.

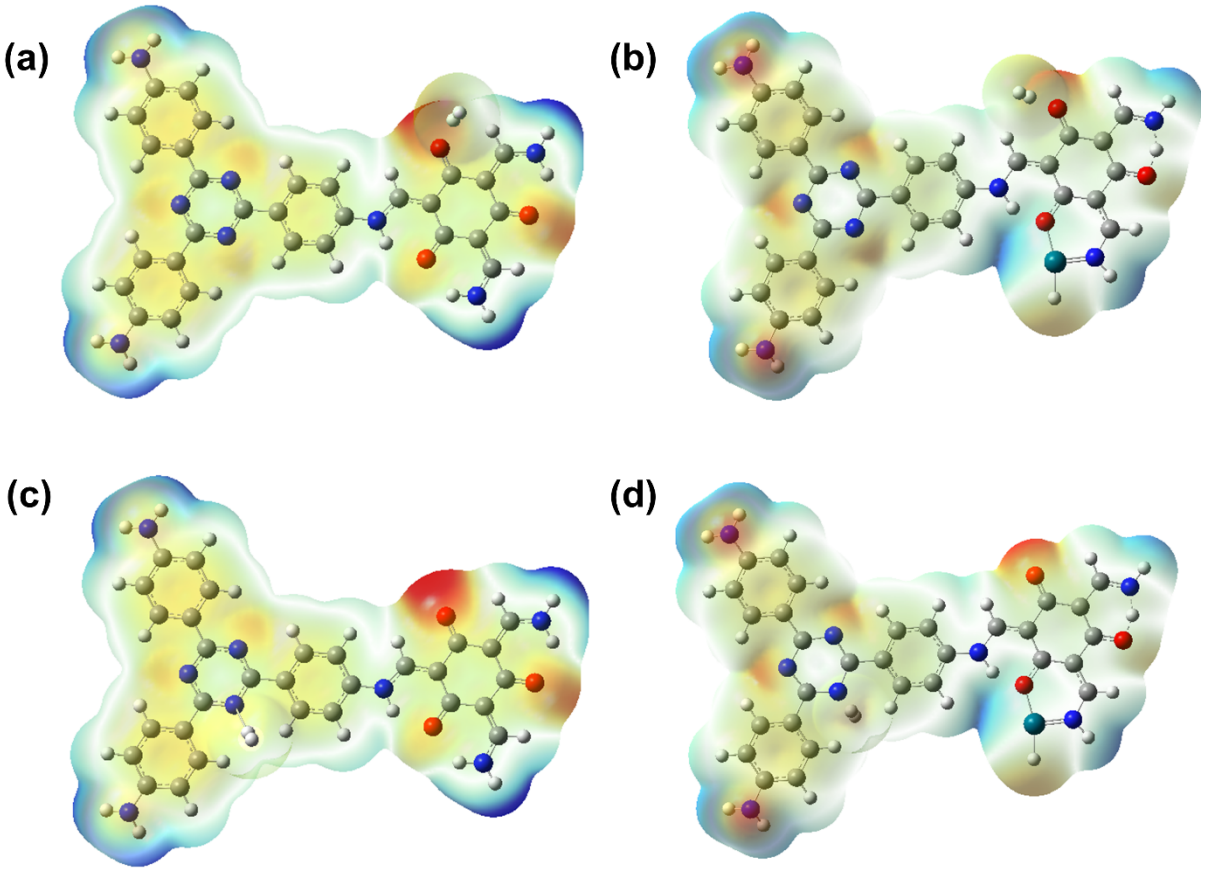


Figure S18. Electrostatic potential graphs of COFs at Site-1 (a) TAPT-COF-H_2, (b) Pd@TAPT-COF-H_2, and Site-2, (c) TAPT-COF-H_2 and (d) Pd@TAPT-COF-H_2.

