Supporting Information

Enhanced selective gold recovery from e-waste via synergistic hetero-atom controlled quasi-planar benzoxazine-based covalent organic frameworks

Sushil Kumar[a ǂ], Mahira Bashri [a ǂ], Safa Gaber [a], José I. Martínez[b], Matthew J. O'Connor[c], Sabu Varghese[c], Blaž Belec[d], Gisha Elizabeth Luckachan, and Dinesh Shetty*[a,e]

[a] *Department of Chemistry, Khalifa University, Abu Dhabi 127788, United Arab Emirates*
[b] *Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), C/Sor Juana Inés de la Cruz 3, 28049 Madrid, Spain*
[c] *Core Technology Platform, New York University Abu Dhabi (NYUAD), Saadiyat Island, 129188, Abu Dhabi, United Arab Emirates*
[d] *Materials Research Laboratory, University of Nova Gorica, Vipavska 11c, Slovenia*
[e] *Center for Catalysis & Separations (CeCaS), Khalifa University of Science & Technology, Abu Dhabi 127788, UAE*

*Corresponding author.
E-mail address: dinesh.shetty@ku.ac.ae (Dr. Dinesh Shetty)

Contents

Section S1. Materials and methods

The precursor materials 1,3,5-triformyl-2,4-dihydroxybenzene (Tra) and1,3,5-Trifrormyl-2-hydroxybenzene (Tpa) were synthesized using the previously reported literature protocols.1 All other commercially available reagents and solvents purchased from Sigma-Aldrich, TCI chemicals and Fisher Scientific chemical suppliers were used as received. The reactions were performed in oven-dried glassware under ambient atmosphere.

Instruments details and sample preparation

Powder X-ray diffraction (PXRD) data collection was performed using a Bruker D8 ADVANCE equipped with high-intensity Microfocus rotating anode X-ray generator and Cu Kα (α = 1.54 Å) with a Ni filter as a radiation source. PXRD data were recorded in the 2θ = 5 – 40o using a Quartz holder at a scan speed of 1° min-1 and a step size of 0.01° with the help of Diffrac Plus XRD commander software. Fourier transform infrared (FTIR) spectra were recorded against wavenumber (cm–1) scale using a ThermoScientific Nicolet iS10 spectrometer equipped with a universal Zn-Se ATR (attenuated total reflection) accessory. Solid state 13C Cross Polarization Magic Angle Spinning (CP-MAS) NMR were measured on BrukerAvance III 400 MHz Wide Bore instrument. Thermogravimetric analyses (TGA) were carried under N2 atmosphere at a heating rate of 10 ºC min–1 within a temperature range of 30−900 °C using a TGA 209 F1 analyzer (Netzsch). Prior to the measurement the samples were dried under high vacuum for 12 h. Before collecting TGA data the samples were activated by heating at 100 oC for ~1 h at TGA instrument only. Morphology of the membranes was determined from SEM measurements performed with a Magellan FEI 400 scanning electron microscope. For sample preparation, a isopropanol suspension of COFs were drop casted on a clean unit of Silicon wafer. To avoid charging during SEM analyses, we coated all the ICONs samples with a 3 nm thick layer of Iridium using Q150T S sputter prior to analyses. N2 gas uptake analyses were performed at 77K using a liquid nitrogen bath (77 K) on a Micromeritics ASAP 2420 BET instrument. Samples were thoroughly outgassed for 12 h at 140 °C under high vacuum prior to the gas adsorption studies. The surface areas were evaluated using Brunauer-Emmett-Teller (BET) model applied between P/P0 values of 0.05 and 0.3. The pore size distributions were calculated using the non-localized density functional theory (NLDFT) method.

Theoretical methods and atomistic modelling

Density Functional Theory (DFT) calculations were conducted to study the structural and electronic properties, including the Electron Localization Function (ELF), of PGBpy-COF and PGBD-COF systems, as well as their interaction with the $[AuCl_4]^-$ ion. The molecular building blocks involved in the COF systems and the $[AuCl_4]^-$ ion were pre-optimized using DFT as implemented in the localized basis set Gaussian16 package [1] within M06-2X/6-311++G(d,p) [2-4] theory level, allowing full geometric flexibility and confirming equilibrium configurations via frequency calculations. Periodic boundary conditions were applied to model 2D layered systems, followed by structural and cell optimizations for stacked 3D models. The 2D networks were constructed using the plane-wave QUANTUM ESPRESSO atomistic simulation code [5] with the GGA-PBESol exchange-correlation functional [6], Grimme DFT-D3 vdW corrections [7], and ultra-soft pseudopotentials [8]. Brillouin zone sampling employed optimal Monkhorst-Pack grids of [2×2×1] (2D) and [2×2×8] (3D) [9], with plane-wave cutoffs of 50 Ry (for wave functions) and 350 Ry (for electron density). Atomic relaxations and cell optimizations used a conjugate gradient algorithm, reducing forces below 0.02 eV $Å^{-1}$ and the net cell strain below 0.1 GPa.

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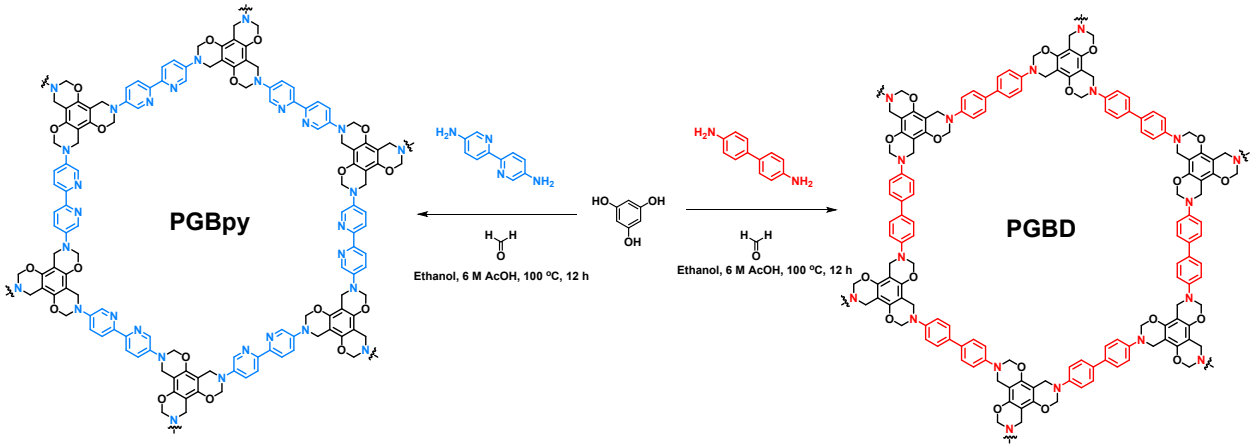
Section S2. Synthesis of PGBpy and PGBD

PGBpy or PGBD: To a thick-walled pressure tube, Bpy (0.22 g, 1.18 mmol) or BD (0.21 g, 1.18 mmol) and phloroglucinol were (0.10 g, 0.79 mmol) were mixed together in 5 mL of ethanol. After sonication for 5 minutes, 50 µL of 6 M acetic acid was added followed by addition of 37% of aqueous formaldehyde (2.37 mmol) solution. After performing sonication for 15 minutes, the tube was subjected to heating at 100 °C for 12 h to afford PGBpy as solid. The obtained material was purified by Soxhlet using THF and methanol. The obtained COFs were dried in an oven at 90 °C for 12 h prior to characterization studies. Yield (62%).



Scheme 1. Synthesis procedure of PGBpy and PGBD.

Section S3. Gold adsorption studies

Adsorption isotherm: 20 mL $AuCl_3$ solutions with concentrations ranging from 1 to 2000 mg L^{-1} was allowed to adsorb with 2 mg of COF until reaches equilibrium. The samples were filtered using 0.45 µm Nylon syringe filters and change in metal concentrations were monitored *via* ICP-MS analysis.

Adsorption constant was calculated using the following equation.

$$Q_e = (C_0\text{-}C_e) \times V/M$$

Where C_0 and C_e are the initial and equilibrium concentrations, M is the mass of adsorbent in g, and V is the volume of solution in litre.

Linear Langmuir isotherm fitting was done using the following equation.

$$C_e/Q_e = (Q_m \times K_a)^{-1} + C_e/Q_m$$

Linear Freundlich isotherm fitting was done using the following equation.

$$\ln Q_e = \ln K_f + 1/n \ln C_e$$

Where Q_m is the maximum adsorption capacity, K_a, n and K_f are the adsorption constants.

Adsorption kinetics: Into a 100 mL, 50 mg L^{-1} $AuCl_3$ solution, 10 mg of COF was added. Several samplings were collected with respect to time from 0 to 48 hours and filtered using 0.45 µm Nylon syringe filters. The filtrate samples were analysed using ICP-MS to obtain residual metal concentration.

Uptake efficiency was calculated using the following equation.

$$R_e\ (\%) = ((C_0\text{-}C_e) \times 100)/C_e$$

Pseudo first oder kinetic fittings were done using the following equation.

$$\ln(Q_e\text{-}Q_t) = \ln Q_e - k_1 t$$

Pseudo second order fittings were done using the following equation.

$$t/Q_t = (k_2\, Q_e^2)^{-1} + t/Q_e$$

Where, t is the time (min) and k_1 and k_2 are the pseudo first and second order rate constants, Q_e and Q_t are the adsorption capacity (mg g^{-1}) at equilibrium and time t respectively.

Selectivity test: 100 mL of mixed metal ions solution with 50 mg L^{-1} each of Au^{3+}, Al^{3+}, Cr^{3+}, Co^{3+}, Cd^{2+}, Zn^{2+} and Cu^{2+} was freshly prepared. 10 mg COF was added allowed to adsorb for 48 hours. Samplings were done at specific time intervals. The samples were filtered using 0.45 µm Nylon syringe filters and change in metal concentrations were monitored *via* ICP-MS analysis.

The distribution co-efficient (K_d) of each metal ions (in L g^{-1}) towards the PGBpy COF was calculated as follows;

$$K_d = ((C_0\text{-}C_e) \times V)/M \times C_e = Q_e/C_e$$

Additionally, the selectivity of COFs towards Au ions were determined by calculating the separation factor ($\alpha_{(Au/M)}$) of Au ions with respect to each competing metal ions.

$$\alpha_{(Au/M)} = K_d(Au)/K_d(M)$$

Where, M is the competing metal ion.

***p*H study:** 2 mg each of COF were added to 10 mL 50 mg L^{-1} $AuCl_3$ solutions prepared at varying *p*Hs (2,4,6,8,10 and 12) and stirred for 48 hours. The initial and final concentrations of the $AuCl_3$ solutions were analysed using ICP-MS after filtering the samples using 0.45 µm Nylon syringe filters. Subsequently, uptake efficiencies were calculated.

Regeneration experiment: First, 50 mL, 20 mg L^{-1} $AuCl_3$ solution were added with 10 mg of COF and allowed to stir for 48 hours. The gold adsorbed COF was thoroughly washed and dried. For desorption, the gold adsorbed COF was added into the stripping solution (mixed solution of 50 mL, 1M Thiourea and 1M HCl) and allowed stir for 12 hours. The regenerated COF was washed with DI water for several times and reused for further adsorption cycles. The experiment was repeated for up to 10 cycles for PGBpy and 5 cycles for PGBD. Residual metal concentrations were analyzed after each adsorption and respective uptake efficiencies were calculated.

E-waste analysis: the e-waste leaching solution was prepared by soaking the central processing unit (CPU) in 50 mL aqua regia for 24 hours. The leaching solution was further diluted to a *p*H = 2. A 20 mL e-waste leaching solution was treated with 2 mg COF with constant stirring for 48 hours. The samples were filtered using 0.45 µm Nylon syringe filters and change in metal concentrations were monitored *via* ICP-MS analysis.

Section S4. FTIR spectroscopic characterization studies

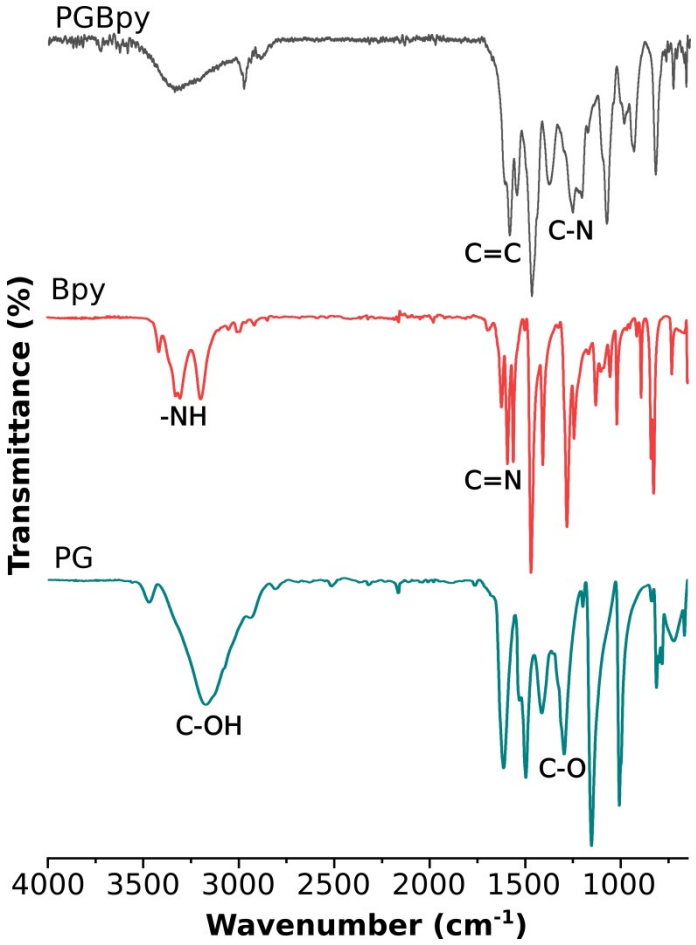


Figure S1. Comparison of FTIR spectra of **PGBpy** with starting material i.e. **Bpy** and **PG** suggest the no contamination from starting material in the final **PGBpy** product.

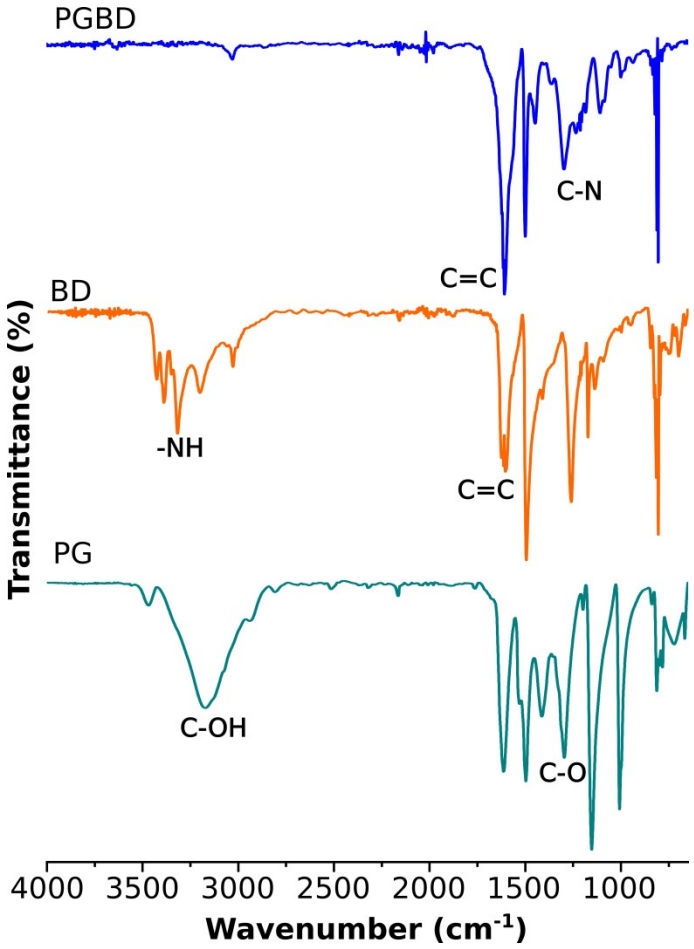


Figure S2. Comparison of FTIR spectra of **PGBD** with starting material i.e. **BD** and **PG** suggest the no contamination from starting material in the final **PGBD** product.

Section S5. PXRD and Pawley refinement studies

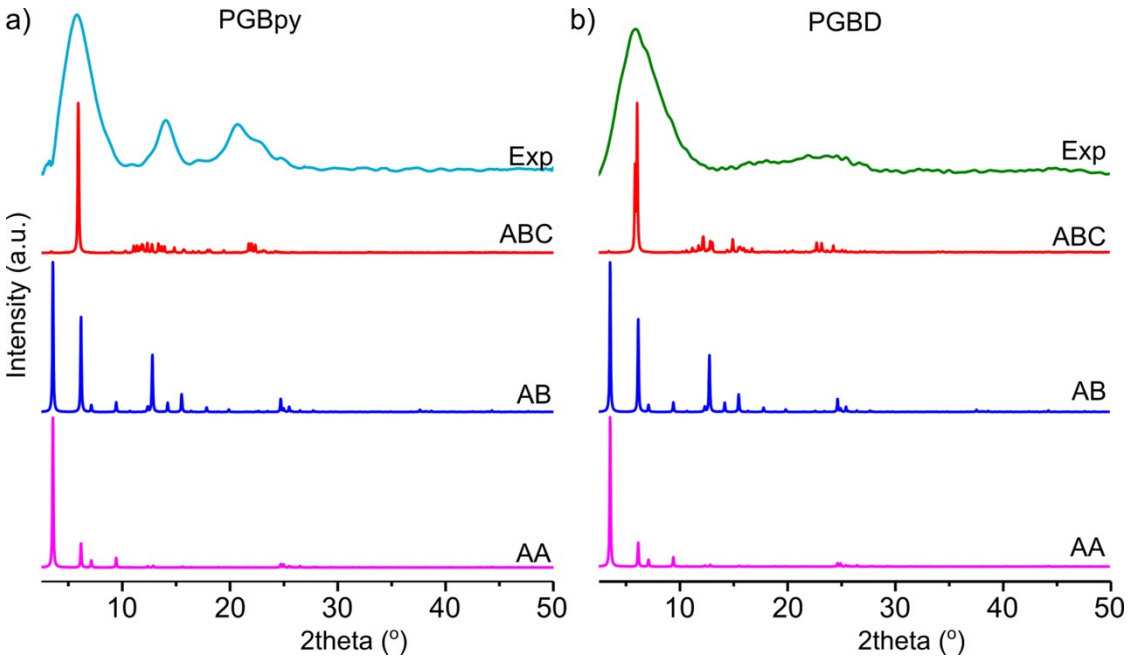


Figure S3. Comparison of experimental PXRD of a) PGBpy and b) PGBD with their respective pxrd pattern generated from simulated model showed good agreement with ABC model while disagreement with eclipsed AA and staggered AB models.

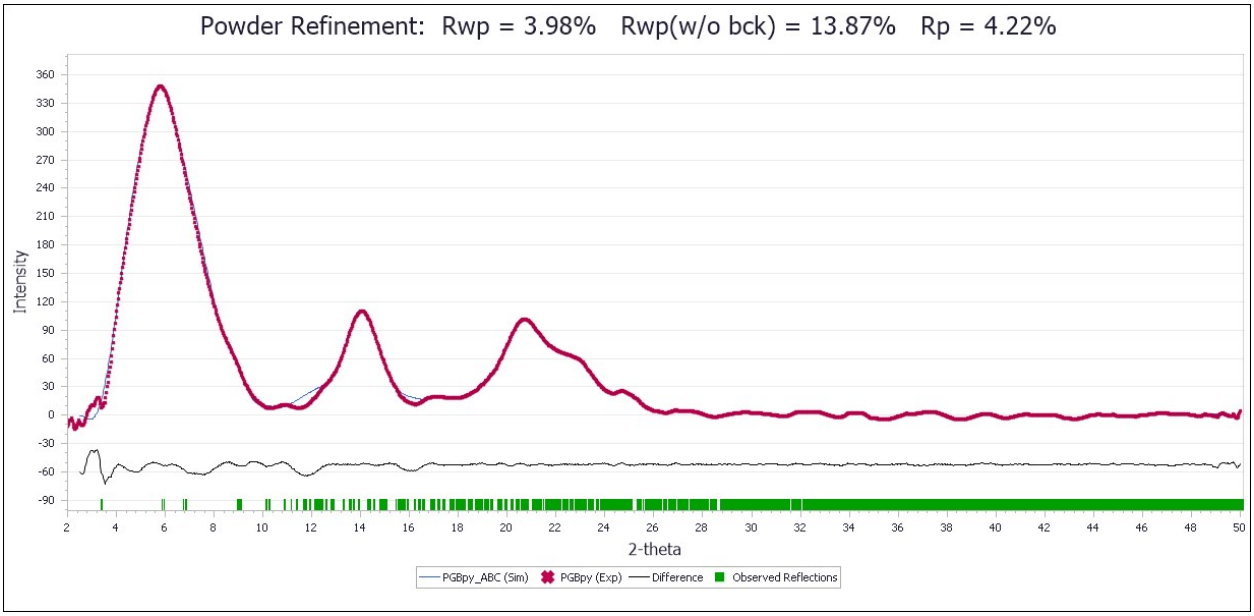


Figure S4. Experimental PXRD pattern of **PGBpy** after Pawley refinement studies shows a good agreement with the simulated ABC model structure.