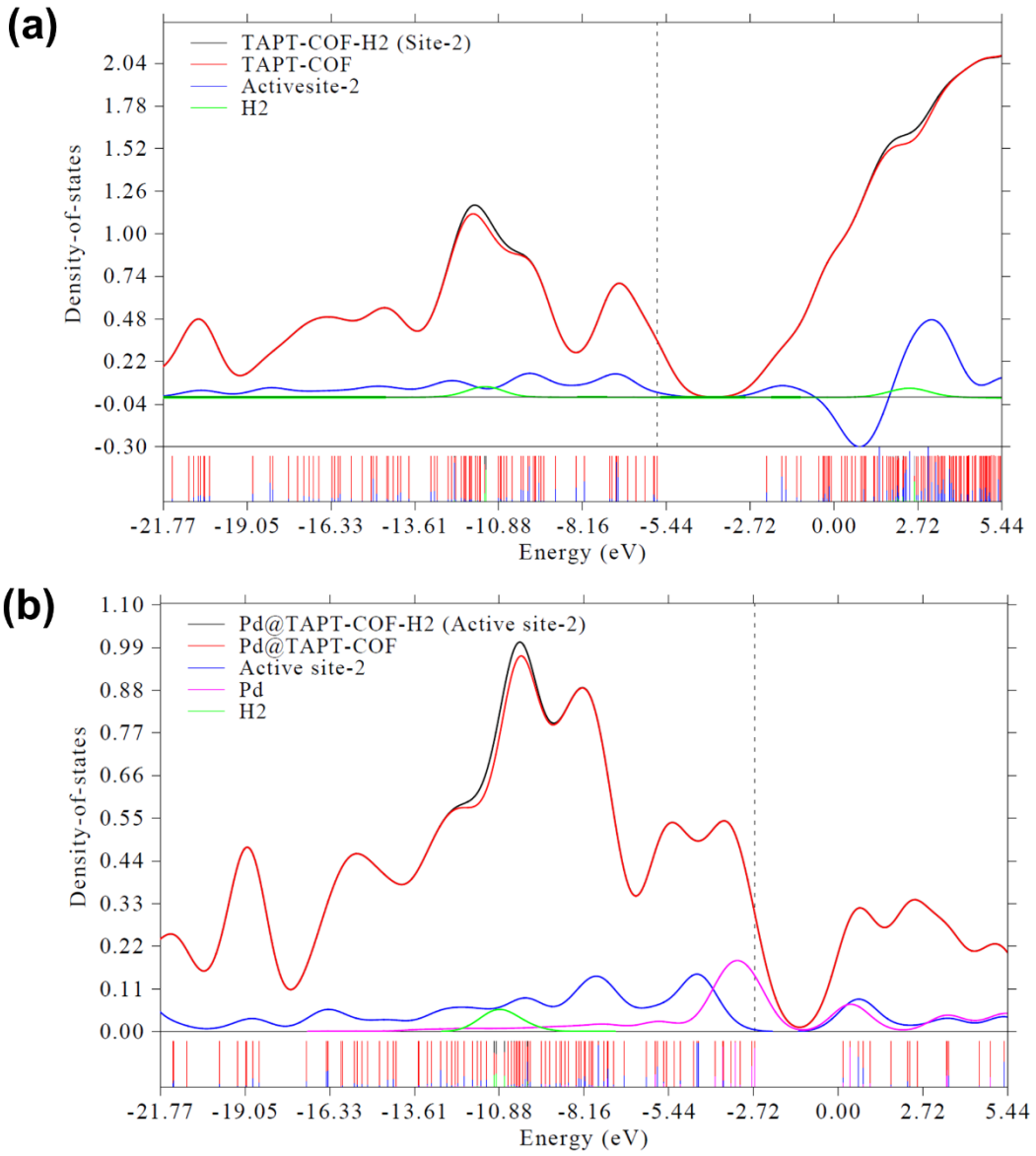


Figure S19. Projected density of states (PDOS) analysis of H_2 adsorption at active site-2 in (a) TAPT-COF and (b) Pd@TAPT-COF. (a) PDOS of TAPT-COF (black), TAPT-COF-H_2 (red), active site-1 (blue), and H_2 molecule (green) indicates weak interaction between H_2 and pristine COF, (b) PDOS of Pd@TAPT-COF (black), Pd@TAPT-COF-H_2 (red), active site-1 (blue), Pd (magenta), and H_2 molecule (green) indicates significant changes in electronic states upon H_2 adsorption.

S4. TABLES

Table S1. Optimized atomic coordinates in Cartesian format (A^0) for the unit cell of COFs used in DFT calculations.

COF Type	Lattice parameters (A°)	d-Spacing (A°)		Space Group
		Peak		
TAPT-COF	a=b=20.07, c= 4 α= 90, β=90, and γ=120	(100) (110) (210) (001)	15.42 8.94 4.74 3.37	P1(Hexagonal)
Pd@TAPT-COF	a=b=20.07, c= 4 α= 90, β=90, and γ=120	(110 shifted) Pd (111) Pd (200) Pd (220) Pd (311) Pd (222)	23.27 2.91 2.25 1.94 1.74 1.37	P1(Hexagonal)

TAPT-COF			
C	-4.61537	1.09924	0.03375
C	-2.51235	-0.12575	0.03321
C	-4.40619	1.20824	0.05053
N	-3.28278	-1.21951	0.03504
N	-5.1769	0.11475	0.04703
N	-3.07422	1.08798	0.03705
C	-5.05266	2.60558	0.07058
C	-4.24577	3.75148	0.07222
C	-6.44798	2.7307	0.0877
C	-4.83515	5.02282	0.09127
H	-3.1801	3.65595	0.05908
C	-7.03722	4.00188	0.10765
H	-7.06352	1.85546	0.08577
C	-6.23085	5.14799	0.1099
H	-4.21968	5.8979	0.09155
H	-8.10292	4.09749	0.12101
C	-5.50282	-2.35808	0.01536
C	-6.89874	-2.23223	0.01319
C	-4.91412	-3.62967	-0.0004
C	-7.70555	-3.37805	-0.00794

H	-7.34857	-1.26132	0.02749
C	-5.72091	-4.77548	-0.023
H	-3.84848	-3.72547	0.00451
C	-7.11673	-4.64946	-0.02732
H	-8.7712	-3.282	-0.00957
H	-5.27131	-5.74626	-0.03714
C	-0.97832	-0.26374	0.02707
C	-0.1715	0.88204	-0.00067
C	-0.38908	-1.53502	0.0493
C	1.22457	0.75617	-0.0086
H	-0.62153	1.85298	-0.01634
C	1.00656	-1.66046	0.04696
H	-1.00484	-2.41004	0.06857
C	1.81339	-0.51512	0.01654
H	1.84072	1.63062	-0.0333
H	1.45628	-2.63111	0.0681
N	-7.96333	-5.85106	-0.05214
H	-8.82154	-5.64479	-0.5223
H	-7.48622	-6.5849	-0.53624
N	-6.84896	6.48135	0.13205
H	-6.25446	7.13229	-0.34014
H	-7.73594	6.44513	-0.32836
C	4.05204	0.44008	-0.03931
H	3.60782	1.41239	-0.08612
C	5.40098	0.30958	-0.03157
C	6.2996	1.55874	-0.10269
C	6.03505	-1.09126	0.04925
C	7.83203	1.40621	-0.09318
C	7.5671	-1.24375	0.06337
C	8.46545	0.00499	-0.00987
O	5.30042	-2.11151	0.10445
O	9.71717	-0.11957	-0.00147
O	5.78231	2.70398	-0.16872
C	8.14328	-2.51902	0.14308
H	9.20784	-2.62564	0.15273
C	8.6507	2.5422	-0.16049
H	8.21154	3.51627	-0.21856
N	3.27711	-0.64953	0.01117
H	3.69444	-1.55759	0.04493
N	9.98186	2.40831	-0.15214
H	10.39229	1.49813	-0.09727
H	10.56656	3.2183	-0.20083
N	7.36204	-3.60321	0.20769

H	7.773	-4.5131	0.26545
H	6.36709	-3.50369	0.19832
TAPT-COF-H_2 (site -1)			
C	-4.61537	-1.09924	0.03375
C	-2.51235	-0.12575	0.03321
C	-4.40619	1.20824	0.05053
N	-3.28278	-1.21951	0.03504
N	-5.1769	0.11475	0.04703
N	-3.07422	1.08798	0.03705
C	-5.05266	2.60558	0.07058
C	-4.24577	3.75148	0.07222
C	-6.44798	2.7307	0.0877
C	-4.83515	5.02282	0.09127
H	-3.1801	3.65595	0.05908
C	-7.03722	4.00188	0.10765
H	-7.06352	1.85546	0.08577
C	-6.23085	5.14799	0.1099
H	-4.21968	5.8979	0.09155
H	-8.10292	4.09749	0.12101
C	-5.50282	-2.35808	0.01536
C	-6.89874	-2.23223	0.01319
C	-4.91412	-3.62967	-0.0004
C	-7.70555	-3.37805	-0.00794
H	-7.34857	-1.26132	0.02749
C	-5.72091	-4.77548	-0.023
H	-3.84848	-3.72547	0.00451
C	-7.11673	-4.64946	-0.02732
H	-8.7712	-3.282	-0.00957
H	-5.27131	-5.74626	-0.03714
C	-0.97832	-0.26374	0.02707
C	-0.1715	0.88204	-0.00067
C	-0.38908	-1.53502	0.0493
C	1.22457	0.75617	-0.0086
H	-0.62153	1.85298	-0.01634
C	1.00656	-1.66046	0.04696
H	-1.00484	-2.41004	0.06857
C	1.81339	-0.51512	0.01654
H	1.84072	1.63062	-0.0333
H	1.45628	-2.63111	0.0681
N	-7.96333	-5.85106	-0.05214
H	-8.82154	-5.64479	-0.5223
H	-7.48622	-6.5849	-0.53624
N	-6.84896	6.48135	0.13205

H	-6.25446	7.13229	-0.34014
H	-7.73594	6.44513	-0.32836
C	4.05204	0.44008	-0.03931
H	3.60782	1.41239	-0.08612
C	5.40098	0.30958	-0.03157
C	6.2996	1.55874	-0.10269
C	6.03505	-1.09126	0.04925
C	7.83203	1.40621	-0.09318
C	7.5671	-1.24375	0.06337
C	8.46545	0.00499	-0.00987
O	5.30042	-2.11151	0.10445
O	9.71717	-0.11957	-0.00147
O	5.78231	2.70398	-0.16872
C	8.14328	-2.51902	0.14308
H	9.20784	-2.62564	0.15273
C	8.6507	2.5422	-0.16049
H	8.21154	3.51627	-0.21856
N	3.27711	-0.64953	0.01117
H	3.69444	-1.55759	0.04493
N	9.98186	2.40831	-0.15214
H	10.39229	1.49813	-0.09727
H	10.56656	3.2183	-0.20083
N	7.36204	-3.60321	0.20769
H	7.773	-4.5131	0.26545
H	6.36709	-3.50369	0.19832
H	5.4219	4.2051	-0.42361
H	4.8219	4.2051	-0.42361

Pd@TAPT-COF			
C	-5.25816	-1.08108	0.002584
C	-3.31424	0.199006	0.002252
C	-5.3929	1.246137	0.00286
N	-3.85848	-1.08762	0.002202
N	-6.09693	0.037847	0.002138
N	-4.00327	1.414179	0.002515
C	-6.21963	2.50394	0.003791
C	-5.5956	3.779275	0.002273
C	-7.63785	2.436184	0.003762
C	-6.35913	4.951948	-0.00061
H	-4.4977	3.822525	0.000615