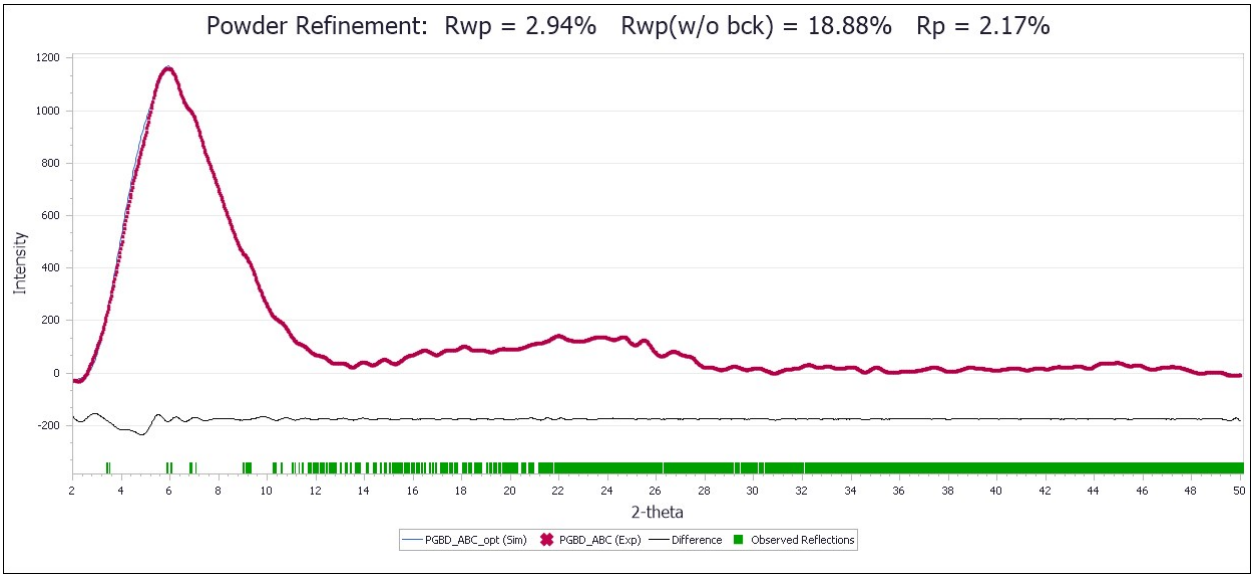


Figure S5. Experimental PXRD pattern of **PGBD** after Pawley refinement studies shows a good agreement with the simulated ABC model structure.

Section S6. Fractional atomic coordinates and unit cell parameters

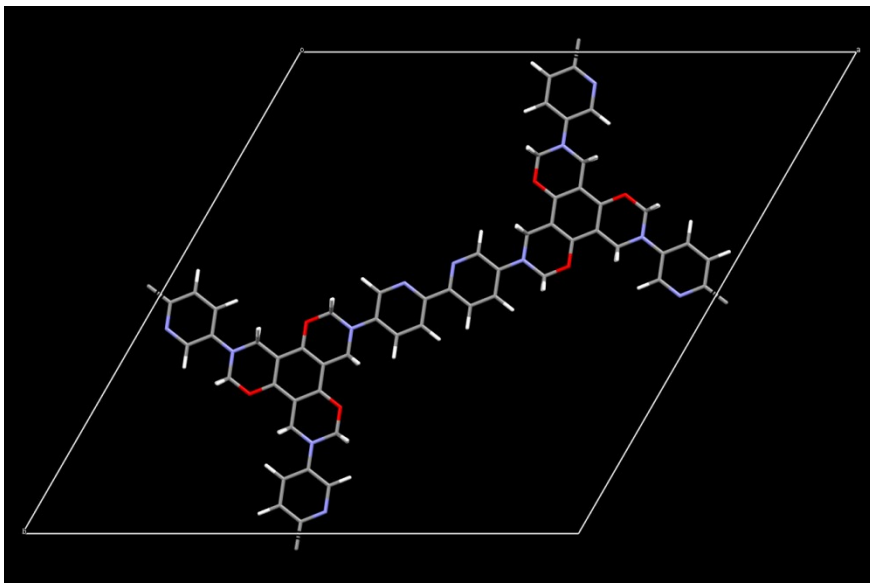


Figure S6. Unit cell structure of **PGBpy** calculated for eclipsed AA model.

Table S1. Fractional atomic coordinates and unit cell parameters of **PGBpy**calculated for eclipsed AA model.

PGBpy: Model **AA**; Space group***P*1**											
Unit cell parameters: a = 28.6 Å, b = 28.6 Å, c = 3.6 Å; α = 90°, β = 90°, γ = 120°											
Atoms	X	Y	Z	**Atoms**	X	Y	Z	**Atoms**	X	Y	Z
C1	1.5081	-0.96873	0	**N41**	1.18937	-0.37759	0	**H81**	1.78509	-0.56867	-0.25856
N2	1.56251	-0.93469	0	**C42**	1.13495	-0.41162	0	**H82**	1.6488	-0.46482	0
C3	1.58297	-0.88026	0	**C43**	1.37276	-0.22141	0	**H83**	1.58638	-0.42731	0
C4	1.54902	-0.85987	0	**N44**	1.42686	-0.18775	0	**H84**	1.51158	-0.62691	0
C5	1.4946	-0.89391	0	**C45**	1.44732	-0.13332	0	**H85**	1.54718	-0.4038	0
C6	1.47414	-0.94834	0	**C46**	1.10099	-0.39123	0	**H86**	1.48476	-0.36628	0
N7	1.56916	-0.80581	0	**N47**	1.04658	-0.42527	0	**H87**	1.34757	-0.5285	0
C8	1.62358	-0.77178	0	**C48**	1.02611	-0.4797	0	**H88**	1.4273	-0.35385	-0.2522
C9	1.64404	-0.71734	0	**C49**	1.06007	-0.50009	0	**H89**	1.4256	-0.35279	0.25856
C10	1.69846	-0.68331	0	**C50**	1.11449	-0.46605	0	**H90**	1.21294	-0.42556	0.25205
C11	1.7186	-0.62925	0	**O51**	1.26393	-0.28949	0	**H91**	1.21116	-0.42452	-0.25856
C12	1.68465	-0.60886	0	**O52**	1.44068	-0.2622	0	**H92**	1.3556	-0.21103	0.25225
C13	1.63055	-0.64252	0	**O53**	1.73241	-0.7037	0	**H93**	1.35833	-0.2093	-0.25856
C14	1.61008	-0.69695	0	**O54**	1.55567	-0.73099	0	**H94**	1.11809	-0.34568	0
C15	1.59684	-0.62228	0	**O55**	1.70511	-0.55443	0	**H95**	1.04298	-0.54565	0
N16	1.61673	-0.56808	0	**O56**	1.29123	-0.43876	0	**H96**	1.14298	-0.48311	0
C17	1.58278	-0.54769	0	**C57**	1.20983	-0.32316	0	**H97**	1.19266	-0.31277	0.25225
C18	1.77302	-0.59521	0	**C58**	1.46082	-0.20814	0	**H98**	1.1954	-0.31105	-0.25856
N19	1.80698	-0.6156	0	**C59**	1.32519	-0.45915	0	**H99**	1.48839	-0.19088	0.25205
C20	1.86139	-0.58156	0	**C60**	1.6714	-0.53419	0	**H100**	1.48736	-0.19369	-0.25856
C21	1.60324	-0.49326	0	**C61**	1.78651	-0.67003	0	**H101**	1.31481	-0.48673	0.25205
C22	1.56928	-0.47286	0	**C62**	1.53521	-0.78542	0	**H102**	1.31303	-0.48569	-0.25856
C23	1.51487	-0.5069	0	**C63**	1.89535	-0.60196	0	**H103**	1.68183	-0.50658	0.25195
N24	1.49472	-0.56096	0	**C64**	1.94977	-0.56792	0	**H104**	1.68362	-0.50764	-0.25856
C25	1.52868	-0.58135	0	**C65**	1.96991	-0.51386	0	**H105**	1.80368	-0.68041	0.25225
C26	1.48116	-0.48666	0	**N66**	1.93595	-0.49347	0	**H106**	1.80094	-0.68214	-0.25856
C27	1.50162	-0.43223	0	**C67**	1.88185	-0.52713	0	**H107**	1.50765	-0.80263	0.2522
C28	1.46766	-0.41184	0	**C68**	1.50174	-0.09928	0	**H108**	1.50867	-0.79987	-0.25856
C29	1.41325	-0.44588	0	**N69**	1.5222	-0.04485	0	**H109**	1.87826	-0.64751	0

C30	1.3931	-0.49993	0	**C70**	1.48825	-0.02446	0	**H110**	1.97826	-0.58498	0
N31	1.42706	-0.52033	0	**C71**	1.43383	-0.0585	0	**H111**	1.8535	-0.50992	0
N32	1.37929	-0.42549	0	**C72**	1.41337	-0.11293	0	**H112**	1.53023	-0.11634	0
C33	1.39975	-0.37106	0	**H73**	1.62854	-0.85183	0	**H113**	1.40534	-0.04144	0
C34	1.3658	-0.35067	0	**H74**	1.46611	-0.87685	0	**H114**	1.36781	-0.14136	0
C35	1.38626	-0.29624	0	**H75**	1.42858	-0.97677	0	**C1**	1.5081	0.03127	0
C36	1.3523	-0.27584	0	**H76**	1.6408	-0.78212	-0.2521	**C48**	2.02611	-0.4797	0
C37	1.29788	-0.30988	0	**H77**	1.64187	-0.77932	0.25856	**C65**	0.96991	-0.51386	0
C38	1.27742	-0.36431	0	**H78**	1.56923	-0.63964	0.2518	**C70**	1.48825	-1.02446	0
C39	1.31138	-0.3847	0	**H79**	1.5703	-0.63673	-0.25856				
C40	1.22332	-0.39798	0	**H80**	1.78335	-0.56766	0.2522				

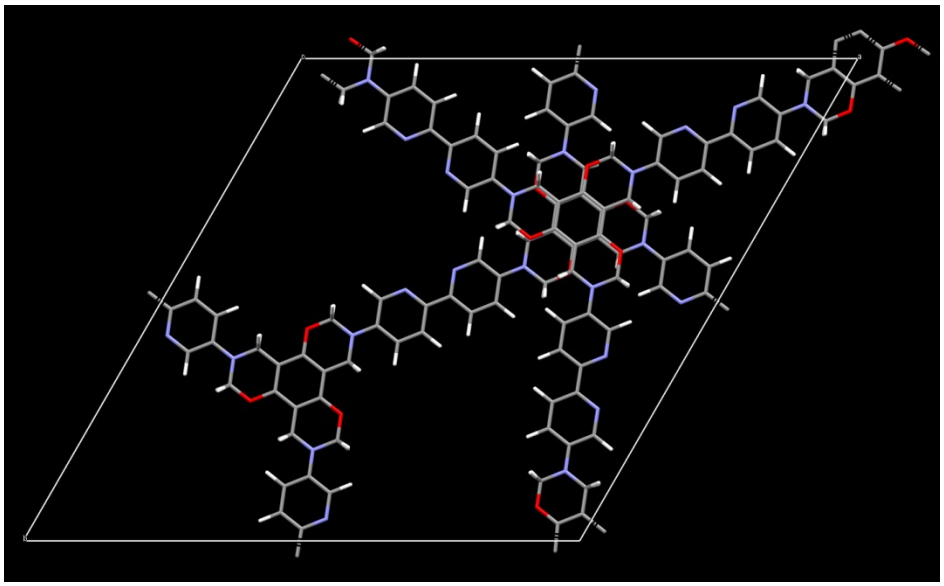


Figure S7. Unit cell structure of **PGBpy** calculated for staggered ABC model.

Table S 2. Fractional atomic coordinates and unit cell parameters of PGBpy calculated for staggered AB model.

PGBpy: Model **AB**; Space group ***P*1**											
Unit cell parameters: a = 28.6 Å, b = 28.6 Å, c = 7.2 Å; α = 90°, β = 90°, γ = 120°											
Atoms	X	Y	Z	**Atoms**	X	Y	Z	**Atoms**	X	Y	Z
C1	2.03481	-1.0195	-0.76372	**H195**	1.76163	-0.69104	-0.88969	**C111**	0.31087	0.61491	0.70833
C2	2.05509	-0.9651	-0.76372	**H196**	1.75984	-0.68996	-0.63444	**C112**	0.22282	0.60164	0.70833
C3	2.02098	-0.94489	-0.76372	**H197**	1.54683	-0.7639	-0.63762	**N113**	0.18886	0.62203	0.70833
C4	1.9666	-0.97908	-0.76372	**H198**	1.54508	-0.7629	-0.89299	**C114**	0.13444	0.58799	0.70833
C5	1.93249	-0.95886	-0.76372	**H199**	1.68877	-0.54936	-0.63759	**C115**	0.37226	0.7782	0.70833
N6	1.95277	-0.90446	-0.76372	**H200**	1.69151	-0.54762	-0.89299	**N116**	0.42636	0.81186	0.70833
C7	1.91867	-0.88425	-0.76372	**H201**	1.45116	-0.68445	-0.76372	**C117**	0.44682	0.86629	0.70833
C8	1.93895	-0.82984	-0.76372	**H202**	1.37695	-0.88447	-0.76372	**C118**	0.10049	0.60838	0.70833
C9	1.90484	-0.80963	-0.76372	**H203**	1.47691	-0.82166	-0.76372	**N119**	0.04607	0.57434	0.70833
C10	1.85045	-0.84382	-0.76372	**H204**	1.18835	-0.84946	-0.76372	**C120**	0.02561	0.51991	0.70833
N11	1.83017	-0.89822	-0.76372	**H205**	1.2141	-0.98666	-0.76372	**C121**	0.05956	0.49952	0.70833
C12	1.86428	-0.91844	-0.76372	**H206**	1.31405	-0.92385	-0.76372	**C122**	0.11398	0.53356	0.70833
C13	1.81635	-0.82361	-0.76372	**H207**	1.11946	-0.90659	-0.88848	**O123**	0.26342	0.71012	0.70833
C14	1.83663	-0.7692	-0.76372	**H208**	1.11567	-0.90892	-0.63444	**O124**	0.44017	0.73742	0.70833
C15	1.80227	-0.74884	-0.76372	**H209**	1.13852	-1.02037	-0.63621	**O125**	0.73191	0.29592	0.70833
C16	1.74788	-0.78303	-0.76372	**H210**	1.13691	-1.02138	-0.89299	**O126**	0.55516	0.26862	0.70833
C17	1.7276	-0.83743	-0.76372	**H211**	1.52594	-0.6515	-0.63766	**O127**	0.7046	0.44518	0.70833
N18	1.76196	-0.8578	-0.76372	**H212**	1.52874	-0.64973	-0.89299	**O128**	0.29073	0.56085	0.70833

N19	1.71403	-0.76297	-0.76372	**H213**	1.82213	-0.5283	-0.63762	**C129**	0.20932	0.67646	0.70833
C20	1.73406	-0.70842	-0.76372	**H214**	1.82113	-0.53106	-0.89299	**C130**	0.46031	0.79147	0.70833
C21	1.69995	-0.6882	-0.76372	**H215**	1.64905	-0.8246	-0.63774	**C131**	0.32468	0.54046	0.70833
C22	1.72024	-0.6338	-0.76372	**H216**	1.64725	-0.82355	-0.89299	**C132**	0.6709	0.46543	0.70833
C23	1.68613	-0.61359	-0.76372	**H217**	2.01747	-0.84278	-0.63747	**C133**	0.78601	0.32958	0.70833
C24	1.63174	-0.64778	-0.76372	**H218**	2.01915	-0.84374	-0.89299	**C134**	0.5347	0.21419	0.70833
C25	1.61146	-0.70218	-0.76372	**H219**	1.86378	-0.45369	-0.76372	**C135**	0.89484	0.39766	0.70833
C26	1.64556	-0.72239	-0.76372	**H220**	1.7383	-0.37902	-0.76372	**C136**	0.94926	0.4317	0.70833
C27	1.55707	-0.73637	-0.76372	**H221**	1.70117	-0.47954	-0.76372	**C137**	0.9694	0.48575	0.70833
N28	1.52296	-0.71616	-0.76372	**H222**	1.96153	-0.19023	-0.76372	**N138**	0.93545	0.50614	0.70833
C29	1.46857	-0.75034	-0.76372	**H223**	1.79892	-0.21609	-0.76372	**C139**	0.88135	0.47248	0.70833
C30	1.7061	-0.55956	-0.76372	**H224**	1.76172	-0.31596	-0.76372	**C140**	0.50124	0.90033	0.70833
N31	1.76048	-0.52537	-0.76372	**H225**	1.97391	-0.12047	-0.88977	**N141**	0.5217	0.95476	0.70833
C32	1.78077	-0.47097	-0.76372	**H226**	1.97497	-0.11767	-0.63444	**C142**	0.48774	0.97515	0.70833
C33	1.43421	-0.72998	-0.76372	**H227**	1.84057	-0.14147	-0.88982	**C143**	0.43332	0.94112	0.70833
N34	1.37982	-0.76417	-0.76372	**H228**	1.84228	-0.14252	-0.63444	**C144**	0.41286	0.88669	0.70833
C35	1.35954	-0.81857	-0.76372	**C1**	2.03481	-0.0195	-0.76372	**H145**	0.62803	0.14779	0.70833
C36	1.3939	-0.83894	-0.76372	**C2**	1.05509	-0.9651	-0.76372	**H146**	0.4656	0.12276	0.70833
C37	1.44829	-0.80475	-0.76372	**C4**	1.9666	0.02092	-0.76372	**H147**	0.42807	0.02284	0.70833
C38	1.30572	-0.85254	-0.76372	**C45**	2.10819	-0.93474	-0.76372	**H148**	0.6403	0.2175	0.58227
N39	1.27136	-0.83218	-0.76372	**O48**	1.06891	-1.03972	-0.76372	**H149**	0.64137	0.2203	0.8376
C40	1.21697	-0.86636	-0.76372	**C51**	2.12227	-1.00951	-0.76372	**H150**	0.56873	0.35997	0.83423
C41	1.19669	-0.92077	-0.76372	**C69**	1.97689	-1.05581	-0.76372	**H151**	0.5698	0.36288	0.57905
C42	1.23105	-0.94113	-0.76372	**C70**	1.94278	-1.0356	-0.76372	**H152**	0.78284	0.43195	0.83443
C43	1.28543	-0.90694	-0.76372	**C73**	0.50759	0.03088	0.70833	**H153**	0.78459	0.43094	0.57905
N44	1.1423	-0.95496	-0.76372	**N74**	0.56201	0.06492	0.70833	**H154**	0.64829	0.53479	0.70833
C45	1.10819	-0.93474	-0.76372	**C75**	0.58247	0.11935	0.70833	**H155**	0.58587	0.57231	0.70833
O46	1.59763	-0.62756	-0.76372	**C76**	0.54851	0.13975	0.70833	**H156**	0.51108	0.37271	0.70833
O47	1.77431	-0.59999	-0.76372	**C77**	0.49409	0.10571	0.70833	**H157**	0.54668	0.59582	0.70833
O48	2.06891	-1.03972	-0.76372	**C78**	0.47363	0.05128	0.70833	**H158**	0.48425	0.63333	0.70833
O49	2.04095	-0.89086	-0.76372	**N79**	0.56866	0.1938	0.70833	**H159**	0.34706	0.47111	0.70833
O50	1.62528	-0.7768	-0.76372	**C80**	0.62307	0.22784	0.70833	**H160**	0.4268	0.64576	0.58223
C51	1.12227	-1.00951	-0.76372	**C81**	0.64353	0.28227	0.70833	**H161**	0.42509	0.64682	0.8376
C52	1.54324	-0.66175	-0.76372	**C82**	0.69795	0.31631	0.70833	**H162**	0.21243	0.57405	0.83435
C53	1.79459	-0.54558	-0.76372	**C83**	0.7181	0.37036	0.70833	**H163**	0.21066	0.5751	0.57905
C54	1.65939	-0.79701	-0.76372	**C84**	0.68414	0.39075	0.70833	**H164**	0.35509	0.78858	0.83445
C55	2.00716	-0.87027	-0.76372	**C85**	0.63004	0.35709	0.70833	**H165**	0.35783	0.79031	0.57905
C56	1.83516	-0.43678	-0.76372	**C86**	0.60958	0.30266	0.70833	**H166**	0.11758	0.65394	0.70833
N57	1.85544	-0.38238	-0.76372	**C87**	0.59633	0.37733	0.70833	**H167**	0.04247	0.45397	0.70833
C58	1.82133	-0.36216	-0.76372	**N88**	0.61623	0.43154	0.70833	**H168**	0.14247	0.5165	0.70833
C59	1.76669	-0.3962	-0.76372	**C89**	0.58227	0.45193	0.70833	**H169**	0.19216	0.68684	0.83445
C60	1.74666	-0.45075	-0.76372	**C90**	0.77251	0.4044	0.70833	**H170**	0.19489	0.68857	0.57905
C61	1.84137	-0.30761	-0.76372	**N91**	0.80647	0.38401	0.70833	**H171**	0.48788	0.80873	0.83435
N62	1.89601	-0.27357	-0.76372	**C92**	0.86089	0.41805	0.70833	**H172**	0.48685	0.80592	0.57905
C63	1.91604	-0.21902	-0.76372	**C93**	0.60273	0.50636	0.70833	**H173**	0.3143	0.51288	0.83435
C64	1.88193	-0.19881	-0.76372	**C94**	0.56878	0.52675	0.70833	**H174**	0.31253	0.51392	0.57905
C65	1.82754	-0.233	-0.76372	**C95**	0.51436	0.49271	0.70833	**H175**	0.68132	0.49303	0.8343
C66	1.80726	-0.2874	-0.76372	**N96**	0.49422	0.43866	0.70833	**H176**	0.68312	0.49197	0.57905
N67	1.90222	-0.1444	-0.76372	**C97**	0.52817	0.41827	0.70833	**H177**	0.80318	0.3192	0.83445
C68	1.95661	-0.11021	-0.76372	**C98**	0.48065	0.51295	0.70833	**H178**	0.80044	0.31747	0.57905
C69	1.97689	-0.05581	-0.76372	**C99**	0.50111	0.56738	0.70833	**H179**	0.50715	0.19699	0.83443
C70	1.94278	-0.0356	-0.76372	**C100**	0.46716	0.58777	0.70833	**H180**	0.50816	0.19974	0.57905
O71	1.88839	-0.06979	-0.76372	**C101**	0.41274	0.55374	0.70833	**H181**	0.87775	0.3521	0.70833
C72	1.86811	-0.12419	-0.76372	**C102**	0.3926	0.49968	0.70833	**H182**	0.97775	0.41464	0.70833
H187	1.90495	-0.97614	-0.63762	**N103**	0.42655	0.47929	0.70833	**H183**	0.85299	0.4897	0.70833
H188	1.90596	-0.97339	-0.89299	**N104**	0.37879	0.57413	0.70833	**H184**	0.52973	0.88328	0.70833
H189	1.98449	-0.80128	-0.76372	**C105**	0.39925	0.62856	0.70833	**H185**	0.40483	0.95817	0.70833
H190	1.92179	-0.7641	-0.76372	**C106**	0.36529	0.64895	0.70833	**H186**	0.3673	0.85825	0.70833
H191	1.84733	-0.96397	-0.76372	**C107**	0.38575	0.70338	0.70833	**C73**	0.50759	1.03088	0.70833

H192	1.88217	-0.74064	-0.76372	**C108**	0.3518	0.72377	0.70833	**C120**	1.02561	0.51991	0.70833
H193	1.81922	-0.70331	-0.76372	**C109**	0.29738	0.68973	0.70833	**C137**	-0.0306	0.48575	0.70833
H194	1.68206	-0.86599	-0.76372	**C110**	0.27692	0.6353	0.70833	**C142**	0.48774	-0.02485	0.70833

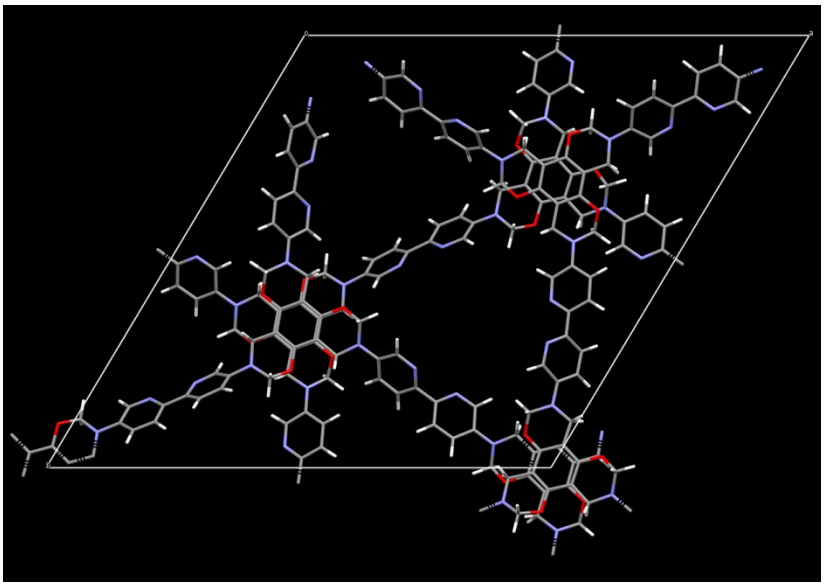


Figure S8. Unit cell structure of **PGBpy** calculated for ABC model.