C	-8.41209	3.601795	0.00084
H	-8.11203	1.444981	0.003445
C	-7.78191	4.879477	-0.00333
H	-5.8711	5.935018	-0.00303
H	-9.50807	3.543207	-0.00034
C	-5.93421	-2.42594	0.00335
C	-7.35077	-2.5224	0.003977
C	-5.16717	-3.62072	0.001061
C	-7.98526	-3.76961	0.000974
H	-7.93621	-1.59257	0.004246
C	-5.79018	-4.87372	-0.00194
H	-4.07164	-3.53692	-0.0011
C	-7.2118	-4.96601	-0.00397
H	-9.08067	-3.83794	0.000325
H	-5.19192	-5.79388	-0.00496
C	-1.80806	0.285777	0.001688
C	-1.15769	1.547314	0.001665
C	-1.01767	-0.89343	0.001545
C	0.239697	1.640614	0.001153
H	-1.78003	2.452964	0.002375
C	0.379308	-0.81699	0.001022
H	-1.53011	-1.86537	0.002147
C	1.026936	0.453528	0.000743
H	0.724606	2.623693	0.001355
H	0.987665	-1.73056	0.001068
N	-7.857	-6.24907	0.090019
H	-8.80952	-6.2405	-0.349
H	-7.28276	-7.00832	-0.35033
N	-8.57097	6.079445	0.090696
H	-8.08795	6.900052	-0.3491
H	-9.51587	5.961149	-0.34894
C	3.301947	1.5832	-0.00049
H	2.872392	2.598125	-0.00067
C	4.684189	1.421832	-0.00083
C	5.55588	2.679428	-0.00157
C	5.294381	0.090549	-0.00038
C	7.034772	2.425924	-0.00125
C	6.717377	-0.09999	-0.00045
C	7.607069	1.102704	-0.00074
O	4.487404	-1.02445	0.000184
O	8.929353	0.899422	-0.00053
O	5.044524	3.84101	-0.0025
C	7.323886	-1.38118	-0.0002

H	8.426101	-1.41677	-0.00014
C	7.948697	3.530256	-0.00124
H	7.544801	4.561789	-0.00136
N	2.459432	0.477998	-4.1E-05
H	3.054831	-0.41878	0.000426
N	9.267887	3.266281	-0.00104
H	9.358416	2.008117	-0.00068
H	9.90816	4.10023	-0.00071
N	6.647012	-2.59423	-0.00019
H	7.317552	-3.40646	-0.00015
H	4.855794	-4.34296	-0.0005
Pd	4.919613	-2.76847	0.000054

Pd@TAPT-COF-H_2 (site-1)			
C	-5.25994	-1.0868	-0.00349
C	-3.31732	0.190656	-0.00172
C	-5.39301	1.238148	-0.00502
N	-3.86113	-1.09504	-0.00167
N	-6.09798	0.031475	-0.00607
N	-4.0042	1.40582	-0.00341
C	-6.2166	2.493358	-0.00614
C	-5.58945	3.765759	-0.00645
C	-7.63347	2.424001	-0.00943
C	-6.35155	4.938274	-0.01126
H	-4.49162	3.803788	-0.00568
C	-8.40612	3.589581	-0.01435
H	-8.1045	1.431591	-0.01076
C	-7.77362	4.865367	-0.01708
H	-5.8645	5.921403	-0.01284
H	-9.50185	3.533836	-0.01824
C	-5.93513	-2.4278	-0.00293
C	-7.35066	-2.5204	-0.00458
C	-5.16715	-3.62045	-0.0033
C	-7.98547	-3.76645	-0.00788
H	-7.93168	-1.5881	-0.00592
C	-5.79065	-4.87221	-0.00659
H	-4.07216	-3.5331	-0.00384
C	-7.21175	-4.96186	-0.01069

H	-9.08042	-3.83591	-0.01045
H	-5.19478	-5.79346	-0.00828
C	-1.81466	0.276291	-0.00022
C	-1.16732	1.538117	-0.00018
C	-1.02876	-0.9045	0.002018
C	0.229259	1.63072	0.000986
H	-1.79316	2.441049	-0.00029
C	0.36736	-0.82854	0.003209
H	-1.54615	-1.87351	0.002931
C	1.011962	0.442191	0.002057
H	0.717748	2.611714	0.003149
H	0.978865	-1.73976	0.004955
N	-7.85758	-6.24373	0.082252
H	-8.80859	-6.23315	-0.35964
H	-7.28236	-7.00198	-0.35819
N	-8.5614	6.065318	0.074188
H	-8.07556	6.88409	-0.36554
H	-9.50437	5.946434	-0.36905
C	3.283133	1.564001	-0.01246
H	2.852866	2.577043	-0.02764
C	4.665512	1.390263	-0.01035
C	5.556976	2.625772	-0.02486
C	5.254486	0.051522	-0.0036
C	7.026614	2.349197	-0.05398
C	6.671567	-0.1653	-0.02338
C	7.579372	1.019023	-0.05243
O	4.429693	-1.04955	0.017913
O	8.897654	0.795465	-0.07411
O	5.076951	3.804172	-0.0161
C	7.257252	-1.45518	-0.01892
H	8.35835	-1.50668	-0.03575
C	7.954597	3.44088	-0.07502
H	7.562219	4.476587	-0.07144
N	2.442042	0.462789	0.004036
H	3.03895	-0.43598	0.015163
N	9.268572	3.157801	-0.09796
H	9.341644	1.897446	-0.0904

H	9.920482	3.98237	-0.11023
N	6.561721	-2.65602	0.004508
H	7.218063	-3.4793	0.004377
Pd	4.832726	-2.80041	0.031195
H	4.763531	-4.37368	0.049715
H	3.217216	4.648159	1.645932
H	3.718973	4.416734	1.158359

Pd@TAPT-COF-H_2 Site-2			
C	5.223497	-1.05695	0.002925
C	3.277494	0.219838	-0.00551
C	5.353084	1.268067	-0.03465
N	3.824144	-1.06537	0.023308
N	6.059374	0.062138	-0.02349
N	3.964085	1.434475	-0.03326
C	6.175336	2.523661	-0.05497
C	5.546971	3.795477	-0.06701
C	7.592329	2.455481	-0.05913
C	6.308002	4.968548	-0.08131
H	4.449112	3.832493	-0.06212
C	8.3639	3.621633	-0.07335
H	8.064225	1.463532	-0.04834
C	7.730212	4.896871	-0.08283
H	5.820136	5.951238	-0.08925
H	9.459685	3.566888	-0.07526
C	5.901186	-2.39616	0.014019
C	7.316473	-2.48259	0.063299
C	5.139781	-3.59259	-0.02513
C	7.957153	-3.72535	0.078578
H	7.892311	-1.54755	0.092271
C	5.769394	-4.84119	-0.01077
H	4.045269	-3.5139	-0.06577
C	7.189769	-4.92442	0.044298
H	9.051653	-3.78952	0.119609
H	5.178298	-5.76502	-0.0402
C	1.775587	0.305399	-0.00289
C	1.131006	1.568137	0.041331
C	0.985881	-0.87232	-0.04804
C	-0.26499	1.664715	0.045204
H	1.759427	2.468715	0.072437

C	-0.40985	-0.79222	-0.04496
H	1.496974	-1.84344	-0.08694
C	-1.05175	0.479265	0.002906
H	-0.7507	2.646312	0.080912
H	-1.02351	-1.70126	-0.08029
N	7.84464	-6.20233	-0.03582
H	8.779509	-6.19117	0.439196
H	7.257874	-6.96702	0.377369
N	8.516243	6.096077	-0.19359
H	8.032499	6.920201	0.238289
H	9.462299	5.983667	0.244645
C	-3.32241	1.605831	0.045894
H	-2.89743	2.621654	0.081758
C	-4.70297	1.433413	0.041779
C	-5.58702	2.677595	0.087853
C	-5.29667	0.09852	-0.00526
C	-7.06086	2.406068	0.079713
C	-6.71497	-0.11038	-0.01099
C	-7.61791	1.078714	0.03259
O	-4.476	-1.00507	-0.04577
O	-8.93713	0.859149	0.026297
O	-5.09013	3.844531	0.129599
C	-7.30621	-1.39649	-0.05634
H	-8.40762	-1.44346	-0.05683
C	-7.98561	3.498877	0.119837
H	-7.59136	4.53318	0.156295
N	-2.48059	0.503805	0.005007
H	-3.07825	-0.39323	-0.02624
N	-9.30138	3.220514	0.111338
H	-9.37835	1.962567	0.066307
H	-9.95066	4.046551	0.141214
N	-6.61527	-2.59982	-0.10013
H	-7.27515	-3.41974	-0.12878
Pd	-4.8866	-2.75232	-0.10753
H	-4.82124	-4.32524	-0.16374
H	3.128685	-2.09978	1.86766
H	2.931898	-2.37788	2.515035

Pd@TAPT-COF-H_2 (site-3)			
C	5.15096	-1.0666	0.047193
C	3.227454	0.238527	0.000211
C	5.317569	1.255604	-0.02211
N	3.751632	-1.05371	0.041246
N	6.00468	0.039599	0.018426
N	3.931058	1.443347	-0.03363
C	6.159608	2.498088	-0.05675
C	5.551651	3.779175	-0.0941
C	7.575283	2.407653	-0.04995
C	6.331274	4.939815	-0.12248
H	4.454536	3.833604	-0.09714
C	8.365331	3.561181	-0.0782
H	8.03128	1.408703	-0.01922
C	7.752061	4.845827	-0.11312
H	5.8591	5.929789	-0.14989
H	9.460101	3.489127	-0.07164
C	5.805078	-2.41661	0.089285
C	7.219009	-2.53116	0.104374
C	5.017851	-3.59661	0.116923
C	7.833755	-3.78639	0.14746
H	7.814998	-1.6086	0.084121
C	5.621325	-4.85726	0.159627
H	3.9243	-3.49242	0.106703
C	7.040887	-4.96898	0.177386
H	8.927386	-3.87309	0.160608
H	5.010638	-5.7685	0.18216
C	1.724499	0.345292	-0.0082
C	1.098852	1.617051	-0.05706
C	0.922745	-0.8247	0.032274
C	-0.29676	1.729216	-0.06562
H	1.739763	2.508649	-0.08909
C	-0.47326	-0.72936	0.024379
H	1.42649	-1.80016	0.069904
C	-1.09337	0.551936	-0.02407
H	-0.77154	2.716462	-0.10623
H	-1.10629	-1.62761	0.059056
N	7.666652	-6.2626	0.125534
H	8.613841	-6.25606	0.575455
H	7.074845	-7.00022	0.57865
N	8.55786	6.030748	-0.23839