Table S3. Fractional atomic coordinates and unit cell parameters of **PGBpy** calculated for ABC model.

PGBpy: Model **ABC**; Space group ***P*1**											
Unit cell parameters: a = 30.10 Å, b = 30.04 Å, c = 8.15 Å; α = 92.57°, β = 92.44°, γ = 120.67°											
Atoms	X	Y	Z	**Atoms**	X	Y	Z	**Atoms**	X	Y	Z
C1	1.91148	-0.90082	0.09705	**C75**	1.10618	-0.79999	0.46508	**C144**	1.07966	-0.0268	0.48746
C2	1.93182	-0.84765	0.1391	**C76**	1.14568	-0.76116	0.57562	**C145**	0.51721	0.03452	0.82755
N3	1.8995	-0.82834	0.15089	**N77**	1.16277	-0.7103	0.55757	**N146**	0.56257	0.06158	0.75644
C4	1.84681	-0.85895	0.12532	**C78**	1.14286	-0.69465	0.43422	**C147**	0.58272	0.11219	0.72656
C5	1.82477	-0.91268	0.09322	**C79**	1.10376	-0.73241	0.31955	**C148**	0.55628	0.13842	0.76578
C6	1.85705	-0.93337	0.0789	**C80**	1.08558	-0.78486	0.33597	**C149**	0.51053	0.11191	0.84475
C7	1.81458	-0.8345	0.13335	**C81**	1.16439	-0.63826	0.42303	**C150**	0.49084	0.06006	0.87532
N8	1.83493	-0.78738	0.21875	**N82**	1.21153	-0.60431	0.50404	**N151**	0.57498	0.1908	0.72233
C9	1.80822	-0.76193	0.22983	**C83**	1.23435	-0.55205	0.4997	**C152**	0.63085	0.2271	0.71912
C10	1.75776	-0.78394	0.15122	**C84**	1.20964	-0.53046	0.40841	**C153**	0.64308	0.28255	0.72103
C11	1.73632	-0.83202	0.06026	**C85**	1.16063	-0.56526	0.3245	**C154**	0.69497	0.32269	0.72296
C12	1.76453	-0.85742	0.05065	**C86**	1.13772	-0.61866	0.33347	**C155**	0.70737	0.37487	0.73674
N13	1.72824	-0.75826	0.16524	**N87**	1.23418	-0.47462	0.39893	**C156**	0.66742	0.3865	0.7366
C14	1.75425	-0.70183	0.15883	**C88**	1.29143	-0.44279	0.40971	**C157**	0.61503	0.34617	0.72863
C15	1.71646	-0.68252	0.15754	**C89**	1.31144	-0.38567	0.40208	**C158**	0.60277	0.29414	0.71889
C16	1.73561	-0.62893	0.16733	**C90**	1.36533	-0.35076	0.408	**C159**	0.57205	0.35876	0.73285
C17	1.70071	-0.61044	0.16787	**C91**	1.38456	-0.29714	0.41721	**N160**	0.59162	0.4147	0.72972
C18	1.64694	-0.64542	0.15947	**C92**	1.35003	-0.27835	0.41373	**C161**	0.55692	0.43451	0.75112
C19	1.62759	-0.69925	0.15057	**C93**	1.29607	-0.31325	0.406	**C162**	0.76358	0.41833	0.74776
C20	1.66245	-0.71775	0.15332	**C94**	1.27684	-0.36688	0.39949	**N163**	0.79928	0.39858	0.72867
C21	1.56959	-0.73697	0.14251	**C95**	1.25877	-0.29329	0.40972	**C164**	0.8548	0.43194	0.76736
N22	1.53967	-0.71048	0.15591	**N96**	1.28525	-0.23656	0.41133	**C165**	0.55568	0.46984	0.64645
C23	1.48358	-0.74071	0.14245	**C97**	1.25431	-0.21223	0.41647	**N166**	0.52427	0.48963	0.67141
C24	1.72069	-0.55304	0.18456	**C98**	1.44217	-0.25932	0.44259	**C167**	0.49254	0.4764	0.79549
N25	1.77775	-0.52197	0.19405	**N99**	1.47379	-0.28409	0.43051	**C168**	0.49164	0.44002	0.90037
C26	1.80322	-0.46704	0.17232	**C100**	1.53003	-0.25097	0.44234	**C169**	0.52396	0.41957	0.87816

C27	1.45569	-0.7362	0.26757	**C101**	1.25286	-0.18323	0.28912	**C170**	0.4607	0.50142	0.81425
C28	1.40152	-0.7653	0.25427	**C102**	1.222	-0.16061	0.29384	**N171**	0.46108	0.53282	0.69819
C29	1.37463	-0.79917	0.11363	**C103**	1.19262	-0.16664	0.42817	**C172**	0.43383	0.5579	0.70619
N30	1.4026	-0.80335	-0.00573	**N104**	1.19459	-0.19527	0.54984	**C173**	0.40363	0.55203	0.83702
C31	1.45554	-0.77542	0.00513	**C105**	1.22416	-0.21789	0.54716	**C174**	0.40275	0.52018	0.95851
C32	1.317	-0.83231	0.09442	**C106**	1.15889	-0.14376	0.4421	**C175**	0.43109	0.49495	0.94806
C33	1.28479	-0.82275	0.19066	**C107**	1.16117	-0.1063	0.34037	**N176**	0.37385	0.57767	0.84642
C34	1.23119	-0.85708	0.17415	**C108**	1.12802	-0.0868	0.35919	**C177**	0.40042	0.63442	0.84383
C35	1.20886	-0.90053	0.05934	**C109**	1.09287	-0.10354	0.48065	**C178**	0.3631	0.65451	0.8484
C36	1.24227	-0.90725	-0.04029	**C110**	1.09242	-0.14053	0.58161	**C179**	0.38212	0.70827	0.8593
N37	1.29455	-0.87378	-0.01954	**N111**	1.12481	-0.15932	0.55977	**C180**	0.34688	0.7264	0.84983
O38	1.61311	-0.62584	0.15866	**N112**	1.05922	-0.0824	0.50347	**C181**	0.29314	0.69125	0.83995
O39	1.78967	-0.59446	0.17707	**O113**	1.37029	-0.22455	0.42818	**C182**	0.27411	0.63786	0.83704
O40	1.64278	-0.77141	0.15081	**O114**	1.39947	-0.36989	0.41871	**C183**	0.30896	0.6194	0.84081
C41	1.56618	-0.65717	0.23194	**O115**	0.97171	-0.10183	0.51582	**C184**	0.21633	0.59998	0.8246
C42	1.80674	-0.54532	0.26303	**O116**	1.22337	-0.40064	0.40424	**N185**	0.1848	0.62505	0.83415
C43	1.67721	-0.78527	0.23016	**C117**	1.01055	-0.11201	0.58112	**C186**	0.12841	0.59274	0.8303
C44	1.85317	-0.44023	0.11639	**C118**	1.33725	-0.20834	0.35364	**C187**	0.36631	0.78365	0.85312
C45	1.87749	-0.38691	0.10086	**C119**	1.44894	-0.33801	0.3589	**N188**	0.42323	0.81558	0.88074
C46	1.85098	-0.36071	0.13612	**C120**	1.20366	-0.45217	0.33382	**C189**	0.4484	0.87109	0.87069
N47	1.80219	-0.38737	0.18516	**C121**	1.56096	-0.26239	0.3446	**C190**	0.0985	0.61012	0.90945
C48	1.77822	-0.43887	0.20504	**N122**	1.61342	-0.22989	0.35362	**C191**	0.04446	0.57908	0.90214
C49	1.87414	-0.30502	0.11854	**C123**	1.63793	-0.18503	0.4528	**C192**	0.01991	0.5294	0.82124
C50	1.92335	-0.26882	0.19477	**C124**	1.60904	-0.17187	0.55187	**N193**	0.04896	0.5124	0.74839
C51	1.94178	-0.2159	0.18761	**C125**	1.55541	-0.20511	0.548	**C194**	0.10154	0.54233	0.74972
C52	1.91159	-0.19897	0.10212	**C126**	1.6947	-0.15156	0.45972	**O195**	0.25904	0.71017	0.82434
C53	1.86318	-0.23717	0.02247	**N127**	1.72552	-0.17088	0.50587	**O196**	0.4361	0.74332	0.87698
N54	1.8456	-0.28829	0.03524	**C128**	1.77825	-0.1407	0.52566	**O197**	0.73395	0.31003	0.70904
N55	1.92946	-0.14418	0.09647	**C129**	1.80293	-0.08759	0.49889	**O198**	0.55024	0.25445	0.70951
C56	1.98547	-0.10702	0.09282	**C130**	1.77151	-0.06791	0.44252	**O199**	0.6806	0.43864	0.74592
C57	1.99792	-0.05198	0.07859	**C131**	1.71742	-0.09954	0.42565	**O200**	0.28886	0.56567	0.83107
C58	1.95901	-0.03934	0.09302	**N132**	1.85874	-0.05413	0.53233	**C201**	0.21057	0.6804	0.89153
O59	1.90889	-0.07701	0.12556	**C133**	1.89299	-0.076	0.53186	**C202**	0.45136	0.79268	0.9592
C60	1.89179	-0.12775	0.05374	**C134**	1.96391	0.01801	0.52555	**C203**	0.32232	0.55039	0.90798
C61	2.04911	-0.01281	0.05921	**O135**	1.92678	0.0335	0.53513	**C204**	0.64237	0.4475	0.66755
C62	2.0611	0.03895	0.05225	**C136**	1.88129	-0.00131	0.6102	**C205**	0.7781	0.34804	0.63596
C63	2.02128	0.05086	0.05643	**C137**	2.03936	-0.01128	0.50558	**C206**	0.53955	0.20502	0.6411
C64	1.97057	0.01187	0.08293	**C138**	2.05378	0.04105	0.50079	**C207**	0.8862	0.41121	0.81301
O65	2.03287	0.10192	0.03836	**C139**	2.01595	0.0557	0.50921	**C208**	0.94025	0.44276	0.8315
C66	1.98985	0.10575	-0.02813	**O140**	2.10558	0.07765	0.47835	**C209**	0.96297	0.49575	0.81102
N67	1.94536	0.07871	0.06964	**C141**	2.12272	0.12917	0.54368	**N210**	0.93202	0.51587	0.77571
C68	1.92816	0.02459	0.09922	**N142**	2.08675	0.14585	0.48464	**C211**	0.87928	0.48575	0.75418
O69	2.0881	-0.02573	0.05819	**C143**	2.03073	0.11152	0.49601	**C212**	0.49758	0.8989	0.81135
C70	2.13327	0.0088	-0.01818	**C144**	2.07966	-0.0268	0.48746	**C213**	0.52106	0.95239	0.79969
N71	2.15332	0.06283	0.04422	**H301**	1.16241	-0.77124	0.67758	**C214**	0.49507	0.97834	0.84677
C72	2.11663	0.08195	0.0464	**H302**	1.0879	-0.72202	0.2163	**N215**	0.44757	0.95066	0.90484
H259	1.97324	-0.82128	0.16188	**H303**	1.05605	-0.81359	0.2464	**C216**	0.42407	0.89877	0.91829
H260	1.78309	-0.93873	0.07937	**H304**	1.27177	-0.52803	0.56775	**H217**	0.61845	0.13122	0.66729
H261	1.839	-0.97474	0.05023	**H305**	1.13976	-0.55188	0.24897	**H218**	0.48987	0.1312	0.88203
H262	1.82625	-0.72508	0.30235	**H306**	1.09941	-0.6439	0.27146	**H219**	0.45491	0.04	0.93341
H263	1.69796	-0.84959	-0.00456	**H307**	1.30571	-0.45655	0.3084	**H220**	0.64425	0.21752	0.60662
H264	1.74754	-0.89395	-0.0234	**H308**	1.30842	-0.44694	0.52742	**H221**	0.65232	0.22319	0.82735
H265	1.77551	-0.69077	0.04683	**H309**	1.23677	-0.3062	0.51909	**H222**	0.55224	0.34421	0.84539
H266	1.78266	-0.68259	0.26795	**H310**	1.23034	-0.31076	0.30037	**H223**	0.54315	0.33791	0.6257
H267	1.56145	-0.76228	0.24476	**H311**	1.44998	-0.23876	0.56571	**H224**	0.77334	0.44094	0.86854
H268	1.55729	-0.76178	0.02559	**H312**	1.45316	-0.23045	0.35012	**H225**	0.76813	0.44429	0.64965
H269	1.70719	-0.54402	0.29836	**H313**	1.27499	-0.1788	0.18477	**H226**	0.57958	0.48171	0.54457
H270	1.70401	-0.54309	0.07735	**H314**	1.22105	-0.13955	0.19167	**H227**	0.46673	0.42711	0.99917
H271	1.47592	-0.71074	0.37715	**H315**	1.22449	-0.23974	0.6477	**H228**	0.52369	0.39284	0.96274

H272	1.3816	-0.7618	0.35545	**H316**	1.18843	-0.09124	0.24816	**H229**	0.43524	0.58174	0.60946
H273	1.47555	-0.77996	-0.09398	**H317**	1.13029	-0.05871	0.27736	**H230**	0.38053	0.51523	1.06282
H274	1.3002	-0.78923	0.27797	**H318**	1.06715	-0.15395	0.6799	**H231**	0.42974	0.47139	1.04544
H275	1.20777	-0.84965	0.25406	**H319**	1.01809	-0.10119	0.71509	**H232**	0.42142	0.64648	0.73215
H276	1.22706	-0.93904	-0.13456	**H320**	0.99496	-0.15436	0.55954	**H233**	0.4297	0.65251	0.9509
H277	1.5753	-0.6572	0.36492	**H321**	1.35518	-0.1659	0.3844	**H234**	0.20756	0.57398	0.92543
H278	1.54108	-0.63991	0.2169	**H322**	1.33413	-0.21583	0.21884	**H235**	0.20625	0.57643	0.706
H279	1.79991	-0.55077	0.39416	**H323**	1.4735	-0.35498	0.39039	**H236**	0.34868	0.79351	0.95321
H280	1.84926	-0.52044	0.25802	**H324**	1.44406	-0.33875	0.22386	**H237**	0.35296	0.79207	0.73553
H281	1.68213	-0.77427	0.36375	**H325**	1.16267	-0.47494	0.36379	**H238**	0.11631	0.64737	0.97936
H282	1.6594	-0.82802	0.21273	**H326**	1.20441	-0.45213	0.19857	**H239**	0.02212	0.59327	0.96219
H283	1.87321	-0.46031	0.08181	**H327**	1.5437	-0.29647	0.25862	**H240**	0.12169	0.52636	0.68664
H284	1.91599	-0.36656	0.05818	**H328**	1.62803	-0.1367	0.6338	**H241**	0.2169	0.68481	1.02682
H285	1.7398	-0.45741	0.24771	**H329**	1.5342	-0.19469	0.62873	**H242**	0.18613	0.69692	0.85369
H286	1.94636	-0.28134	0.26413	**H330**	1.80053	-0.15805	0.56702	**H243**	0.44213	0.78758	1.08863
H287	1.97908	-0.18871	0.25217	**H331**	1.78848	-0.02815	0.41166	**H244**	0.49411	0.81814	0.95987
H288	1.83904	-0.2268	-0.05018	**H332**	1.69351	-0.08365	0.38606	**H245**	0.32631	0.55956	1.04235
H289	1.99968	-0.11923	-0.01246	**H333**	1.88083	-0.10466	0.42401	**H246**	0.30423	0.50773	0.88265
H290	2.00698	-0.10724	0.20653	**H334**	1.88949	-0.09611	0.64502	**H247**	0.65544	0.48927	0.69177
H291	1.88602	-0.12868	-0.08175	**H335**	1.85363	0.01302	0.60453	**H248**	0.6393	0.43867	0.53283
H292	1.85373	-0.15413	0.10042	**H336**	1.89214	-0.00117	0.74135	**H249**	0.80684	0.33524	0.6288
H293	1.97826	0.08757	-0.15587	**H337**	2.16227	0.15516	0.50594	**H250**	0.76619	0.35101	0.50819
H294	2.00234	0.14729	-0.0337	**H338**	2.12531	0.13099	0.67938	**H251**	0.49816	0.17596	0.6522
H295	1.89489	-0.0019	0.00992	**H339**	2.00847	0.11327	0.3859	**H252**	0.5451	0.20687	0.50829
H296	1.91468	0.01706	0.2236	**H340**	2.01951	0.1253	0.6057	**H253**	0.86915	0.37059	0.83342
H297	2.12344	0.0047	-0.15192	**H341**	2.11313	-0.00377	0.57998	**H254**	0.96411	0.42608	0.86257
H298	2.16273	-0.00282	0.00651	**H342**	2.09402	-0.01642	0.36587	**H255**	0.85689	0.50378	0.7219
H299	2.11947	0.10268	-0.06448	**C73**	1.94928	-0.03474	0.5253	**H256**	0.51744	0.8792	0.77076
H300	2.12641	0.10948	0.15545	**C74**	1.98716	-0.04915	0.5188	**H257**	0.55885	0.97298	0.75256
C1	1.91148	0.09918	0.09705	**C75**	2.10618	0.20001	0.46508	**H258**	0.38653	0.87958	0.96667
C35	2.20886	0.09947	0.05934	**N112**	2.05922	-0.0824	0.50347	**C145**	0.51721	1.03452	0.82755
N67	1.94536	-0.92129	0.06964	**C133**	0.89299	-0.076	0.53186	**C192**	1.01991	0.5294	0.82124
N71	1.15332	-0.93717	0.04422	**C134**	0.96391	0.01801	0.52555	**C209**	-0.03703	0.49575	0.81102
C73	0.94928	-0.03474	0.5253	**C137**	1.03936	-0.01128	0.50558	**C214**	0.49507	-0.02166	0.84677
C74	0.98716	-0.04915	0.5188	**N142**	1.08675	-0.85415	0.48464				

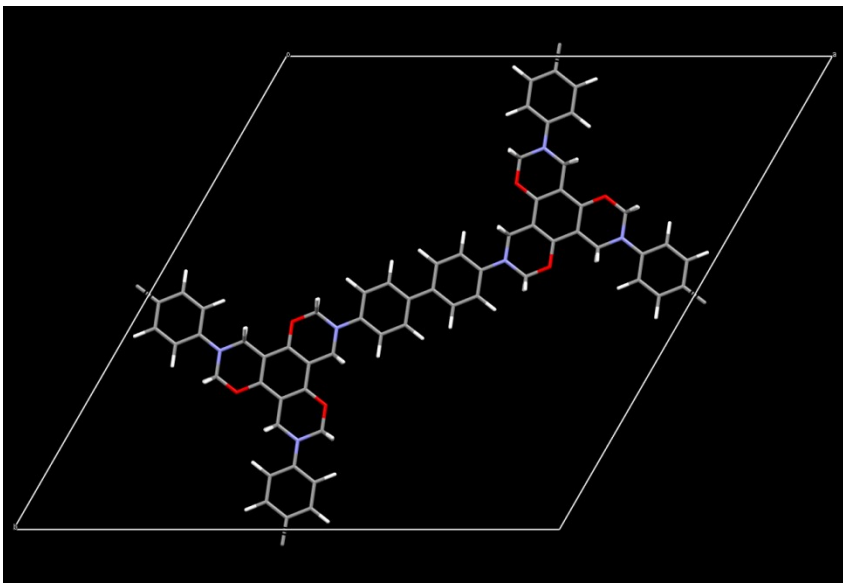


Figure S9. Unit cell structure of **PGBD** elucidated for eclipsed AA model.

Table S4. Fractional atomic coordinates and unit cell parameters of **PGBD** calculated for eclipsed AA model.