H	8.084592	6.868795	0.178176
H	9.498936	5.910111	0.208434
C	-3.34659	1.67209	-0.02127
H	-2.93955	2.697446	-0.01048
C	-4.74807	1.468693	-0.00776
C	-5.63202	2.680968	0.062573
C	-5.28659	0.121789	-0.01055
C	-7.14422	2.347514	0.177536
C	-6.72585	-0.14925	0.04147
C	-7.60786	0.952041	0.138015
O	-4.4057	-0.91459	-0.02208
O	-8.98421	0.654913	0.164432
O	-5.19767	3.866032	0.054186
C	-7.24122	-1.501	0.004881
H	-8.31274	-1.64477	0.200935
C	-8.02298	3.359895	0.360244
N	-2.52912	0.577268	-0.0317
H	-3.20464	-0.33143	-0.01602
N	-8.85185	4.308733	0.249689
H	-9.43222	1.578468	0.180676
H	-9.1372	4.747139	1.189731
N	-6.46375	-2.59284	-0.3184
H	-7.09423	-3.43613	-0.35903
Pd	-4.69849	-2.7701	-0.19299
H	-4.81486	-4.28219	-0.48235
H	-3.32506	-3.09352	0.526872

Table S2. Deconvoluted O1s XPS peak areas for C=O and C-O groups, and their corresponding C=O/C-O ratios for TAPT-COF and Pd@TAPT-COF

COF	C=O Peak Area%	C-O Peak Area%	C=O/C-O Ratio
TAPT-COF	65.1	34.8	1.87
Pd@TAPT-COF	79.6	20.4	3.90

Table S3. AFM results of COFs.

S. No	Material	Mean surface roughness (Sa)
1.	TAPT-COF	14.39nm
2.	Pd@TAPT-COF	16.23nm

Table S4. Brunauer-Emmett-Teller (BET) details of COFs**.**

Sample	Specific area (m^2/g)	Pore size (nm)	Pore Volume (cc/g)
TAPT-COF	200 m^2/g	45.7 nm	0.271241
Pd@TAPT-COF	150 m^2/g	42.1 nm	0.229689

Target Gas	Concentration (ppm)	Sensing Material: TAPT- COF			
		Response (R_a/R_g)	Response time (sec)	Recovery time (sec)	Recovery (%)
Hydrogen	1	1.14	6	4	99.3
Hydrogen	5	1.21	8	12	99.5
Hydrogen	10	1.34	22	21	99.8
Hydrogen	25	1.68	20	22	99.6
Hydrogen	50	5.83	18	17	99.6
					Avg: 99.56

Table S5. Response, Response time, and Recovery times of TAPT-COF compounds for concentrations of Hydrogen gas at room temperature.

Table S6. Response, Response time, and Recovery times of Pd@TAPT-COF compounds for concentrations of Hydrogen gas at room temperature.

Target Gas	**Concentration (ppm)**	**Sensing Material: Pd@TAPT-COF**			
		Response (R_a/R_g)	**Response time (sec)**	**Recovery time (sec)**	**Recovery (%)**
Hydrogen	1	1.4	4	3	97.15
Hydrogen	5	2.2	5	6	97.48
Hydrogen	10	3.2	10	12	98.78
Hydrogen	25	5.3	11	14	99.49
Hydrogen	50	10	16	18	99.64
					Avg: 99.70

Table S7. Response, Response time, and Recovery times of TAPT-COF for Hydrogen gas concentrations at different temperatures.

Target Gas	**Temperature**	**Sensing material: TAPT-COF**			
		Response (R_a/R_g)	**Response time (sec)**	**Recovery time (sec)**	**Recovery (%)**
Hydrogen	50 °C	2	4	5	99.4
Hydrogen	100 °C	4	20	13	99.5
Hydrogen	150 °C	6	18	15	99.8
					Avg:99.6

Table S8. Response, Response time, and Recovery times of Pd@TAPT-COF for Hydrogen gas concentrations at different temperatures.

Target Gas	**Temperature**	**Sensing material: Pd@TAPT-COF**			
		Response (R_a/R_g)	**Response time (sec)**	**Recovery time (sec)**	**Recovery (%)**
Hydrogen	50 °C	3	4	6	99.6
Hydrogen	100 °C	5	13	15	99.7
Hydrogen	150 °C	8	17	15	99.8
					Avg:99.8

Table S9. Geometrically optimized COFs energy values.

Sl. No.	Sample Name	Optimized energy (Before Hydrogen Sensing)	Optimized energy (After Hydrogen Sensing Energy)
1.	TAPT-COF	-1822.01 Hartree	-1823.18 Hartree
2.	Pd@TAPT-COF	-6689.59 Hartree	-6690.92 Hartree

Table S10. The total energy and absorption energy are computed from TAPT-COF and Pd@TAPT-COF-H_2 at Site-1.

Site-1 (-C=O-H_2)	**Energy (kJ/mol)**	**E_{ads} (kJ/mol)**	**E_{ads} (eV)**
H_2	-3035.07		
TAPT-COF	-4783687.25		
TAPT-COF-H_2	-4786780.09	-57.77	-0.599
Pd@TAPT-COF	-17561695.43		
Pd@TAPT-COF-H_2	-17569571.03	-484.57	-5.022

Table S11. The total energy and adsorption energy are computed from TAPT-COF and Pd@TAPT-COF-H_2 at Site-2.