PGBD: Model **AA**; Space group ***P*1**											
Unit cell parameters: a = 28.6 Å, b = 28.6 Å, c = 3.6 Å; α = 90°, β = 90°, γ = 120°											
Atoms	X	Y	Z	**Atoms**	X	Y	Z	**Atoms**	X	Y	Z
C1	1.5081	-0.96873	0	**C43**	1.37276	-0.22141	0	**H85**	1.44918	-0.58953	0
C2	1.56251	-0.93469	0	**N44**	1.42686	-0.18775	0	**H86**	1.51158	-0.62691	0
C3	1.58297	-0.88026	0	**C45**	1.44732	-0.13332	0	**H87**	1.54718	-0.4038	0
C4	1.54902	-0.85987	0	**C46**	1.10099	-0.39123	0	**H88**	1.48476	-0.36628	0
C5	1.4946	-0.89391	0	**C47**	1.04658	-0.42527	0	**H89**	1.34757	-0.5285	0
C6	1.47414	-0.94834	0	**C48**	1.02611	-0.4797	0	**H90**	1.40997	-0.56588	0
N7	1.56916	-0.80581	0	**C49**	1.06007	-0.50009	0	**H91**	1.4273	-0.35385	-0.2522
C8	1.62358	-0.77178	0	**C50**	1.11449	-0.46605	0	**H92**	1.4256	-0.35279	0.25856
C9	1.64404	-0.71734	0	**O51**	1.26393	-0.28949	0	**H93**	1.21294	-0.42556	0.25205
C10	1.69846	-0.68331	0	**O52**	1.44068	-0.2622	0	**H94**	1.21116	-0.42452	-0.25856
C11	1.7186	-0.62925	0	**O53**	1.73241	-0.7037	0	**H95**	1.3556	-0.21103	0.25225
C12	1.68465	-0.60886	0	**O54**	1.55567	-0.73099	0	**H96**	1.35833	-0.2093	-0.25856
C13	1.63055	-0.64252	0	**O55**	1.70511	-0.55443	0	**H97**	1.11809	-0.34568	0
C14	1.61008	-0.69695	0	**O56**	1.29123	-0.43876	0	**H98**	1.01808	-0.40821	0
C15	1.59684	-0.62228	0	**C57**	1.20983	-0.32316	0	**H99**	1.04298	-0.54565	0
N16	1.61673	-0.56808	0	**C58**	1.46082	-0.20814	0	**H100**	1.14298	-0.48311	0
C17	1.58278	-0.54769	0	**C59**	1.32519	-0.45915	0	**H101**	1.19266	-0.31277	0.25225
C18	1.77302	-0.59521	0	**C60**	1.6714	-0.53419	0	**H102**	1.1954	-0.31105	-0.25856
N19	1.80698	-0.6156	0	**C61**	1.78651	-0.67003	0	**H103**	1.48839	-0.19088	0.25205
C20	1.86139	-0.58156	0	**C62**	1.53521	-0.78542	0	**H104**	1.48736	-0.19369	-0.25856
C21	1.60324	-0.49326	0	**C63**	1.89535	-0.60196	0	**H105**	1.31481	-0.48673	0.25205
C22	1.56928	-0.47286	0	**C64**	1.94977	-0.56792	0	**H106**	1.31303	-0.48569	-0.25856
C23	1.51487	-0.5069	0	**C65**	1.96991	-0.51386	0	**H107**	1.68183	-0.50658	0.25195
C24	1.49472	-0.56096	0	**C66**	1.93595	-0.49347	0	**H108**	1.68362	-0.50764	-0.25856
C25	1.52868	-0.58135	0	**C67**	1.88185	-0.52713	0	**H109**	1.80368	-0.68041	0.25225
C26	1.48116	-0.48666	0	**C68**	1.50174	-0.09928	0	**H110**	1.80094	-0.68214	-0.25856
C27	1.50162	-0.43223	0	**C69**	1.5222	-0.04485	0	**H111**	1.50765	-0.80263	0.2522
C28	1.46766	-0.41184	0	**C70**	1.48825	-0.02446	0	**H112**	1.50867	-0.79987	-0.25856
C29	1.41325	-0.44588	0	**C71**	1.43383	-0.0585	0	**H113**	1.87826	-0.64751	0
C30	1.3931	-0.49993	0	**C72**	1.41337	-0.11293	0	**H114**	1.97826	-0.58498	0
C31	1.42706	-0.52033	0	**H73**	1.59101	-0.95175	0	**H115**	1.95305	-0.44791	0
N32	1.37929	-0.42549	0	**H74**	1.62854	-0.85183	0	**H116**	1.8535	-0.50992	0
C33	1.39975	-0.37106	0	**H75**	1.46611	-0.87685	0	**H117**	1.53023	-0.11634	0
C34	1.3658	-0.35067	0	**H76**	1.42858	-0.97677	0	**H118**	1.56776	-0.01642	0
C35	1.38626	-0.29624	0	**H77**	1.6408	-0.78212	-0.2521	**H119**	1.40534	-0.04144	0
C36	1.3523	-0.27584	0	**H78**	1.64187	-0.77932	0.25856	**H120**	1.36781	-0.14136	0
C37	1.29788	-0.30988	0	**H79**	1.56923	-0.63964	0.2518	**C1**	1.5081	0.03127	0
C38	1.27742	-0.36431	0	**H80**	1.5703	-0.63673	-0.25856	**C48**	2.02611	-0.4797	0
C39	1.31138	-0.3847	0	**H81**	1.78335	-0.56766	0.2522	**C65**	0.96991	-0.51386	0
C40	1.22332	-0.39798	0	**H82**	1.78509	-0.56867	-0.25856	**C70**	1.48825	-1.02446	0
N41	1.18937	-0.37759	0	**H83**	1.6488	-0.46482	0				
C42	1.13495	-0.41162	0	**H84**	1.58638	-0.42731	0				

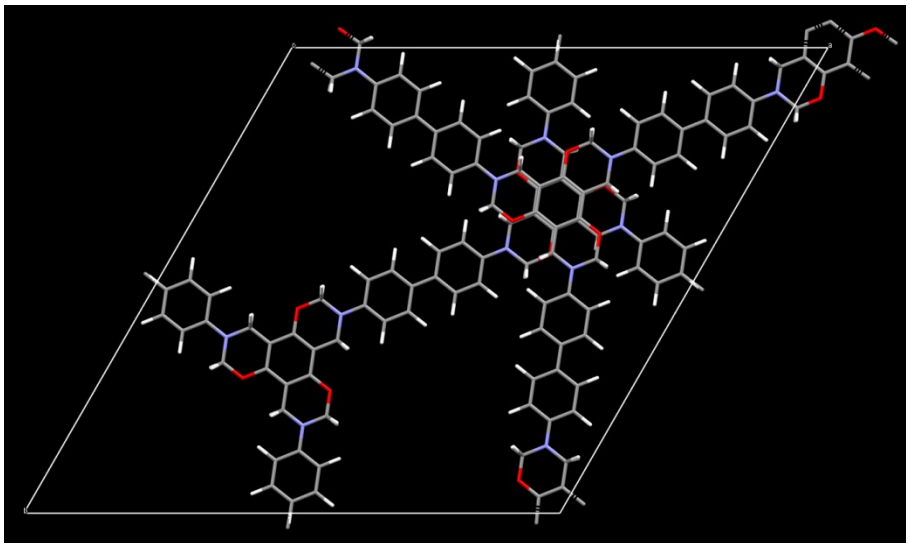


Figure S10. Unit cell structure of **PGBD** calculated for staggered AB model.

Table S5. Fractional atomic coordinates and unit cell parameters calculated for **PGBD** staggered AB model.

PGBD: Model **AB**; Space group ***P*1**											
Unit cell parameters: a = 28.6 Å, b = 28.6 Å, c = 7.2 Å; α = 90°, β = 90°, γ = 120°											
Atoms	X	Y	Z	**Atoms**	X	Y	Z	**Atoms**	X	Y	Z
C1	2.03481	-1.0195	-0.76372	**H207**	1.68877	-0.54936	-0.63759	**C117**	0.44682	0.86629	0.70833
C2	2.05509	-0.9651	-0.76372	**H208**	1.69151	-0.54762	-0.89299	**C118**	0.10049	0.60838	0.70833
C3	2.02098	-0.94489	-0.76372	**H209**	1.45116	-0.68445	-0.76372	**C119**	0.04607	0.57434	0.70833
C4	1.9666	-0.97908	-0.76372	**H210**	1.35121	-0.74726	-0.76372	**C120**	0.02561	0.51991	0.70833
C5	1.93249	-0.95886	-0.76372	**H211**	1.37695	-0.88447	-0.76372	**C121**	0.05956	0.49952	0.70833
N6	1.95277	-0.90446	-0.76372	**H212**	1.47691	-0.82166	-0.76372	**C122**	0.11398	0.53356	0.70833
C7	1.91867	-0.88425	-0.76372	**H213**	1.2883	-0.78664	-0.76372	**O123**	0.26342	0.71012	0.70833
C8	1.93895	-0.82984	-0.76372	**H214**	1.18835	-0.84946	-0.76372	**O124**	0.44017	0.73742	0.70833
C9	1.90484	-0.80963	-0.76372	**H215**	1.2141	-0.98666	-0.76372	**O125**	0.73191	0.29592	0.70833
C10	1.85045	-0.84382	-0.76372	**H216**	1.31405	-0.92385	-0.76372	**O126**	0.55516	0.26862	0.70833
C11	1.83017	-0.89822	-0.76372	**H217**	1.11946	-0.90659	-0.88848	**O127**	0.7046	0.44518	0.70833
C12	1.86428	-0.91844	-0.76372	**H218**	1.11567	-0.90892	-0.63444	**O128**	0.29073	0.56085	0.70833
C13	1.81635	-0.82361	-0.76372	**H219**	1.13852	-1.02037	-0.63621	**C129**	0.20932	0.67646	0.70833
C14	1.83663	-0.7692	-0.76372	**H220**	1.13691	-1.02138	-0.89299	**C130**	0.46031	0.79147	0.70833
C15	1.80227	-0.74884	-0.76372	**H221**	1.52594	-0.6515	-0.63766	**C131**	0.32468	0.54046	0.70833
C16	1.74788	-0.78303	-0.76372	**H222**	1.52874	-0.64973	-0.89299	**C132**	0.6709	0.46543	0.70833
C17	1.7276	-0.83743	-0.76372	**H223**	1.82213	-0.5283	-0.63762	**C133**	0.78601	0.32958	0.70833
C18	1.76196	-0.8578	-0.76372	**H224**	1.82113	-0.53106	-0.89299	**C134**	0.5347	0.21419	0.70833
N19	1.71403	-0.76297	-0.76372	**H225**	1.64905	-0.8246	-0.63774	**C135**	0.89484	0.39766	0.70833
C20	1.73406	-0.70842	-0.76372	**H226**	1.64725	-0.82355	-0.89299	**C136**	0.94926	0.4317	0.70833
C21	1.69995	-0.6882	-0.76372	**H227**	2.01747	-0.84278	-0.63747	**C137**	0.9694	0.48575	0.70833
C22	1.72024	-0.6338	-0.76372	**H228**	2.01915	-0.84374	-0.89299	**C138**	0.93545	0.50614	0.70833
C23	1.68613	-0.61359	-0.76372	**H229**	1.86378	-0.45369	-0.76372	**C139**	0.88135	0.47248	0.70833
C24	1.63174	-0.64778	-0.76372	**H230**	1.90098	-0.35382	-0.76372	**C140**	0.50124	0.90033	0.70833
C25	1.61146	-0.70218	-0.76372	**H231**	1.7383	-0.37902	-0.76372	**C141**	0.5217	0.95476	0.70833
C26	1.64556	-0.72239	-0.76372	**H232**	1.70117	-0.47954	-0.76372	**C142**	0.48774	0.97515	0.70833
C27	1.55707	-0.73637	-0.76372	**H233**	1.9244	-0.29075	-0.76372	**C143**	0.43332	0.94112	0.70833
N28	1.52296	-0.71616	-0.76372	**H234**	1.96153	-0.19023	-0.76372	**C144**	0.41286	0.88669	0.70833
C29	1.46857	-0.75034	-0.76372	**H235**	1.79892	-0.21609	-0.76372	**H145**	0.5905	0.04787	0.70833
C30	1.7061	-0.55956	-0.76372	**H236**	1.76172	-0.31596	-0.76372	**H146**	0.62803	0.14779	0.70833
N31	1.76048	-0.52537	-0.76372	**H237**	1.97391	-0.12047	-0.88977	**H147**	0.4656	0.12276	0.70833
C32	1.78077	-0.47097	-0.76372	**H238**	1.97497	-0.11767	-0.63444	**H148**	0.42807	0.02284	0.70833

C33	1.43421	-0.72998	-0.76372	**H239**	1.84057	-0.14147	-0.88982	**H149**	0.6403	0.2175	0.58227
C34	1.37982	-0.76417	-0.76372	**H240**	1.84228	-0.14252	-0.63444	**H150**	0.64137	0.2203	0.8376
C35	1.35954	-0.81857	-0.76372	**C1**	2.03481	-0.0195	-0.76372	**H151**	0.56873	0.35997	0.83423
C36	1.3939	-0.83894	-0.76372	**C2**	1.05509	-0.9651	-0.76372	**H152**	0.5698	0.36288	0.57905
C37	1.44829	-0.80475	-0.76372	**C4**	1.9666	0.02092	-0.76372	**H153**	0.78284	0.43195	0.83443
C38	1.30572	-0.85254	-0.76372	**C45**	2.10819	-0.93474	-0.76372	**H154**	0.78459	0.43094	0.57905
C39	1.27136	-0.83218	-0.76372	**O48**	1.06891	-1.03972	-0.76372	**H155**	0.64829	0.53479	0.70833
C40	1.21697	-0.86636	-0.76372	**C51**	2.12227	-1.00951	-0.76372	**H156**	0.58587	0.57231	0.70833
C41	1.19669	-0.92077	-0.76372	**C69**	1.97689	-1.05581	-0.76372	**H157**	0.44868	0.41009	0.70833
C42	1.23105	-0.94113	-0.76372	**C70**	1.94278	-1.0356	-0.76372	**H158**	0.51108	0.37271	0.70833
C43	1.28543	-0.90694	-0.76372	**C73**	0.50759	0.03088	0.70833	**H159**	0.54668	0.59582	0.70833
N44	1.1423	-0.95496	-0.76372	**C74**	0.56201	0.06492	0.70833	**H160**	0.48425	0.63333	0.70833
C45	1.10819	-0.93474	-0.76372	**C75**	0.58247	0.11935	0.70833	**H161**	0.34706	0.47111	0.70833
O46	1.59763	-0.62756	-0.76372	**C76**	0.54851	0.13975	0.70833	**H162**	0.40946	0.43373	0.70833
O47	1.77431	-0.59999	-0.76372	**C77**	0.49409	0.10571	0.70833	**H163**	0.4268	0.64576	0.58223
O48	2.06891	-1.03972	-0.76372	**C78**	0.47363	0.05128	0.70833	**H164**	0.42509	0.64682	0.8376
O49	2.04095	-0.89086	-0.76372	**N79**	0.56866	0.1938	0.70833	**H165**	0.21243	0.57405	0.83435
O50	1.62528	-0.7768	-0.76372	**C80**	0.62307	0.22784	0.70833	**H166**	0.21066	0.5751	0.57905
C51	1.12227	-1.00951	-0.76372	**C81**	0.64353	0.28227	0.70833	**H167**	0.35509	0.78858	0.83445
C52	1.54324	-0.66175	-0.76372	**C82**	0.69795	0.31631	0.70833	**H168**	0.35783	0.79031	0.57905
C53	1.79459	-0.54558	-0.76372	**C83**	0.7181	0.37036	0.70833	**H169**	0.11758	0.65394	0.70833
C54	1.65939	-0.79701	-0.76372	**C84**	0.68414	0.39075	0.70833	**H170**	0.01758	0.5914	0.70833
C55	2.00716	-0.87027	-0.76372	**C85**	0.63004	0.35709	0.70833	**H171**	0.04247	0.45397	0.70833
C56	1.83516	-0.43678	-0.76372	**C86**	0.60958	0.30266	0.70833	**H172**	0.14247	0.5165	0.70833
C57	1.85544	-0.38238	-0.76372	**C87**	0.59633	0.37733	0.70833	**H173**	0.19216	0.68684	0.83445
C58	1.82133	-0.36216	-0.76372	**N88**	0.61623	0.43154	0.70833	**H174**	0.19489	0.68857	0.57905
C59	1.76669	-0.3962	-0.76372	**C89**	0.58227	0.45193	0.70833	**H175**	0.48788	0.80873	0.83435
C60	1.74666	-0.45075	-0.76372	**C90**	0.77251	0.4044	0.70833	**H176**	0.48685	0.80592	0.57905
C61	1.84137	-0.30761	-0.76372	**N91**	0.80647	0.38401	0.70833	**H177**	0.3143	0.51288	0.83435
C62	1.89601	-0.27357	-0.76372	**C92**	0.86089	0.41805	0.70833	**H178**	0.31253	0.51392	0.57905
C63	1.91604	-0.21902	-0.76372	**C93**	0.60273	0.50636	0.70833	**H179**	0.68132	0.49303	0.8343
C64	1.88193	-0.19881	-0.76372	**C94**	0.56878	0.52675	0.70833	**H180**	0.68312	0.49197	0.57905
C65	1.82754	-0.233	-0.76372	**C95**	0.51436	0.49271	0.70833	**H181**	0.80318	0.3192	0.83445
C66	1.80726	-0.2874	-0.76372	**C96**	0.49422	0.43866	0.70833	**H182**	0.80044	0.31747	0.57905
N67	1.90222	-0.1444	-0.76372	**C97**	0.52817	0.41827	0.70833	**H183**	0.50715	0.19699	0.83443
C68	1.95661	-0.11021	-0.76372	**C98**	0.48065	0.51295	0.70833	**H184**	0.50816	0.19974	0.57905
C69	1.97689	-0.05581	-0.76372	**C99**	0.50111	0.56738	0.70833	**H185**	0.87775	0.3521	0.70833
C70	1.94278	-0.0356	-0.76372	**C100**	0.46716	0.58777	0.70833	**H186**	0.97775	0.41464	0.70833
O71	1.88839	-0.06979	-0.76372	**C101**	0.41274	0.55374	0.70833	**H187**	0.95254	0.5517	0.70833
C72	1.86811	-0.12419	-0.76372	**C102**	0.3926	0.49968	0.70833	**H188**	0.85299	0.4897	0.70833
H193	1.90495	-0.97614	-0.63762	**C103**	0.42655	0.47929	0.70833	**H189**	0.52973	0.88328	0.70833
H194	1.90596	-0.97339	-0.89299	**N104**	0.37879	0.57413	0.70833	**H190**	0.56726	0.9832	0.70833
H195	1.98449	-0.80128	-0.76372	**C105**	0.39925	0.62856	0.70833	**H191**	0.40483	0.95817	0.70833
H196	1.92179	-0.7641	-0.76372	**C106**	0.36529	0.64895	0.70833	**H192**	0.3673	0.85825	0.70833
H197	1.78463	-0.92678	-0.76372	**C107**	0.38575	0.70338	0.70833	**H241**	0.49053	-0.01467	0.70833
H198	1.84733	-0.96397	-0.76372	**C108**	0.3518	0.72377	0.70833	**H242**	-0.01995	0.49148	0.70833
H199	1.88217	-0.74064	-0.76372	**C109**	0.29738	0.68973	0.70833	**H243**	1.01494	0.51432	0.70833
H200	1.81922	-0.70331	-0.76372	**C110**	0.27692	0.6353	0.70833	**H244**	0.50483	1.02071	0.70833
H201	1.68206	-0.86599	-0.76372	**C111**	0.31087	0.61491	0.70833	**C73**	0.50759	1.03088	0.70833
H202	1.74501	-0.90333	-0.76372	**C112**	0.22282	0.60164	0.70833	**C120**	1.02561	0.51991	0.70833
H203	1.76163	-0.69104	-0.88969	**N113**	0.18886	0.62203	0.70833	**C137**	-0.0306	0.48575	0.70833
H204	1.75984	-0.68996	-0.63444	**C114**	0.13444	0.58799	0.70833	**C142**	0.48774	-0.02485	0.70833
H205	1.54683	-0.7639	-0.63762	**C115**	0.37226	0.7782	0.70833				
H206	1.54508	-0.7629	-0.89299	**N116**	0.42636	0.81186	0.70833				

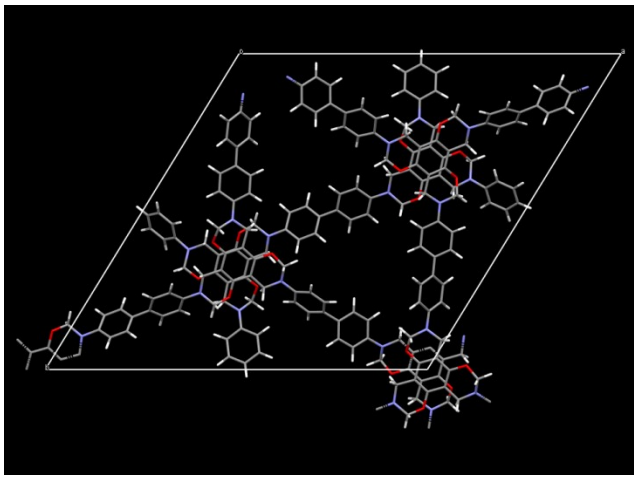


Figure S11. Unit cell diagram of **PGBD** calculated for ABC model.

Table S6. Fractional atomic coordinates and unit cell parameters of **PGBD** calculated for ABC model.