Site-2 (C-N-H_2)	**Energy (kJ/mol)**	**E_{ads} (kJ/mol)**	**E_{ads} (eV)**
H_2	-3035.07		
TAPT-COF	-4783687.25		
TAPT-COF-H_2	-4839164.07	-69.96	-0.725
Pd@TAPT-COF	-17561695.43		
Pd@TAPT-COF-H_2	-17565005.80	-275.30	-2.853

Table S12. HOMO energies (E_{HOMO}), LUMO energies (E_{LUMO}), and energy gap calculated for TAPT-COF and Pd@TAPT-COF.

Sl. No.		**E_{LUMO}**	**E_{HOMO}**	**Energy gap value (eV)**
1	TAPT-COF	-2.1665	-5.7332	3.56
2	Pd@TAPT-COF	-2.6550	-0.1692	2.82
SITE-1(-C=O-H_2)				
3	TAPT-COF-H_2	-2.1758	-5.7470	3.57
4	Pd@TAPT-COF-H_2	-2.6996	-0.1322	2.83
SITE-2 (-C-N-H_2)				
5	TAPT-COF-N-H_2	-2.1725	-5.7367	3.56
6	Pd@TAPT-COF-N-H_2	-2.6642	-0.1540	2.81

Table S13. Second-order perturbation NBO analysis of Pd@TAPT-COF, showing key donor-acceptor interactions. Strong π→ π*, LP→ π*, and LP(O)→Pd interactions indicate effective charge delocalization and metal-ligand coordination, supporting enhanced electronic interaction and sensing activity.

BD (1) C 1 - N 4	σ* C 1 - N 5	2.93	1.08	0.05
π C 1 - N 4	π* C 2 - N 6	32.4	0.27	0.085
π C 2 - N 6	π* C 3 - N 5	31.26	0.27	0.084
π C 3 - N 5	π* C 1 - N 4	31.97	0.27	0.084
π C 7 - C 8	π* C 3 - N 5	20.94	0.22	0.062
π C 7 - C 8	π* C 9 - C 12	23.92	0.27	0.073
π C 7 - C 8	π* C 10 - C 14	21.07	0.26	0.066
π C 9 - C 12	π* C 10 - C 14	22.27	0.27	0.072
π C 10 - C 14	π* C 7 - C 8	25.7	0.29	0.077
π C 17 - C 19	π* C 18 - C 20	23.91	0.27	0.073
π C 17 - C 19	π* C 22 - C 24	21.07	0.26	0.066
BD (2) C 18 - C 20	π* C 22 - C 24	22.27	0.27	0.072
BD (2) C 22 - C 24	π* C 17 - C 19	25.69	0.29	0.077
BD (2) C 27 - C 29	LP (1) C 32	59.03	0.12	0.094
BD (2) C 27 - C 29	π* C 28 - C 30	23.22	0.27	0.073
BD (2) C 28 - C 30	π* C 34 - N 58	35.66	0.2	0.087
BD (2) C 34 - N 58	π* C 43 - C 45	30.43	0.33	0.092
BD (2) C 43 - C 45	LP*(1) C 47	47.41	0.12	0.087
πBD (2) C 48 - C 56	LP (2) N 60	106.91	0.04	0.084
π C 48 - C 56	π* C 46 - O 53	21.86	0.28	0.072
π C 48 - C 56	π* C 50 - O 52	45.47	0.22	0.091
π C 49 - C 54	π* C 50 - O 52	23.77	0.24	0.071
π N 63 -Pd 66	π* C 49 - C 54	40.04	0.3	0.1
LP (1) N 37	π* C 22 - C 24	21.17	0.33	0.081
LP (1) N 40	π* C 10 - C 14	21.16	0.33	0.081
LP (1) O 51	LP*(5)Pd 66	56.77	0.9	0.208
LP (1) O 51	σ* N 58 - H 59	30.26	1.05	0.162
LP (2) O 51	LP*(5)Pd 66	154.16	0.54	0.263
LP (3) O 51	LP (4)Pd 66	22.93	0.13	0.073
LP (2) O 53	σ* C 45 - C 46	24.19	0.55	0.104
LP (2) O 53	σ* C 46 - C 48	21.53	0.59	0.102
LP (1) N 60	σ* O 52 - H 61	199.71	0.67	0.328
LP (2) N 60	π* C 48 - C 56	90.46	0.21	0.126

Table S14. Second-order perturbation NBO analysis of Pd@TAPT-COF-H_2 (Site-1, C=O-H_2 region) showing key donor-acceptor interactions, highlighting strong π→ π*, LP→ π*, and LP → Pd interactions. Notably, strong interactions, such as LP(O) → LP(Pd)* and LP(N) → σ(O-H)* interactions, support weak physisorption of H_2 near the C=O region, contributing to enhanced sensing performance via reversible, non-destructive adsorption.