PGBD: Model **ABC**; Space group ***P*1**											
Unit cell parameters: a = 30.18 Å, b = 29.67 Å, c = 8.08 Å; α = 81.43°, β = 84.38°, γ = 119.79°											
Atoms	X	Y	Z	**Atoms**	X	Y	Z	**Atoms**	X	Y	Z
C1	1.93776	-0.87185	0.09594	**C75**	1.09745	-0.80881	0.51011	**C144**	1.07516	-0.03522	0.492
C2	1.94887	-0.8262	-0.02428	**C76**	1.13395	-0.78155	0.60961	**C145**	0.49629	0.03337	0.78668
C3	1.91667	-0.805	-0.01185	**C77**	1.15679	-0.72673	0.59145	**C146**	0.53099	0.05801	0.89304
C4	1.87212	-0.82974	0.11826	**C78**	1.14288	-0.69804	0.47642	**C147**	0.55457	0.1128	0.88093
C5	1.86096	-0.87491	0.23906	**C79**	1.10464	-0.72514	0.38323	**C148**	0.54462	0.1444	0.75998
C6	1.89379	-0.89542	0.22931	**C80**	1.08216	-0.78001	0.39968	**C149**	0.51021	0.11912	0.65183
C7	1.83717	-0.80855	0.12881	**C81**	1.17009	-0.6396	0.44861	**C150**	0.48582	0.06419	0.66684
C8	1.85398	-0.7595	0.17227	**C82**	1.22446	-0.60904	0.39563	**N151**	0.56943	0.20141	0.74558
C9	1.81967	-0.74117	0.19435	**C83**	1.25066	-0.55366	0.36622	**C152**	0.62404	0.2322	0.76626
C10	1.76776	-0.77136	0.17175	**C84**	1.22314	-0.52762	0.39304	**C153**	0.64426	0.2908	0.74801
C11	1.75229	-0.81915	0.11809	**C85**	1.16865	-0.55872	0.45113	**C154**	0.69644	0.32582	0.75579
C12	1.78642	-0.83791	0.09947	**C86**	1.14228	-0.61417	0.4759	**C155**	0.71509	0.38017	0.7454
N13	1.73129	-0.75379	0.20508	**N87**	1.25052	-0.47017	0.36279	**C156**	0.68155	0.39973	0.7242
C14	1.75086	-0.69774	0.20591	**C88**	1.30564	-0.43981	0.37529	**C157**	0.62905	0.36425	0.71937
C15	1.70906	-0.68417	0.19979	**C89**	1.32317	-0.38339	0.38563	**C158**	0.61065	0.3102	0.72976
C16	1.72185	-0.63181	0.19609	**C90**	1.3746	-0.34929	0.40175	**C159**	0.59199	0.38368	0.70281
C17	1.68482	-0.61699	0.17242	**C91**	1.39086	-0.29737	0.41934	**N160**	0.61619	0.44009	0.70611
C18	1.63392	-0.65579	0.16508	**C92**	1.35524	-0.27986	0.42306	**C161**	0.58334	0.46167	0.73943
C19	1.61993	-0.70916	0.18079	**C93**	1.30428	-0.31322	0.39988	**C162**	0.77101	0.4175	0.7571
C20	1.65749	-0.72358	0.19836	**C94**	1.28836	-0.3648	0.3783	**N163**	0.80258	0.39235	0.75596
C21	1.56517	-0.75043	0.17129	**C95**	1.2661	-0.2945	0.40094	**C164**	0.85776	0.42418	0.75709
N22	1.52886	-0.73086	0.17973	**N96**	1.28894	-0.23932	0.42087	**C165**	0.60099	0.50751	0.80636
C23	1.47427	-0.76669	0.1789	**C97**	1.25631	-0.21639	0.42224	**C166**	0.56915	0.52861	0.83318
C24	1.69935	-0.55978	0.15906	**C98**	1.44631	-0.26034	0.43478	**C167**	0.51866	0.50327	0.79869
N25	1.75303	-0.52593	0.18291	**N99**	1.47971	-0.28311	0.41579	**C168**	0.50029	0.45671	0.73795
C26	1.77797	-0.46853	0.14784	**C100**	1.5341	-0.25171	0.42839	**C169**	0.53231	0.43643	0.70707
C27	1.43518	-0.7613	0.26817	**C101**	1.27438	-0.16529	0.3222	**C170**	0.48497	0.52549	0.82112
C28	1.38316	-0.79287	0.25636	**C102**	1.2424	-0.14379	0.32036	**C171**	0.5019	0.5775	0.73526
C29	1.36877	-0.83114	0.1576	**C103**	1.19122	-0.17323	0.41569	**C172**	0.46788	0.59655	0.74247
C30	1.40673	-0.83899	0.07607	**C104**	1.17279	-0.22432	0.51476	**C173**	0.41622	0.56393	0.83593
C31	1.45894	-0.8072	0.08694	**C105**	1.20531	-0.24524	0.52011	**C174**	0.40035	0.51239	0.92703
C32	1.31494	-0.85966	0.12948	**C106**	1.15778	-0.14994	0.41757	**C175**	0.43419	0.49325	0.91814
C33	1.29295	-0.83042	0.06646	**C107**	1.1763	-0.09961	0.45363	**N176**	0.38018	0.58279	0.83844
C34	1.24237	-0.85637	0.03695	**C108**	1.14324	-0.07968	0.47272	**C177**	0.3987	0.63737	0.85804
C35	1.21243	-0.91229	0.07001	**C109**	1.09082	-0.1095	0.45469	**C178**	0.35768	0.65215	0.85238

C36	1.23429	-0.94164	0.13656	**C110**	1.07391	-0.15801	0.40441	**C179**	0.36939	0.70279	0.87282
C37	1.28544	-0.91546	0.16409	**C111**	1.1067	-0.17849	0.38944	**C180**	0.33104	0.71675	0.86924
O38	1.59806	-0.6403	0.13528	**N112**	1.05486	-0.0916	0.49317	**C181**	0.2803	0.67882	0.85662
O39	1.7722	-0.59447	0.21375	**O113**	1.37092	-0.22953	0.45514	**C182**	0.26927	0.6289	0.82853
O40	1.64339	-0.77687	0.20965	**O114**	1.40849	-0.36858	0.40969	**C183**	0.3081	0.61581	0.82532
C41	1.54572	-0.67865	0.21955	**O115**	0.96602	-0.1151	0.52658	**C184**	0.21459	0.58764	0.81601
C42	1.77452	-0.55256	0.28524	**O116**	1.23689	-0.39797	0.3589	**N185**	0.1779	0.6062	0.83993
C43	1.67635	-0.79174	0.28659	**C117**	1.00116	-0.12963	0.58729	**C186**	0.12619	0.57685	0.80217
C44	1.83277	-0.4359	0.10989	**C118**	1.34592	-0.20402	0.38015	**C187**	0.34389	0.77197	0.88137
C45	1.85713	-0.38116	0.09807	**C119**	1.46193	-0.32971	0.33952	**N188**	0.39917	0.80664	0.88602
C46	1.8274	-0.35728	0.11511	**C120**	1.22912	-0.44024	0.27841	**C189**	0.42315	0.86396	0.84932
C47	1.77282	-0.38898	0.14178	**C121**	1.57353	-0.25183	0.31875	**C190**	0.0984	0.60227	0.76264
C48	1.74831	-0.44407	0.15904	**C122**	1.6259	-0.22127	0.33049	**C191**	0.04662	0.57302	0.74436
C49	1.85342	-0.29934	0.10395	**C123**	1.64025	-0.18894	0.44904	**C192**	0.02159	0.51778	0.7622
C50	1.89022	-0.27519	0.20517	**C124**	1.60157	-0.18785	0.55668	**C193**	0.04992	0.49254	0.79086
C51	1.91399	-0.22056	0.19729	**C125**	1.54908	-0.21928	0.54793	**C194**	0.10165	0.52173	0.81073
C52	1.90217	-0.18867	0.08529	**C126**	1.69525	-0.15786	0.4657	**O195**	0.24099	0.69113	0.87416
C53	1.86641	-0.21311	-0.0198	**C127**	1.7219	-0.18391	0.50943	**O196**	0.42017	0.73943	0.89038
C54	1.84178	-0.26785	-0.00869	**C128**	1.77257	-0.15529	0.53862	**O197**	0.72882	0.30546	0.78281
N55	1.92624	-0.13209	0.07771	**C129**	1.79823	-0.09971	0.52086	**O198**	0.55759	0.27545	0.73476
C56	1.98173	-0.10061	0.08657	**C130**	1.77213	-0.07346	0.46807	**O199**	0.70075	0.45421	0.71309
C57	2.00106	-0.04235	0.07266	**C131**	1.72076	-0.10242	0.44415	**O200**	0.29681	0.56658	0.79304
C58	1.96562	-0.0246	0.08028	**N132**	1.85023	-0.07052	0.55624	**C201**	0.19015	0.64589	0.94407
O59	1.91222	-0.06048	0.09617	**C133**	1.88544	-0.09107	0.53904	**C202**	0.42461	0.78097	0.96925
C60	1.90018	-0.10397	0.01723	**C134**	1.95469	0.00344	0.53805	**C203**	0.32373	0.54423	0.87304
C61	2.05447	-0.00603	0.05632	**O135**	1.9162	0.01693	0.55838	**C204**	0.67213	0.47453	0.63255
C62	2.07203	0.04753	0.05945	**C136**	1.8657	-0.02645	0.64313	**C205**	0.78221	0.34137	0.70422
C63	2.03659	0.06511	0.06903	**C137**	2.03284	-0.02206	0.50537	**C206**	0.546	0.23018	0.66674
C64	1.9833	0.0291	0.07869	**C138**	2.04607	0.03024	0.50694	**C207**	0.89452	0.4183	0.65503
O65	2.05495	0.11838	0.07443	**C139**	2.00706	0.04306	0.524	**C208**	0.94765	0.44876	0.65623
C66	2.02585	0.13967	0.00433	**O140**	2.09874	0.06952	0.48627	**C209**	0.96549	0.48636	0.75746
N67	1.97008	0.10516	0.08023	**C141**	2.10837	0.11193	0.56765	**C210**	0.92935	0.49314	0.85735
C68	1.94491	0.04769	0.08815	**N142**	2.07707	0.13513	0.5192	**C211**	0.87609	0.46234	0.85755
O69	2.08958	-0.02404	0.03981	**C143**	2.02099	0.09912	0.52744	**C212**	0.47736	0.89771	0.78929
C70	2.14136	0.0162	-0.04569	**C144**	2.07516	-0.03522	0.492	**C213**	0.5011	0.95281	0.76872
N71	2.16025	0.0614	0.03658	**H313**	1.14519	-0.80251	0.70113	**C214**	0.47096	0.97547	0.80149
C72	2.12908	0.08657	0.04781	**H314**	1.18551	-0.70654	0.66697	**C215**	0.41662	0.94252	0.85091
H265	1.98191	-0.80736	-0.12997	**H315**	1.09349	-0.70351	0.29356	**C216**	0.39295	0.88727	0.87617
H266	1.92586	-0.76994	-0.10564	**H316**	1.05404	-0.79931	0.32198	**H217**	0.53914	0.03458	0.98747
H267	1.82705	-0.89393	0.34186	**H317**	1.24658	-0.6281	0.37484	**H218**	0.58008	0.12991	0.96811
H268	1.88483	-0.92951	0.32684	**H318**	1.29248	-0.53135	0.32102	**H219**	0.50234	0.14166	0.55377
H269	1.89328	-0.73606	0.19361	**H319**	1.14634	-0.54044	0.48004	**H220**	0.4594	0.04579	0.58281
H270	1.83383	-0.70382	0.23304	**H320**	1.10035	-0.63735	0.51996	**H221**	0.64899	0.22745	0.6689
H271	1.71392	-0.84224	0.09	**H321**	1.33026	-0.4386	0.26102	**H222**	0.62788	0.21695	0.89455
H272	1.77335	-0.8753	0.06146	**H322**	1.3117	-0.45965	0.49142	**H223**	0.55784	0.35959	0.81061
H273	1.78292	-0.67189	0.09302	**H323**	1.23249	-0.3219	0.50724	**H224**	0.57874	0.3777	0.57972
H274	1.76615	-0.68937	0.32443	**H324**	1.25196	-0.29728	0.27845	**H225**	0.77059	0.43196	0.87558
H275	1.55001	-0.78604	0.27678	**H325**	1.44488	-0.25054	0.56142	**H226**	0.78936	0.45267	0.64796
H276	1.56734	-0.7627	0.04982	**H326**	1.46337	-0.22301	0.33473	**H227**	0.63903	0.52687	0.83985
H277	1.67173	-0.55937	0.25927	**H327**	1.31309	-0.14199	0.24322	**H228**	0.58361	0.56428	0.88255
H278	1.69511	-0.54385	0.03217	**H328**	1.25745	-0.10432	0.24287	**H229**	0.46144	0.43666	0.71026
H279	1.44455	-0.73239	0.34644	**H329**	1.13363	-0.24748	0.5914	**H230**	0.51693	0.40121	0.65554
H280	1.35405	-0.78703	0.32281	**H330**	1.19082	-0.28368	0.60225	**H231**	0.54083	0.60268	0.65766
H281	1.39629	-0.86831	-0.00139	**H331**	1.21582	-0.0766	0.47394	**H232**	0.48207	0.6364	0.67145
H282	1.48701	-0.81382	0.01909	**H332**	1.15873	-0.04157	0.50689	**H233**	0.36169	0.48658	1.00536
H283	1.31537	-0.78727	0.03733	**H333**	1.03522	-0.18055	0.37778	**H234**	0.42064	0.45304	0.98617
H284	1.22701	-0.83239	-0.01386	**H334**	1.09213	-0.21679	0.3565	**H235**	0.43243	0.66626	0.75448
H285	1.21173	-0.98472	0.16923	**H335**	0.99944	-0.1298	0.7254	**H236**	0.4114	0.64124	0.98258
H286	1.30175	-0.9386	0.21477	**H336**	0.98761	-0.17093	0.57628	**H237**	0.20093	0.55121	0.91681

H287	1.54232	-0.6826	0.36018	**H337**	1.35758	-0.16773	0.43072	**H238**	0.21542	0.57735	0.68965
H288	1.52097	-0.66327	0.17561	**H338**	1.3597	-0.19175	0.23916	**H239**	0.31937	0.76899	0.99946
H289	1.75075	-0.56946	0.4161	**H339**	1.48483	-0.34899	0.36511	**H240**	0.33444	0.78937	0.7684
H290	1.81519	-0.52526	0.29633	**H340**	1.46729	-0.31688	0.19876	**H241**	0.11601	0.64465	0.7482
H291	1.6712	-0.79164	0.42444	**H341**	1.18707	-0.46556	0.2781	**H242**	0.02589	0.59352	0.71769
H292	1.66365	-0.83315	0.27928	**H342**	1.24971	-0.42326	0.14387	**H243**	0.0314	0.44986	0.80468
H293	1.85707	-0.45258	0.09019	**H343**	1.56421	-0.27501	0.22204	**H244**	0.12155	0.50051	0.83888
H294	1.89932	-0.3573	0.07412	**H344**	1.6554	-0.22217	0.24513	**H245**	0.18893	0.62799	1.07708
H295	1.7491	-0.37127	0.15414	**H345**	1.612	-0.16337	0.65001	**H246**	0.16167	0.65902	0.95289
H296	1.70614	-0.46743	0.18549	**H346**	1.52052	-0.21832	0.63675	**H247**	0.40528	0.76385	1.10517
H297	1.89979	-0.29886	0.29295	**H347**	1.70292	-0.22668	0.52577	**H248**	0.46633	0.8092	0.96637
H298	1.94086	-0.20384	0.28129	**H348**	1.79116	-0.17707	0.57811	**H249**	0.30834	0.53114	1.01308
H299	1.8574	-0.19007	-0.11164	**H349**	1.79131	-0.03055	0.4441	**H250**	0.31545	0.50858	0.82268
H300	1.81419	-0.28553	-0.09021	**H350**	1.70098	-0.08158	0.40738	**H251**	0.6878	0.5161	0.64481
H301	2.00518	-0.10474	-0.01814	**H351**	1.8829	-0.10654	0.42105	**H252**	0.67859	0.47589	0.4939
H302	1.98848	-0.11574	0.20961	**H352**	1.87305	-0.12434	0.65029	**H253**	0.80417	0.32202	0.74334
H303	1.91325	-0.0888	-0.12308	**H353**	1.83786	-0.0124	0.6478	**H254**	0.78643	0.34872	0.56282
H304	1.85717	-0.13106	0.04741	**H354**	1.86682	-0.04003	0.77797	**H255**	0.50286	0.20419	0.69085
H305	2.03167	0.14369	-0.13624	**H355**	2.15072	0.14223	0.52911	**H256**	0.56121	0.24323	0.5271
H306	2.04122	0.18003	0.02959	**H356**	2.09848	0.09671	0.70814	**H257**	0.88249	0.39057	0.57218
H307	1.92441	0.03871	-0.02071	**H357**	2.00845	0.11358	0.41751	**H258**	0.97497	0.44357	0.5758
H308	1.91571	0.02469	0.20904	**H358**	1.9988	0.09819	0.64747	**H259**	0.94229	0.52171	0.93763
H309	2.1414	0.02995	-0.18181	**H359**	2.0944	-0.02556	0.60321	**H260**	0.84956	0.46829	0.9381
H310	2.16663	-0.00099	-0.04549	**H360**	2.1043	-0.01005	0.37209	**H261**	0.50162	0.88168	0.75831
H311	2.14326	0.1192	-0.06754	**C73**	1.94149	-0.04882	0.53069	**H262**	0.54301	0.97788	0.72617
H312	2.13391	0.10392	0.16231	**C74**	1.9803	-0.06207	0.52139	**H263**	0.39272	0.9595	0.87457
C1	1.93776	0.12815	0.09594	**C75**	2.09745	0.19119	0.51011	**H264**	0.35112	0.8629	0.9206
C35	2.21243	0.08771	0.07001	**N112**	2.05486	-0.0916	0.49317	**C145**	0.49629	1.03337	0.78668
N67	1.97008	-0.89484	0.08023	**C133**	0.88544	-0.09107	0.53904	**C192**	1.02159	0.51778	0.7622
N71	1.16025	-0.9386	0.03658	**C134**	0.95469	0.00344	0.53805	**C209**	-0.03451	0.48636	0.75746
C73	0.94149	-0.04882	0.53069	**C137**	1.03284	-0.02206	0.50537	**C214**	0.47096	-0.02453	0.80149
C74	0.9803	-0.06207	0.52139	**N142**	1.07707	-0.86487	0.5192				

Section S7. SEM images

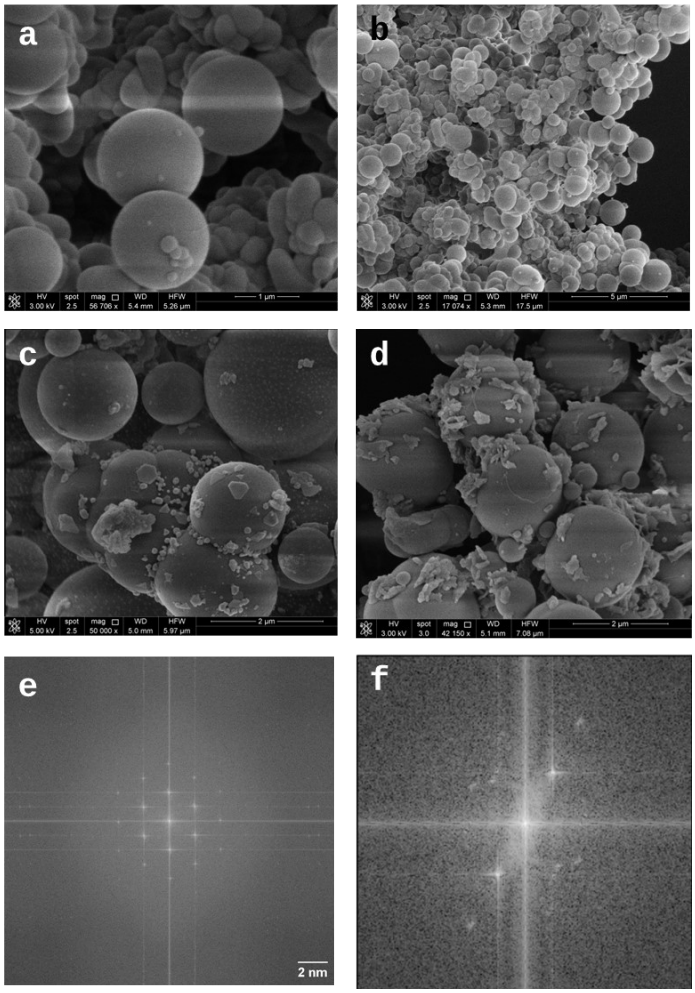


Figure S12. SEM images of (a,b) PGBpy showing presence of small spheres and sheets on the surface, c) Au@PGBpy, d) Au@PGBD, and TEM diffraction pattern of e) Au@PGBpy and f) Au@PGBD..

Section S8. X-ray photoelectron spectroscopic (XPS) studies

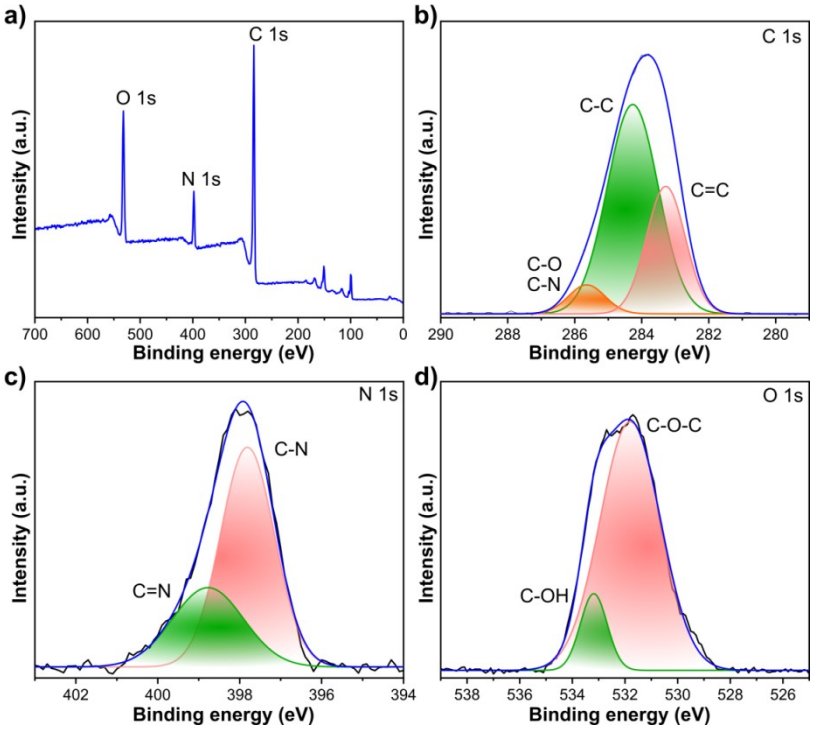


Figure S13. XPS profile of PGBpy a) full survey, and high resolution profile b) C1s, c) N 1s, and d) O 1s.

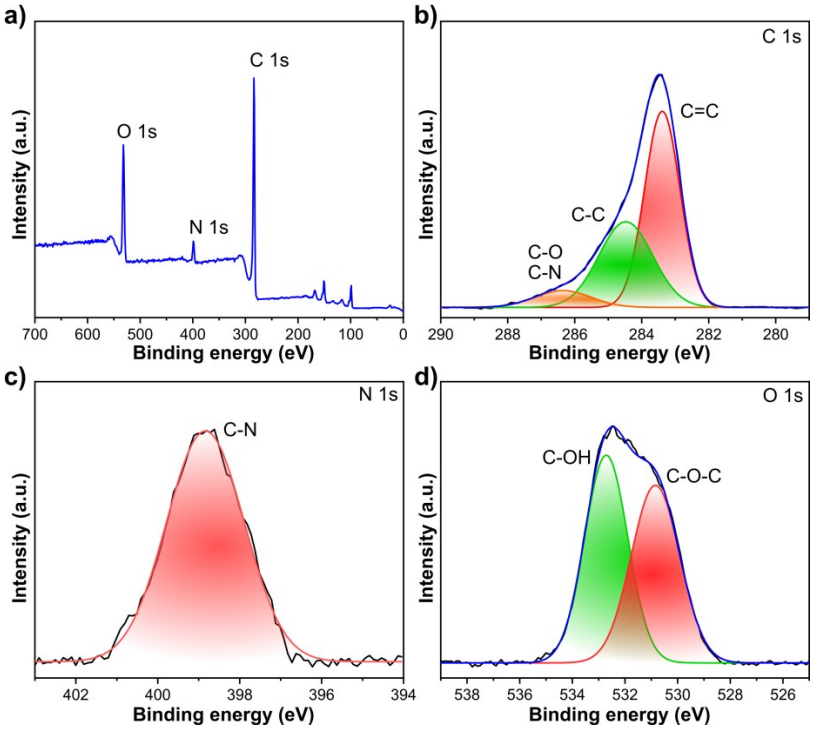


Figure S14. XPS profile of PGBD a) full survey, and high resolution profile b) C1s, c) N 1s, and d) O 1s.

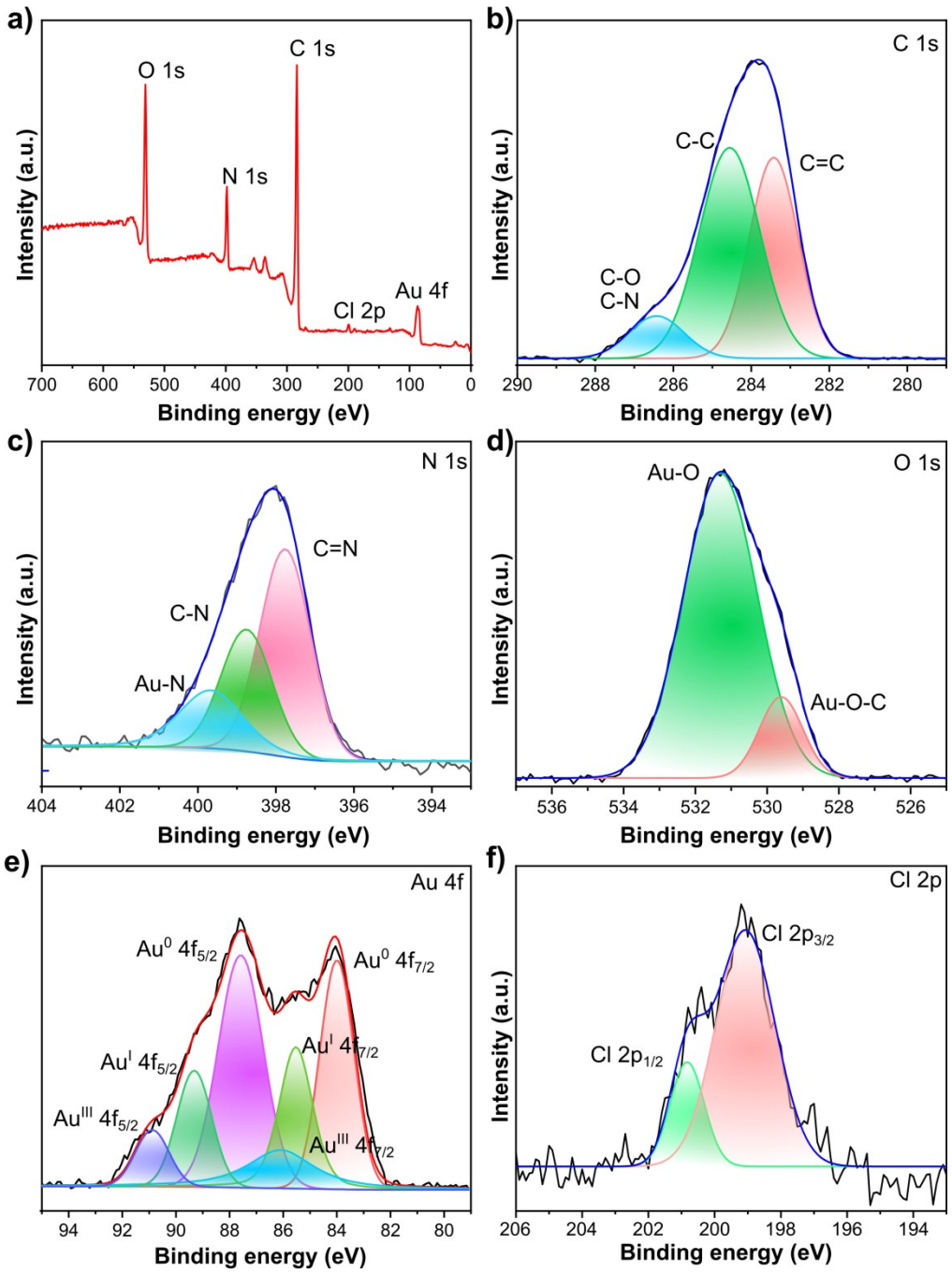


Figure S15. XPS profile of PGBpy recovered after gold adsorption a) full survey, and high-resolution profile b) C1s, c) N 1s, d) O 1s, e) Au 4f, and f) Cl 2p.

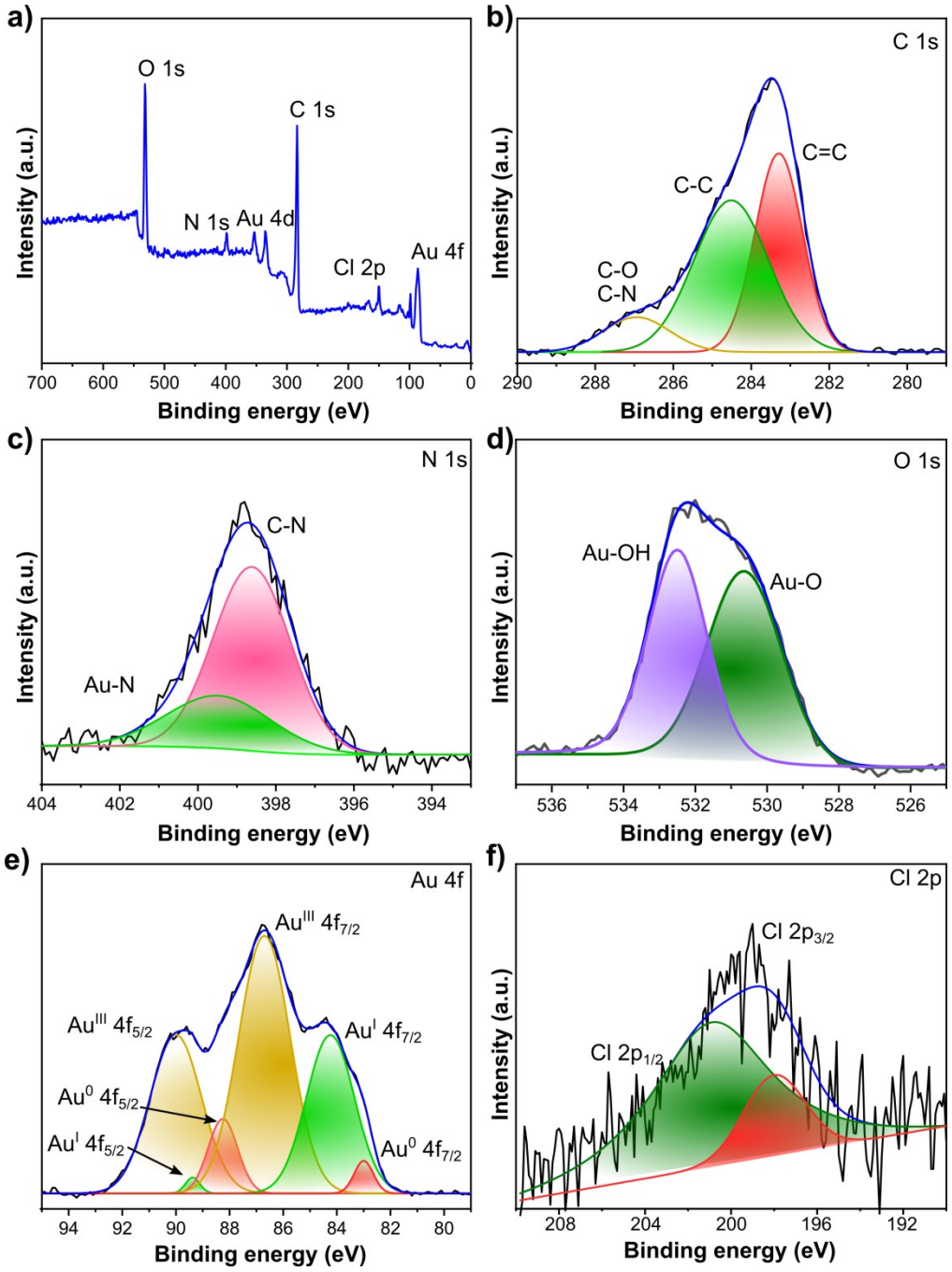


Figure S16. XPS profile of PGBD recovered after gold adsorption a) full survey, and high resolution profile b) C1s, c) N 1s, d) O 1s, e) Au 4f, and f) Cl 2p.

Table S7. Binding energy values observed for our synthesized COF before and after gold adsorption studies.

		PGBpy	**PGBD**		**Au@PGBpy**	**Au@PGBD**
C1s	C=C	283.28	283.38	C=C	283.42	283.29
	C-C	284.26	284.47	C-C	284.55	284.51
	C-O / C-N	285.64	286.34	C-O / C-N	286.42	286.94
N1s	$C=N_{Bpy}$	397.81	-	C=N…Au	397.76	-
	$C-N_{imine}$	398.77	398.82	C-N	398.78	398.64
				C-N…Au	399.68	399.58
O1s	$C-O_{ether}$	531.80	530.84	C-O…Au	529.60	530.64
	C-OH	533.18	532.71	C-OH…Au	531.30	532.49
Au				Au^0 $4f_{7/2}$	83.21	82.99
				Au^{1+} $4f_{7/2}$	83.99	84.23
				Au^{3+} $4f_{7/2}$	85.43	86.70
				Au^0 $4f_{5/2}$	87.48	88.24
				Au^{1+} $4f_{5/2}$	89.37	89.37
				Au^{3+} $4f_{5/2}$	91.39	90.03
Cl				$Cl2p_{3/2}$	199.07	197.96
				$Cl2p_{1/2}$	200.83	200.73

Section S9. Nitrogen gas uptake and pore size distribution profiles

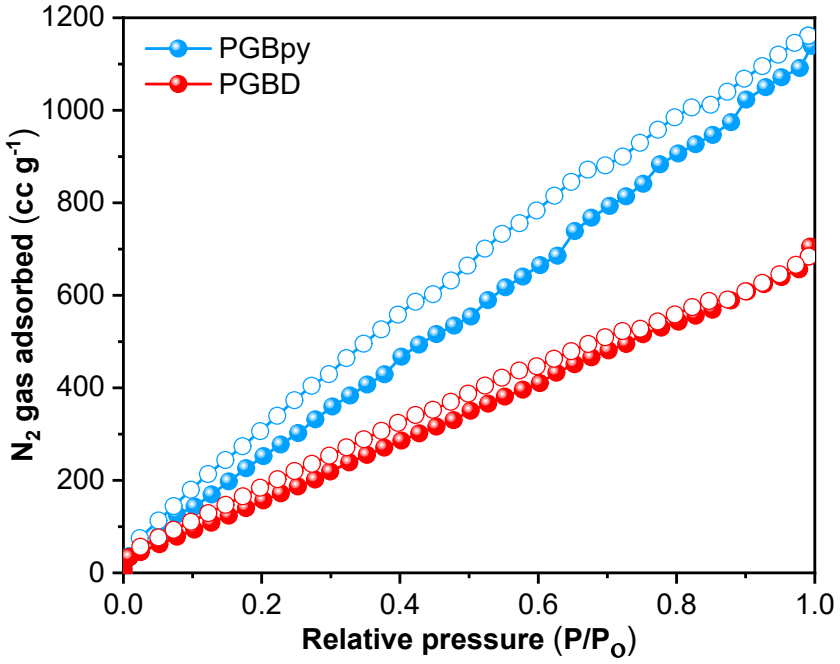


Figure S17. BET isotherm of PGBpy and PGBD suggest their mesoporous nature.

Table S8. Curve fitting data for BET sorption isotherm and summary.

PGBpy		
Relative Pressure, P/Po	**Volume, cc/g**	**BET summary**
2.28E-01	277.4936	Slope = 1.803 1/g Intercept = 4.33E-01 1/g Correlation coefficient (r) = 0.995761 C constant= 5.163 Surface Area = 1557.582 m²/g
2.53E-01	302.2773	
2.78E-01	331.8475	
3.02E-01	359.4928	
3.28E-01	383.4227	
3.53E-01	407.0266	
3.78E-01	429.0504	
4.02E-01	467.369	
PGBD		
2.77E-01	201.5613	**BET summary** Slope = 3.108 1/g Intercept = 6.31E-01 1/g Correlation coefficient (r) = 0.99301 C constant = 5.922 Surface Area = 931.362 m²/g
2.99E-01	219.0527	
3.27E-01	238.6891	
3.52E-01	255.0656	
3.77E-01	270.4776	
4.02E-01	285.9448	
4.28E-01	301.4239	

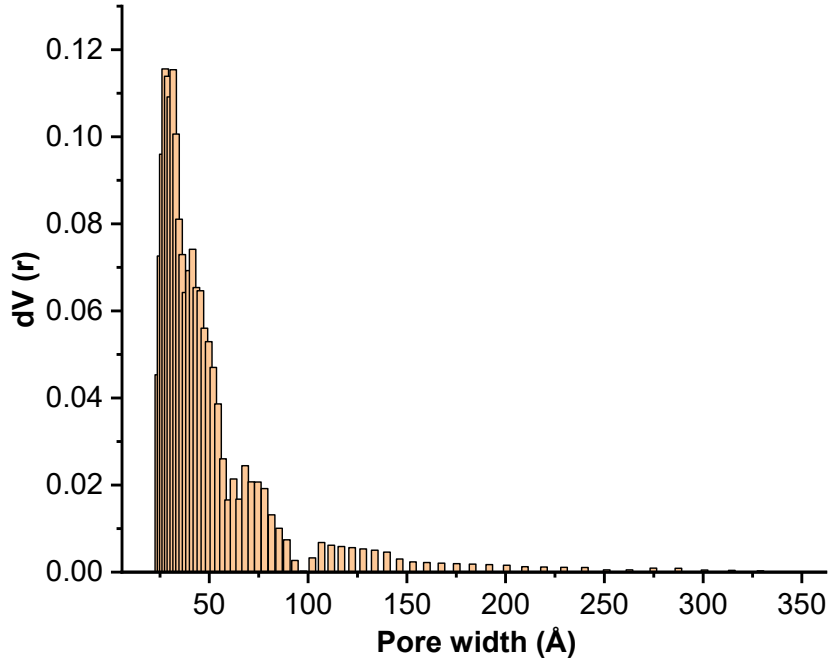


Figure S18 Pore size distribution curve for PGBpy.

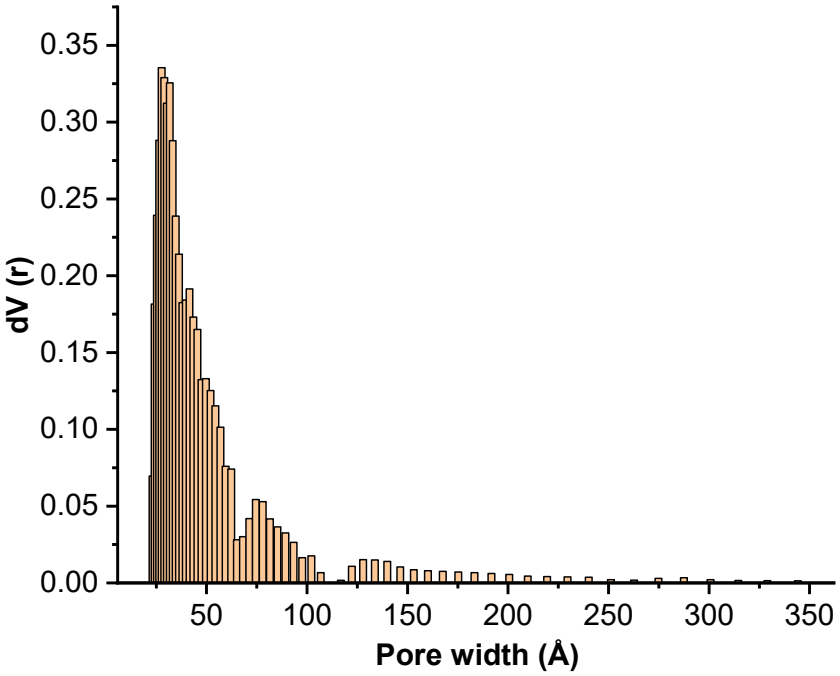


Figure S19. Pore size distribution curve for PGBD.

Section S10. Crystallite size calculation using Debye Scherrer equation

The domain size of the COF crystallites in the form of powder was calculated using Scherrer equation. This equation is generally used to correlate the size of crystallites in a solid to the broadening of the peak in the PXRD pattern. The calculation of integral breadth (β) was performed through Gaussian fitting of the high-intensity first peak that corresponds to the [100] plane. According to our findings, the size of the COF crystallites varies when the synthesis is performed using different green solvents.

The Scherrer equation can be written as:

$$\tau = \frac{K\lambda}{\beta cos\theta} \qquad \text{(eq. 1)}$$

Where, $\tau$is the size of the ordered (crystalline) domains, and K is a dimensionless shape factor with a value close to the unity. The shape factor varies with the actual shape of the crystallite. Herein we considered the shape factor value 0.94 in our calculations.$\lambda$is the X-ray wavelength (1.54178 Å) used for the measurement of the PXRD diffraction pattern of the COFs,β is the line broadening at half of the maximum intensity,θ is the Bragg angle.

PGBpy crystallite size = 2.81 Å

PGBD crystallite size = 1.99 Å

Section S11. Additional characterization data

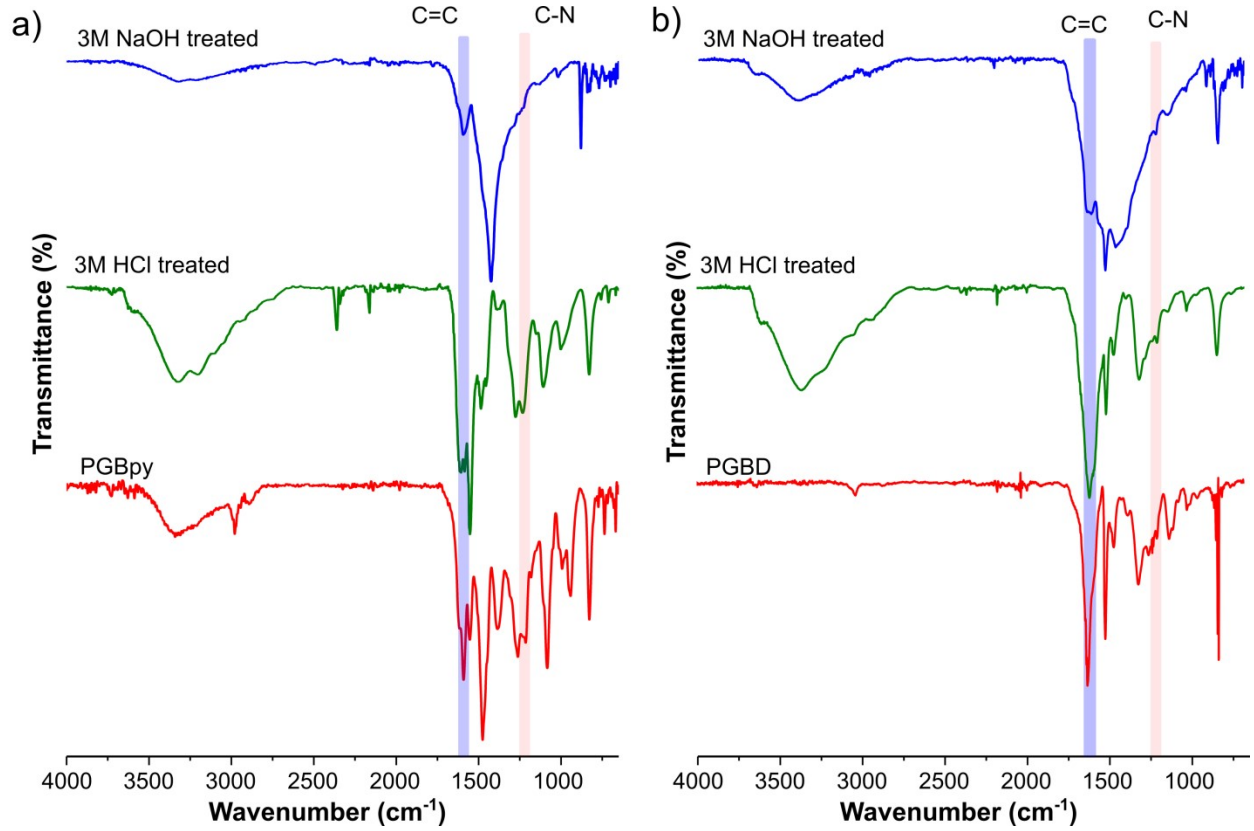


Figure S20. FTIR spectra of a) pristine **PGBpy** and b) PGBD after 3M HCl treatment and 3M NaOH treatment.