π C 1 - N 4	π* C 2 - N 6	32.53	0.27	0.085
π C 2 - N 6	π* C 3 - N 5	31.32	0.27	0.084
π C 3 - N 5	π* C 1 - N 4	32.08	0.27	0.085
π C 7 - C 8	π* C 3 - N 5	21.26	0.23	0.062
π C 7 - C 8	π* C 9 - C 12	23.93	0.28	0.074
π C 7 - C 8	π* C 10 - C 14	21.08	0.26	0.067
π C 9 - C 12	π* C 10 - C 14	22.32	0.27	0.072
π C 10 - C 14	π* C 7 - C 8	25.71	0.29	0.077
π C 17 - C 19	π* C 18 - C 20	23.92	0.28	0.074
π C 17 - C 19	π* C 22 - C 24	21.08	0.26	0.067
π C 18 - C 20	π* C 22 - C 24	22.33	0.27	0.072
π C 22 - C 24	π* C 17 - C 19	25.7	0.29	0.077
π C 27 - C 29	LP (1) C 32	59.34	0.12	0.094
π C 27 - C 29	π* C 28 - C 30	23.14	0.27	0.073
π C 28 - C 30	π* C 34 - N 58	35.66	0.2	0.087
Π C 34 - N 58	π* C 43 - C 45	31.18	0.33	0.093
π N 63 -Pd 65	π* C 49 - C 54	40.24	0.3	0.1
LP (1) N 37	π* C 22 - C 24	21.16	0.33	0.081
LP (1) N 40	π* C 10 - C 14	21.17	0.33	0.081
LP (1) O 51	LP*(5)Pd 65	58.89	0.91	0.212
LP (1) O 51	σ* N 58 - H 59	33.81	1.06	0.172
LP (2) O 51	LP*(5)Pd 65	151.91	0.54	0.26
LP (3) O 51	LP*(1) C 47	99.32	0.14	0.127
LP (3) O 51	LP (4)Pd 65	22.39	0.13	0.073
LP (2) O 53	σ* C 45 - C 46	22.56	0.56	0.102
LP (2) O 53	σ* C 46 - C 48	21.06	0.6	0.102
LP (1) N 60	σ* O 52 - H 61	198.9	0.67	0.327
LP (2) N 60	π* C 48 - C 56	91.13	0.21	0.127

Table S15. Second-order perturbation NBO analysis of Pd@TAPT-COF-H_2 (Site-2, C-N-H_2 region) showing key donor-acceptor interactions, highlighting strong π→ π*, LP→ π*, and LP →Pd interactions. Notable interactions, such as LP(O) →LP(Pd)* and π (N-Pd) →π(C=C)* indicate effective charge delocalization and effective Pd-mediated back-donation, supporting the H_2 Physisorption mechanism at the C-N binding site.

π C 1 - N 4	π * C 2 - N 6	32.46	0.27	0.085
π C 2 - N 6	π * C 3 - N 5	31.36	0.27	0.084
π C 3 - N 5	π * C 1 - N 4	32.3	0.27	0.085
π C 7 - C 8	π * C 3 - N 5	21.35	0.22	0.062
π C 7 - C 8	π * C 9 - C 12	23.92	0.28	0.074
π C 7 - C 8	π * C 10 - C 14	21.07	0.26	0.067
π C 9 - C 12	π * C 10 - C 14	22.33	0.27	0.072
π C 10 - C 14	π * C 7 - C 8	25.74	0.29	0.077
π C 17 - C 19	π * C 1 - N 4	20.31	0.22	0.061
π C 17 - C 19	π * C 18 - C 20	23.92	0.28	0.074
π C 17 - C 19	π * C 22 - C 24	21.04	0.26	0.066
π C 18 - C 20	π * C 22 - C 24	22.32	0.27	0.072
π C 22 - C 24	π * C 17 - C 19	25.75	0.29	0.077
π C 27 - C 29	152. LP (1) C 32	59	0.12	0.094
π C 27 - C 29	π * C 28 - C 30	23.23	0.27	0.073
π C 28 - C 30	π * C 34 - N 58	35.55	0.2	0.087
π C 34 - N 58	π * C 43 - C 45	30.55	0.33	0.092
π C 43 - C 45	LP*(1) C 47	48.35	0.12	0.088
π C 48 - C 56	LP (2) N 60	106.6	0.04	0.084
π C 48 - C 56	π * C 46 - O 53	21.97	0.28	0.073
π C 48 - C 56	π * C 50 - O 52	45.61	0.22	0.092
π C 49 - C 54	LP*(1) C 47	58.79	0.12	0.093
π C 49 - C 54	π * C 50 - O 52	23.9	0.24	0.072
π N 63 -Pd 65	π * C 49 - C 54	40.12	0.3	0.1
LP (1) N 37	π * C 22 - C 24	21.2	0.33	0.081
LP (1) N 40	π * C 10 - C 14	21.23	0.33	0.081
LP (1) O 51	LP*(5)Pd 65	58.61	0.91	0.212
LP (1) O 51	σ* N 58 - H 59	33.19	1.06	0.17
LP (2) O 51	LP*(5)Pd 65	152.78	0.54	0.261
LP (3) O 51	LP*(1) C 47	99.53	0.14	0.127
LP (3) O 51	LP (4)Pd 65	22.6	0.13	0.073
LP (2) O 53	σ* C 45 - C 46	24.1	0.55	0.104
LP (2) O 53	σ* C 46 - C 48	21.53	0.59	0.102
LP (1) N 60	σ* O 52 - H 61	200.03	0.67	0.328
LP (2) N 60	π * C 48 - C 56	90.39	0.21	0.126

LP*(5)Pd 65	σ* N 63 -Pd 65	26.81	0.02	0.047
LP*(5)Pd 65	σ* Pd 65 - H 66	35.76	0.18	0.171
LP*(6)Pd 65	σ* N 63 -Pd 65	21.9	0.13	0.175

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