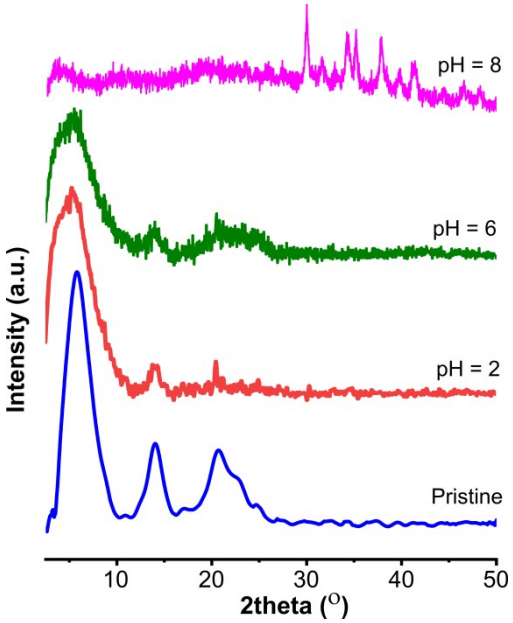


Figure S21. PXRD pattern of the pristine PGBpy COF and sample recovered after treatment at pH 2, 6, and 8.

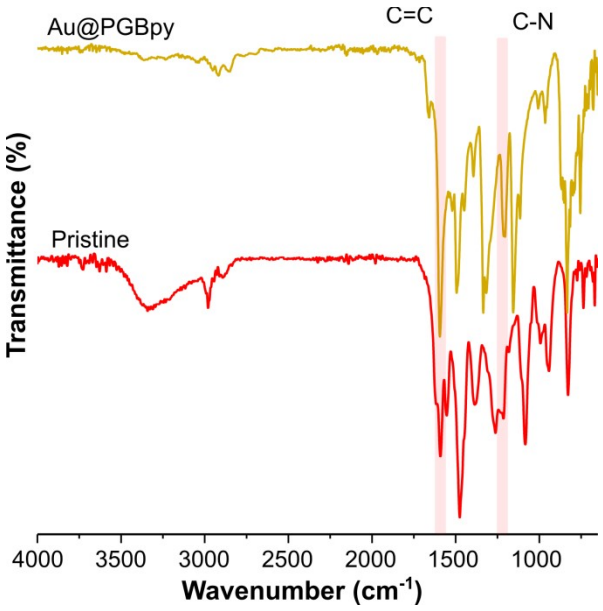


Figure S22. Comparison of FTIR spectra of a) pristine PGBpy and b) Au@PGBpy suggest a notable shift in the C-N stretch due to interaction with gold nanoparticles.

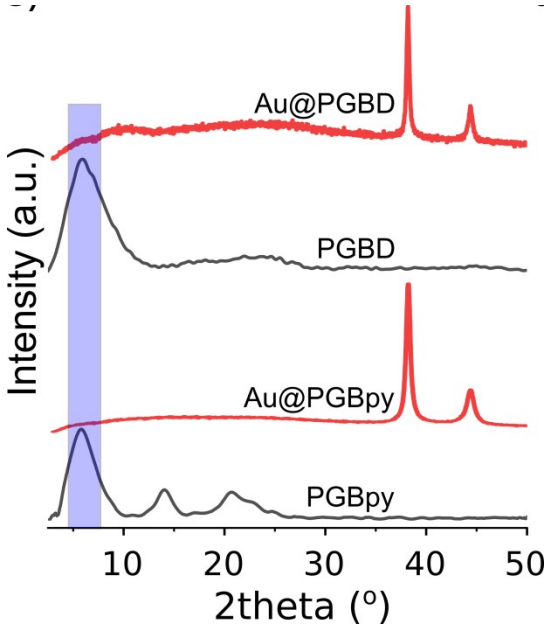


Figure S23.PXRD pattern of Au@PGBpy and Au@PGBD and their comparison with their pristine form.

Section S12. Gold adsorption studies

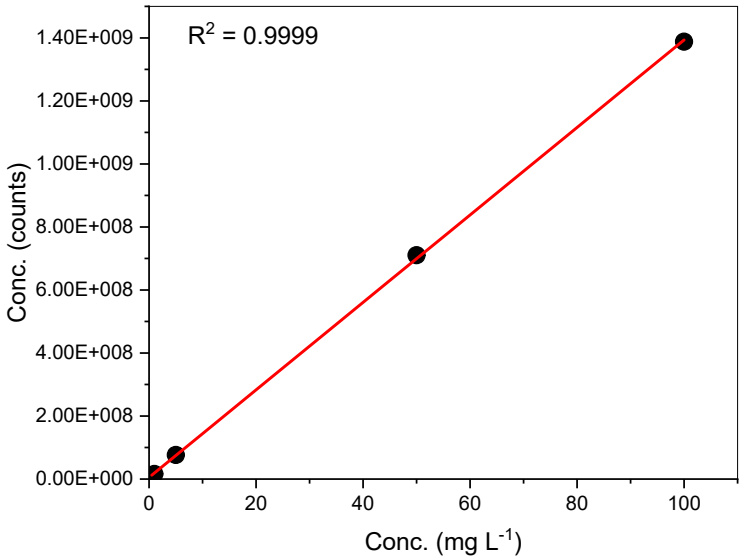


Figure S24. ICP calibration curve using different concentrations of gold chloride solution**.**

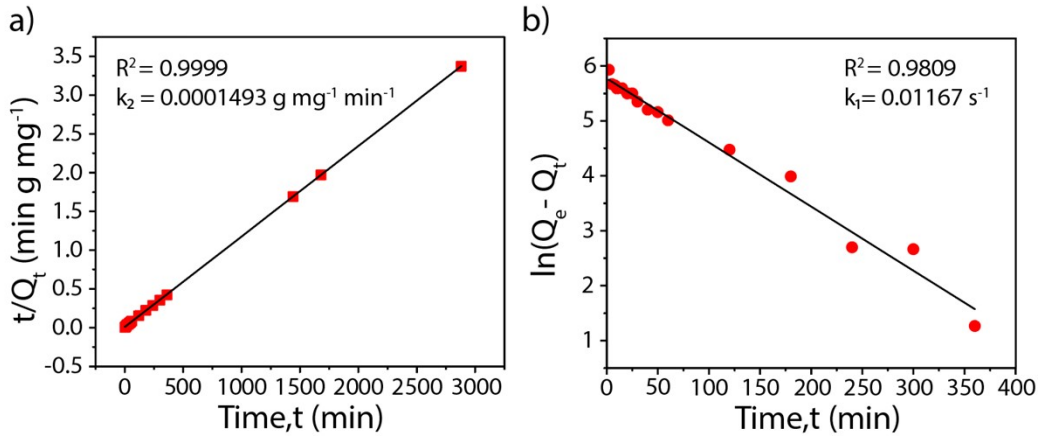


Figure S25. The linear fitting of a) pseudo-second and b) pseudo-first order kinetics for **PGBpy** in Au^{3+} uptake.

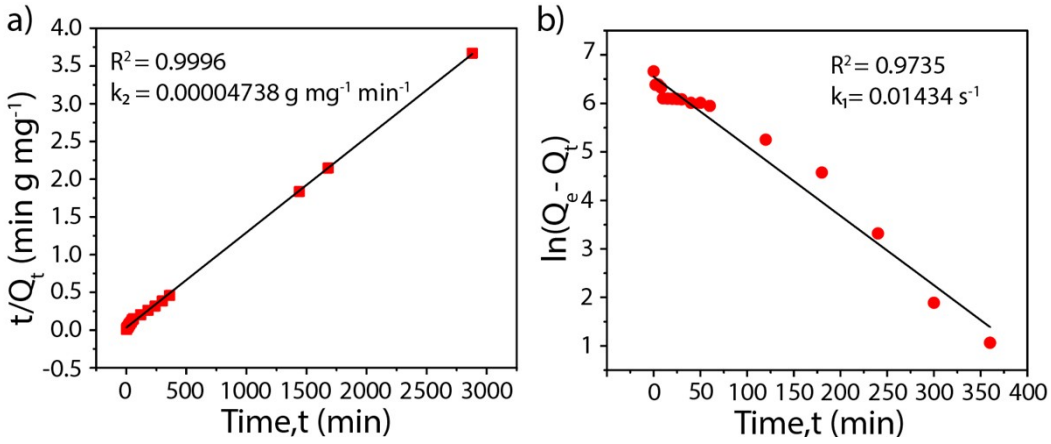


Figure S26. The linear fitting of a) pseudo-second and b) pseudo-first order kinetics for **PGBD** in Au^{3+} uptake.

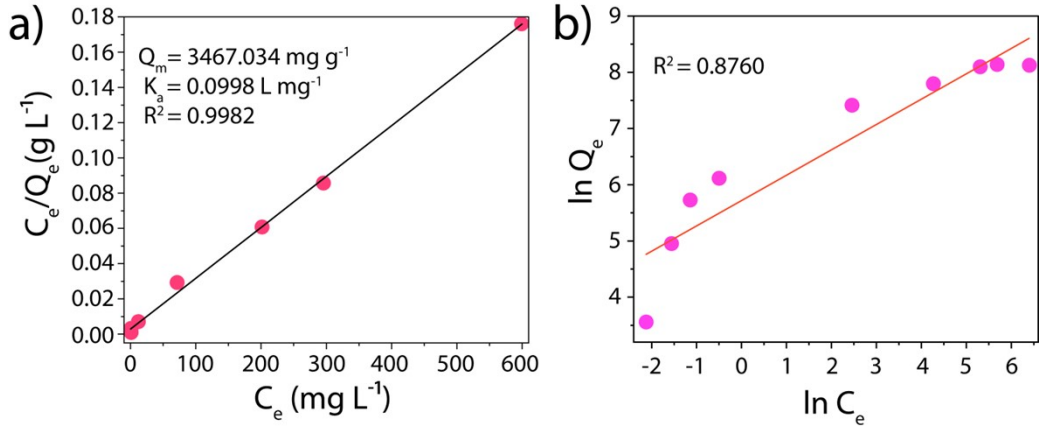


Figure S27. The Linear fitting of a) Langmuir and b) Freundlich isotherms for **PGBpy** in Au^{3+} uptake.

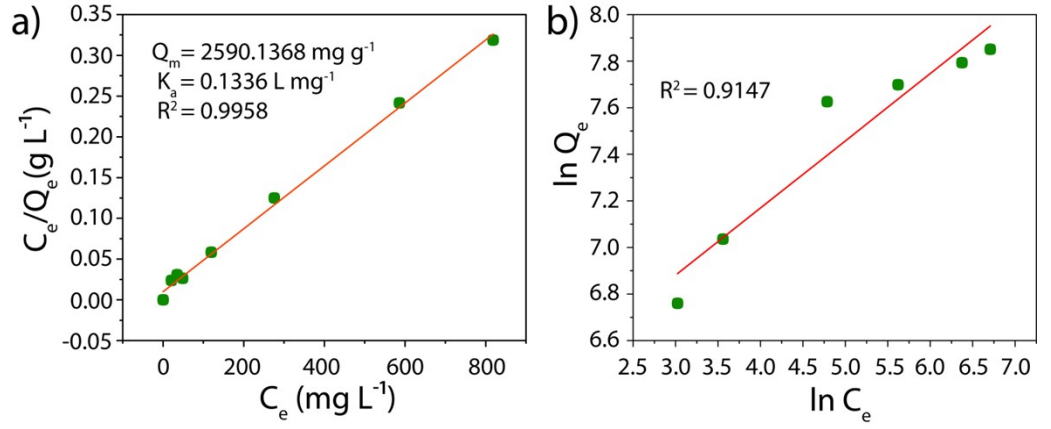


Figure S28. The Linear fitting of a) Langmuir and b) Freundlich isotherms for **PGBD** in Au^{3+} uptake.

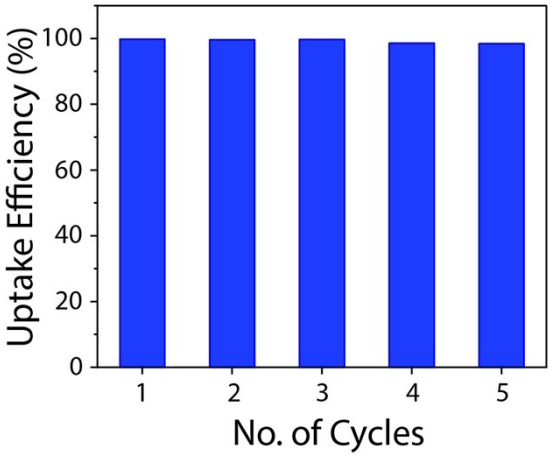


Figure S29. Adsorption performance of PGBD after each regeneration cycle.

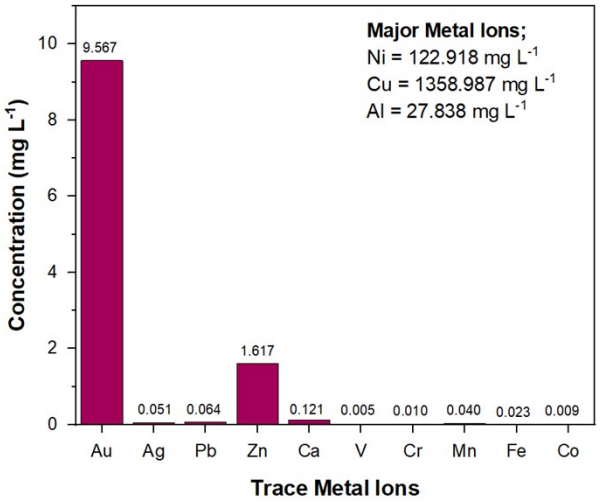


Figure S30. Concentration profile of metal ions in real e-waste leach solution prior to adsorption analysis. Bar graphs display elements present in lower concentrations, while the inset (top right) highlights metal ions with higher concentrations.

Table S9. The calculated selectivity parameters for each competing metal ions in simulated e-waste for PGBpy.

Metal ions (M)	Q_e (mg g^{-1})	K_d (L g^{-1})	$\alpha_{(Au/M)}$
Au	88.58276	53.01309	1
Cu	14.57092	0.391878	135.2795
Cr	12.46112	0.324949	163.1427
Al	7.548128	0.182988	289.7081
Zn	7.53967	0.184073	288.0003
Co	7.287405	0.175873	301.4278
Cd	6.670093	0.158843	333.7456

Table S10. The calculated selectivity parameters for each competing metal ions in real e-waste for PGBpy

Metal ions	**Q_e (mg g^{-1})**	**K_d (L g^{-1})**
Au	18.86038	137.86014
Ag	0.009272	0.199978
Pb	0.004122	0.06654267
Zn	<0.00	<0.00
Ca	<0.00	<0.00
V	<0.00	<0.00
Cr	<0.00	<0.00
Mn	<0.00	<0.00
Fe	<0.00	<0.00
Co	<0.00	<0.00
Ni	<0.00	<0.00
Cu	<0.00	<0.00
Al	<0.00	<0.00

From this, the separation factor for Au ions with respect to Ag and Pb were calculated as;

$\alpha_{(Au/Ag)}$=689.3765

$\alpha_{(Au/Pb)}$= 2071.755

Meanwhile, the separation factor with respect to rest of all metals tends to infinity, indicates the superior selectivity of PGBpy towards Au, compared to other metal ions present in the CPU leaching solution.

Table S11. The calculated selectivity parameters for each competing metal ions in simulated e-waste for PGBD.

Metal ions	**Q_e (mg g^{-1})**	**K_d (L g^{-1})**	**$\alpha_{(Au/M)}$**
Au	85.19579	25.3224	1
Cu	5.051532	0.120441	210.2473
Cr	8.826536	0.219756	115.2297
Al	2.008043	0.045617	555.1057
Zn	3.345807	0.077706	325.8736
Co	4.19237	0.097535	259.6227
Cd	1.822138	0.041025	617.2494

Table S12. The calculated selectivity parameters for each competing metal ions in real e-waste for PGBD

Metal ions	Q_e (mg g^{-1})	Kd (L g^{-1})
Au	55.727	23.27292
Ag	1.817	0.331479

Pb	0.0022	0.053012
Ni	0.004	0.133333
Cu	0.061	0.011821
Zn	<0.00	<0.00
Al	<0.00	<0.00
Ca	<0.00	<0.00
V	<0.00	<0.00
Cr	<0.00	<0.00
Mn	<0.00	<0.00
Fe	<0.00	<0.00
Co	<0.00	<0.00

From this, the separation factor for Au ions with respect to Ag, Pb, Ni and Cu were calculated as follows

$\alpha_{(Au/Ag)} = 70.2094$

$\alpha_{(Au/Pb)} = 439.0118$

$\alpha_{(Au/Ni)} = 174.5469$

$\alpha_{(Au/Cu)} = 1968.835$

Meanwhile, the separation factor with respect to rest of all metals tends to infinity, indicates the superior selectivity of PGBD towards Au, compared to other metal ions present in the CPU leaching solution.

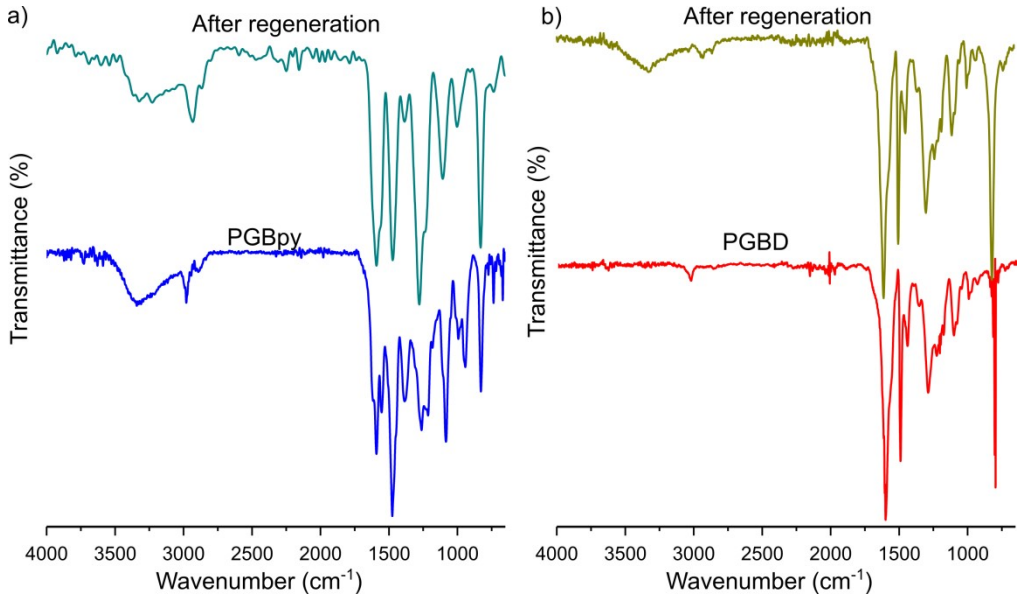


Figure S31. Comparison of PGBpy and PGBD with respective regenerated samples shows negligible change in the FTIR spectra.

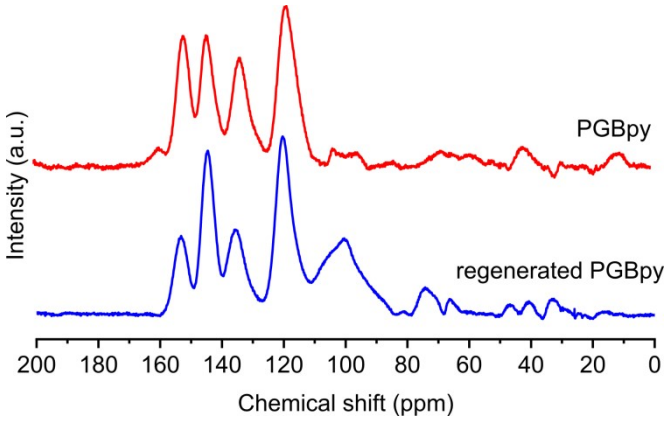


Figure S32. Comparison of solid state ^{13}C NMR of pristine PGBpy with the sample regenerated after gold adsorption studies.

Section S13. Particle size distribution and EDS mapping characterization studies

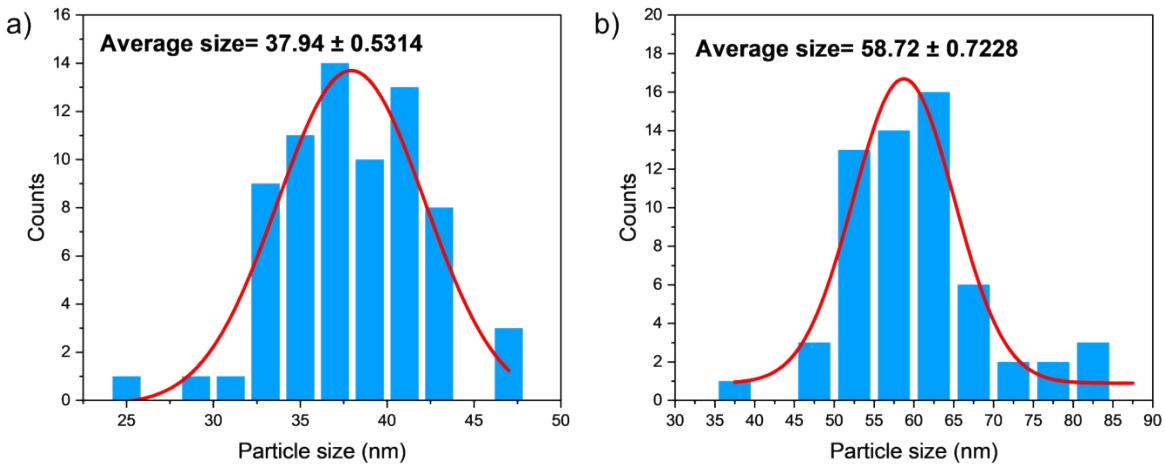


Figure S33. Average gold particle size distribution in a) Au@PGBpy, and b) Au@PGBD.

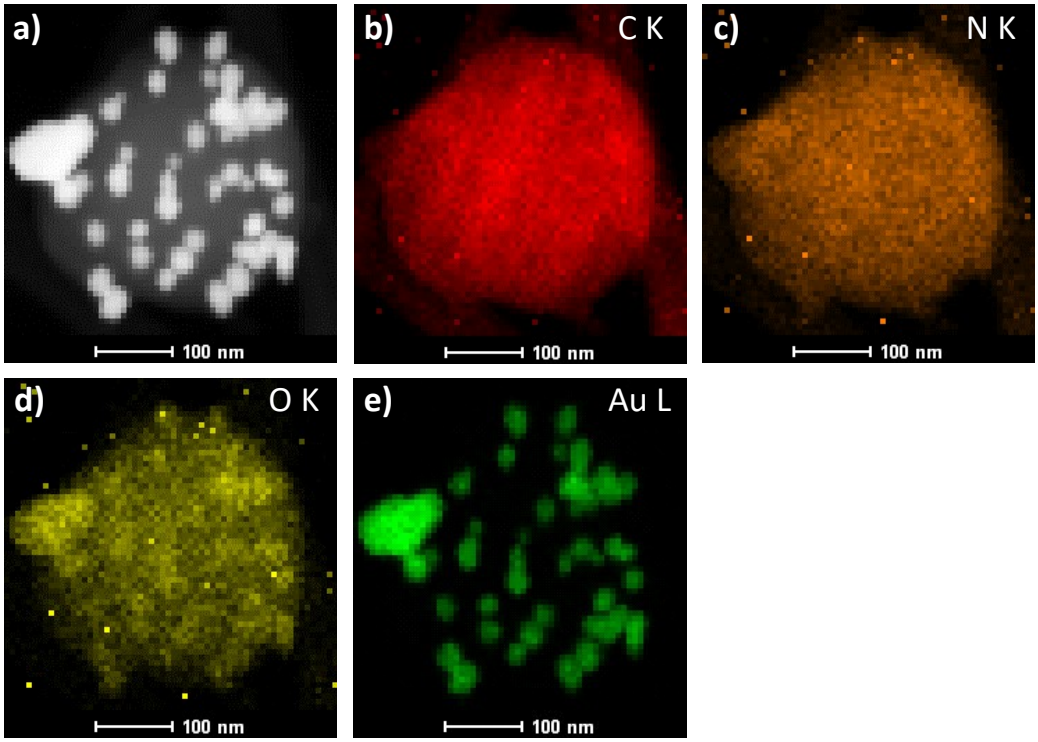


Figure S34. HAADF-STEM-EDS mapping of **Au@PGBpy** sample.

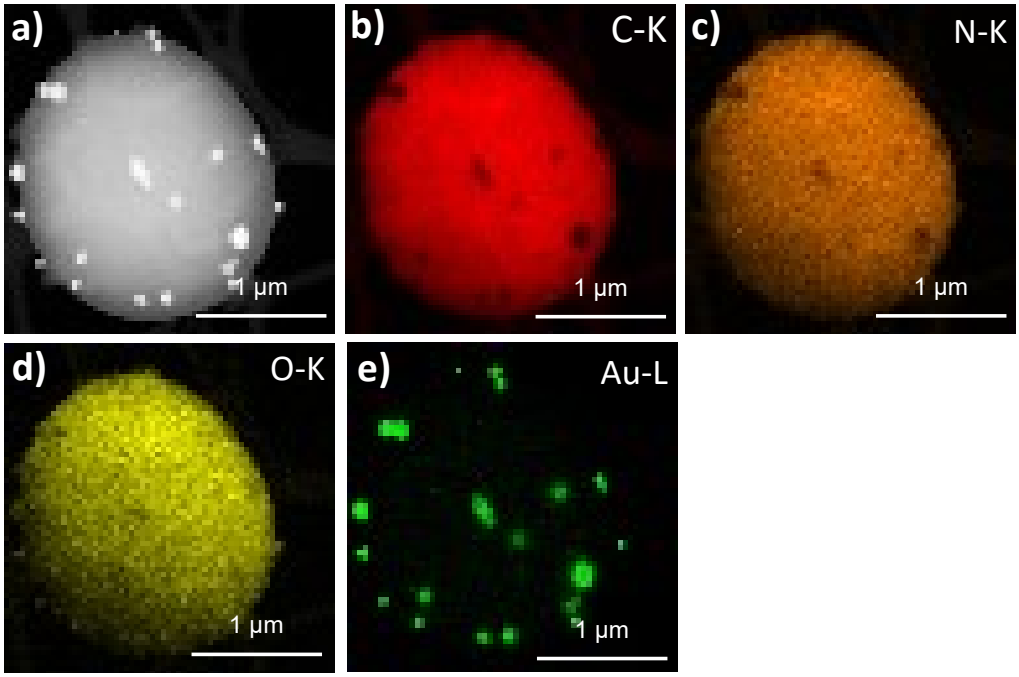


Figure S35. HAADF-STEM-EDS mapping of **Au@PGBD**.

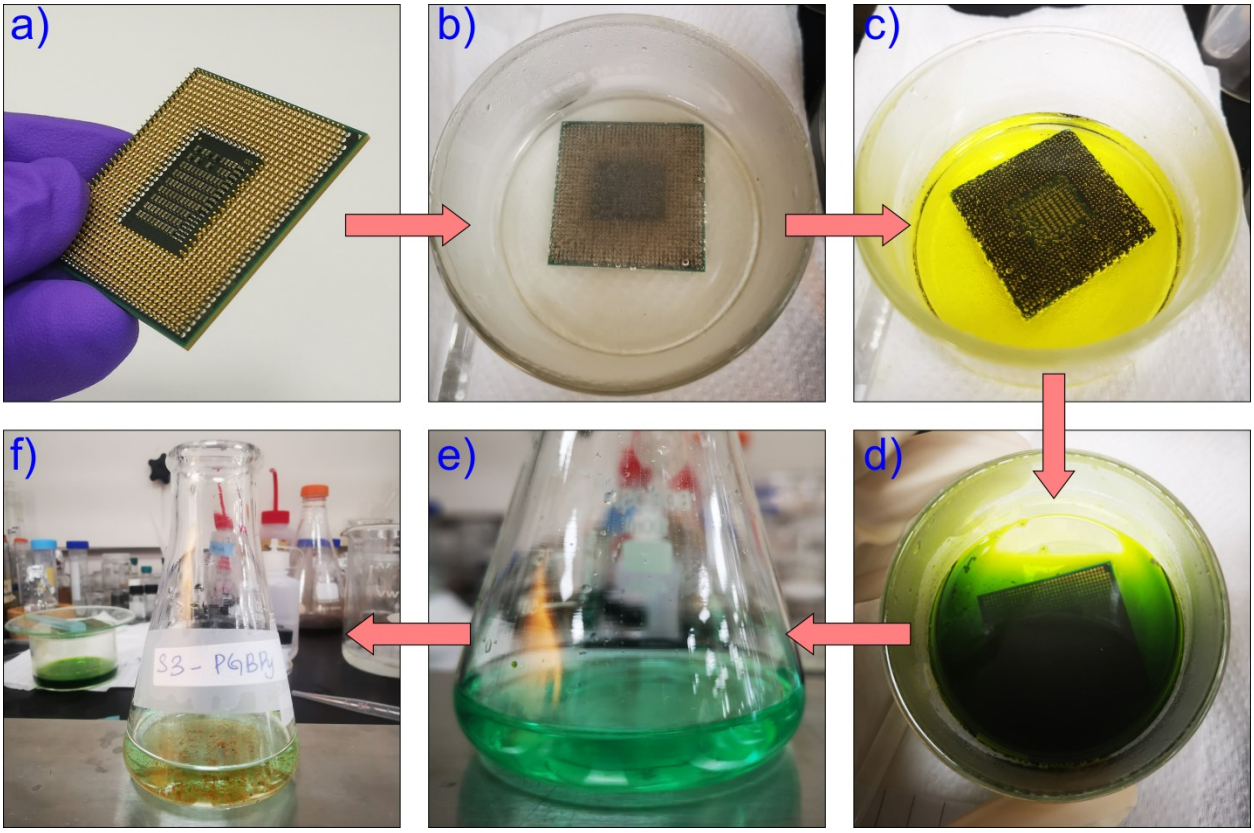


Figure S36. Gold recovery from e-waste using **PGBpy**. a) CPU used as a e-waste source, b) dissolution of metal content of the CPU under acidic conditions, c) solution turned yellow after 10 minutes, d) dark green-yellow solution suggesting complete dissolution of metal content of CPU chip in acidic solution, e) e-waste solution used for gold recovery studies, and f) e-waste solution containing **PGBpy** after gold adsorption.

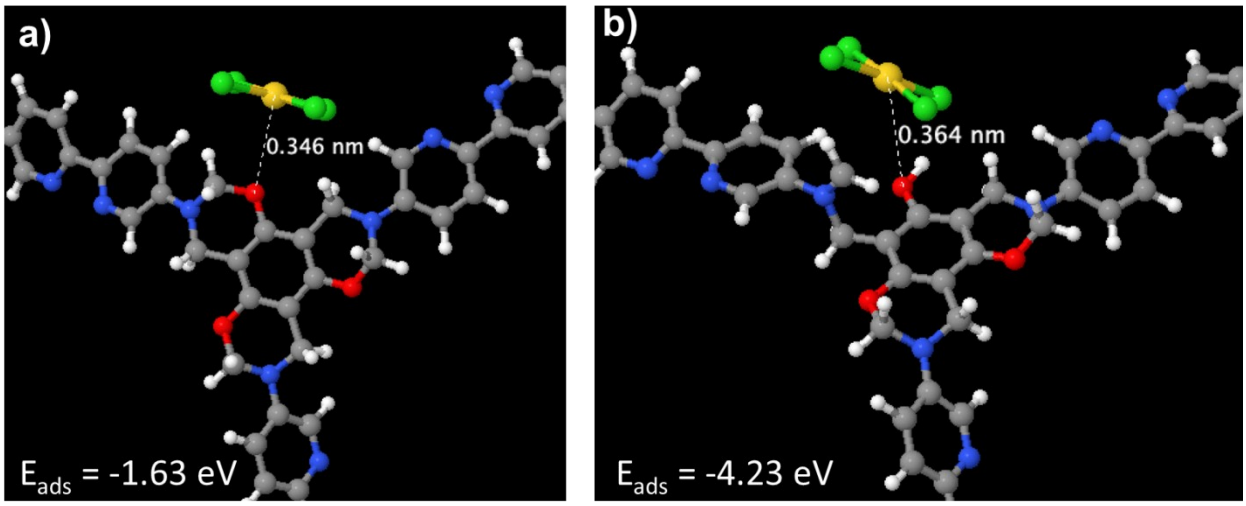


Figure S37. DFT calculation performed for calculating binding energy value $[AuCl_4]^-$ interacting with O_{ether} in **PGBpy** in a) unprotonated, and b) protonated state.

Table S13. Comparison of the equilibrium time and adsorption capacity of various materials employed for gold recovery.

Materials	Equilibrium time (min)	Q_m (mg g^{-1})	Reference
TSC functionalized corn bract	1440	1470	[1]
Methionine MOF	60	598	[2]
UiO-66-BTU	240	680	[3]
JNU-1	0.17	1124	[4]
COP	720	1945	[5]
TpTsc	2880	4400	[6]
DMC	20	~1000	[7]
IM-TUCS	240	933	[8]
TpTGCl	95	1794	[9]
COF-V-DTT	120	652	[10]
COF-V-S-β-CD	240	820	[10]
TTB-COF	1	560	[11]
JNM-100-AO	10	954	[12]
TzDa COF	30	1055	[13]
BMTA-TFPM COF	30	570	[14]
PYTA-COFs	10-60	1752-1180	[15]
NH_2-CTF-1	20	870	[16]

MTpPa-1	180	1737	[17]
S-COF	300	100	[18]
Tp-BTD	3600	3095	[19]
CF-COF	95	1794	[9]
COF-HNU25	8	1725	[20]
TyHz	3	1008	[21]
MoS2-TpTa	360	2565	[22]
ECUT-COF-29	60	3714	[23]
TpDa	360	982	[24]
PGBpy	1440	3467	This work
PGBD	1440	2590	This work

[a] IM-TUCS = thiourea modified chitosan imprinted resin, DMC = dithiocarbamate modified cellulose.

Table S14. Standard electrode reduction potential (V) in water at 25°C under acidic conditions.

S. No.	Metal ion	Reduced state	E^o (V)
1.	$[AuCl_4]^-$	Au^0	1.002
2.	Ag^{1+}	Ag^0	0.80
3.	Pb^{4+}	Pb^{2+}	1.45
4.	Co^{2+}	Co^0	-0.27
5.	Zn^{2+}	Zn^0	-0.76
6.	Ni^{2+}	Ni^0	-0.25
7.	Al^{3+}	Al^0	-1.67
8.	Ca^{2+}	Ca^0	-2.84
9.	V^{3+}	V^{1+}	1.0
10.	Cr^{6+}	Cr^{3+}	1.33
11.	Mn^{7+}	Mn^{2+}	1.51
12.	Fe^{3+}	Fe^{2+}	0.77
13.	Cu^{2+}	Cu^0	0.34

Section S14. Ion adsorption energies and kinetics modeling under acidic conditions

To elucidate the origin of the exceptional selectivity of the PGBpy covalent organic framework (COF) toward Au^{3+} ions under acidic conditions, and as a proof-of-concept, we performed a detailed theoretical investigation combining first-principles adsorption energy calculations and kinetic modeling with the Gaussian16 atomistic simulation package [1]. To include the environmental acidic solvent effect in these new calculations we have adopted an implicit solvation model, the polarizable continuum model (PCM) [J. Tomasi, B. Mennucci, R. Cammi, "Quantum Mechanical Continuum Solvation Models." Chem. Rev. 105(8), 2999-3094 (2005)] for a formic acid solvent, with a pH~3 and a dielectric constant of 57.3, The experimental adsorption process was carried out in strongly acidic media (pH ~ 2-4), in which the bipyridine (Bpy) and amine-based (N_{amine}) coordination sites of the framework are likely protonated, forming -NH^+ species. This protonation significantly alters the electronic properties of these donor atoms, reducing their classical Lewis basicity and changing the nature of metal-ligand interactions within the framework. Therefore, all our additional density functional theory (DFT) calculations of ion–COF interactions were conducted using the protonated COF fragment as the adsorption substrate (see Figure S37).

We evaluated the adsorption energies (ΔE_{ads}) for the representative set of metal ions: Au^{3+}, Cu^{2+}, Co^{2+}, Al^{3+}, Zn^{2+}, Cr^{3+}, and $Cd2^+$. The computed values reveal a clear thermodynamic preference for Au^{3+}, which binds coplanarly to the Bpy moiety with an adsorption energy of -2.07 eV, significantly stronger than Cu^{2+} (-1.23 eV), Co^{2+} (-0.68 eV), Al^{3+} (-0.31 eV), and significantly above the weakly bound Zn^{2+}, Cr^{3+}, and Cd^{2+} (-0.09 to -0.05 eV). These results indicate that even in the presence of protonation, the COF retains a strong thermodynamic affinity for Au^{3+}.

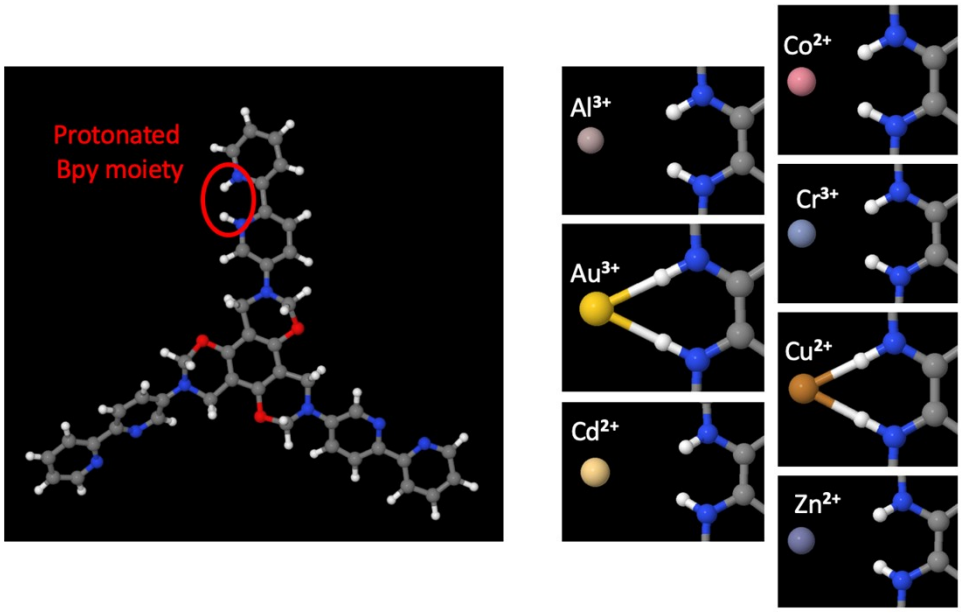


Figure S38. (Left) Protonated COF fragment. (Right) Interaction of metal ions with protonated Bpy moiety within the COF fragment.

This pronounced selectivity may be rationalized by several key factors: i) Chemical Softness and Polarizability of Au^{3+}. Au^{3+} is a highly polarizable soft acid, in accordance with Pearson's HSAB theory. Even in its naked ionic form, it exhibits significant electron-cloud deformability and can engage in strong dispersion-enhanced and partially covalent interactions with soft donor atoms, such as nitrogen and oxygen, even when these are protonated. By contrast, harder cations such as Al^{3+} and Cr^{3+}, which are small and highly charged, prefer to coordinate with hard donor atoms (e.g., carboxylates or phosphates), and show negligible affinity for the protonated and flexible N,O-containing environments of the COF, ii) Electrostatic and Hydrogen Bonding Effects in Acidic Media. Although protonation reduces the formal availability of lone pairs on the nitrogen atoms, hydrogen bonding, cation-π interactions, and induced dipole effects remain operative. The protonated NBpy and Namine sites can still polarize around incoming cations, particularly for highly polarizable species like Au^{3+}. These interactions are far more effective for gold than for more hydrated, hard, and symmetrical metal cations such as Zn^{2+} or Al^{3+}, which tend to remain solvated and exhibit weak, non-directional interactions with the framework, and iii) Ionic Size and Desolvation Energies. The effective ionic radius of Au^{3+} (around ~85 pm) is compatible with the pore sizes and local geometry of PGBpy. Moreover, its relatively low hydration energy (compared to Al^{3+} or Cr^{3+}) makes it more readily desolvated and thus more likely to engage in direct interactions with the framework. In contrast, smaller and more hydrated cations, such as Al^{3+} or Co^{3+}, exhibit strong solvation shells in aqueous solution that hinder direct adsorption onto the framework, particularly in the presence of protons that compete for binding.

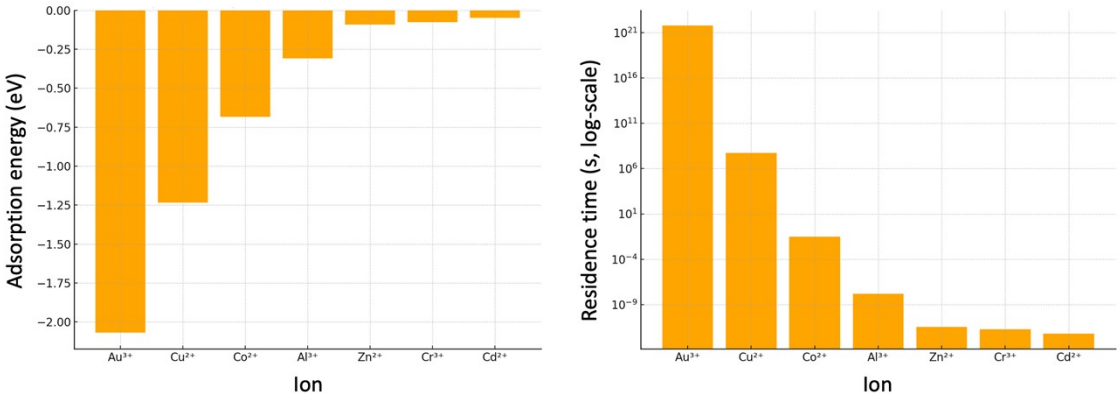


Figure S39. (Left) Adsorption energies, in eV, of metal ions on protonated COF. (Right) Residence time (in s and log-scale at 300 K) of metal ions on protonated COF.

Kinetic Retention – Residence Time Modeling. To assess not only the thermodynamics but also the kinetic persistence of each ion once adsorbed, we calculated the average ion residence time τ by using the Arrhenius expression:

$$\tau = \frac{1}{\nu} e^{\left(\frac{|\Delta E_{ads}|}{k_B T}\right)},$$

where ν is the attempt frequency (typically adopted as 10^{13} s^{-1}), ΔE_{ads} is the ion adsorption energy and T is the temperature (300 K in the present case). The calculated τ for Au^{3+} exceeds 10^{21} s, while for Cu^{2+} it falls several orders of magnitude below 10^{7} s, and for Al^{3+}, Cd^{2+}, Zn^{2+} and Cr^{3+} it drops to microseconds or nanoseconds (see Figure S38 and Table S15). This exponential sensitivity confirms that even moderate differences in ΔE_{ads} lead to orders-of-magnitude differences in retention times, explaining the experimentally observed selectivity under dynamic conditions. The combination of (i) strong thermodynamic interaction of Au^{3+} with the protonated framework, (ii) favorable chemical softness and polarizability of gold, (iii) weak competition from other cations due to charge, size and solvation effects, and (iv) vastly superior kinetic retention, together explain the exceptional selectivity of PGBpy toward Au^{3+} under acidic conditions. These insights offer a predictive framework for the rational design of next-generation adsorbents based on heteroatom-rich, protonation-tolerant COFs for selective metal ion recovery.

It should be noted that the approach employed here - based on static adsorption energy calculations and kinetic modeling via Arrhenius-type expressions - does not fully capture the complexity of ionic competition or dynamic transport phenomena in aqueous media, such as ion–ion correlations, solvent-mediated interactions, or diffusion-limited kinetics. Nevertheless, the combination of adsorption energies and estimated residence times provides a robust and physically meaningful descriptor of ion affinity under acidic conditions. The trends observed are in excellent agreement with the experimental selectivity data, supporting the utility of this theoretical framework for rationalizing and predicting the behavior of COF-based adsorbents.

Table S 15. Adsorption Energies and Residence Times at 300 K.

Ion	**Adsorption Energy (eV)**	**Residence Time (s)**
Au^{3+}	-2.0692	5.768e+21
Cu^{2+}	-1.2346	5.500e+07
Co^{2+}	-0.6844	3.144e-02
Al^{3+}	-0.3082	1.505e-08
Zn^{2+}	-0.0918	3.485e-12
Cr^{3+}	-0.0766	2.239e-13
Cd^{2+}	-0.0481	7.098e-15

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