Electronic Supplementary Information

Catalyst-free and efficient fabrication of highly crystalline fluorinated covalent organic frameworks for selective guest adsorption†

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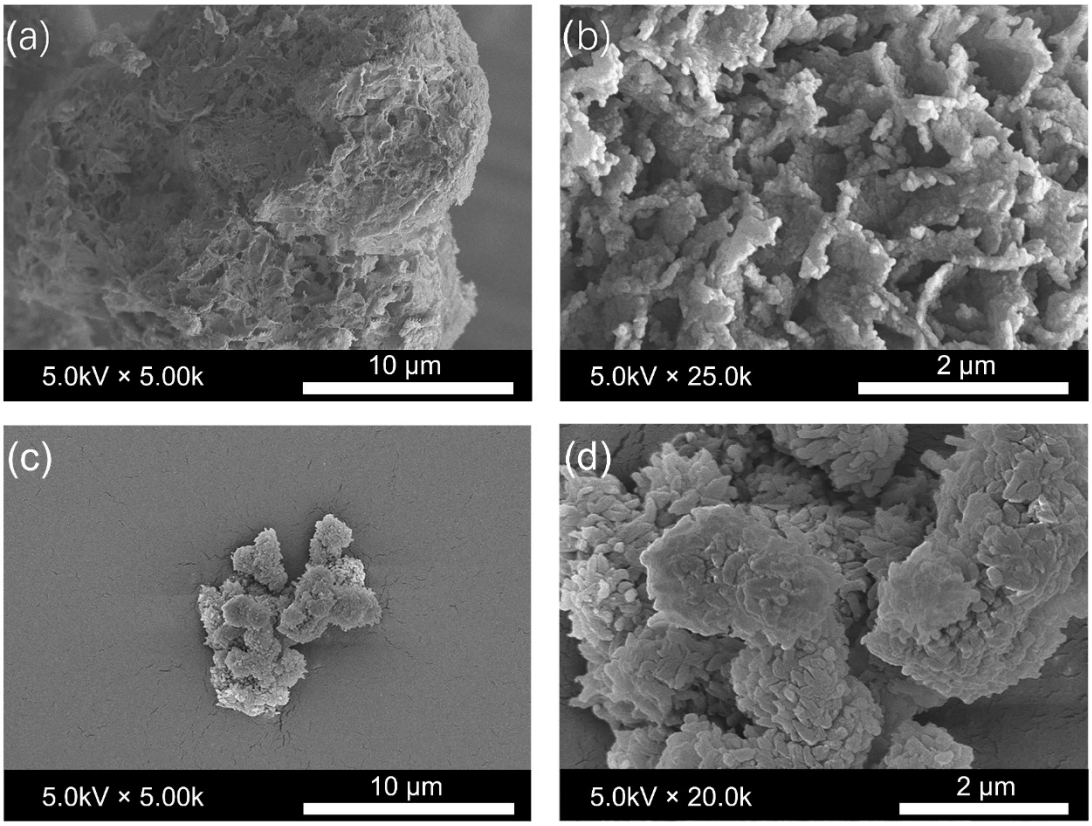


Figure S1.SEM images of (a), (b) SCF-FCOF-1; (c), (d) SCF-FCOF-2. Magnification: a) 5.00k (scale bar: 10µm); b) 25.0k (scale bar: 2µm); c) 5.00k (scale bar: 10µm); d) 20.0k (scale bar: 2µm).

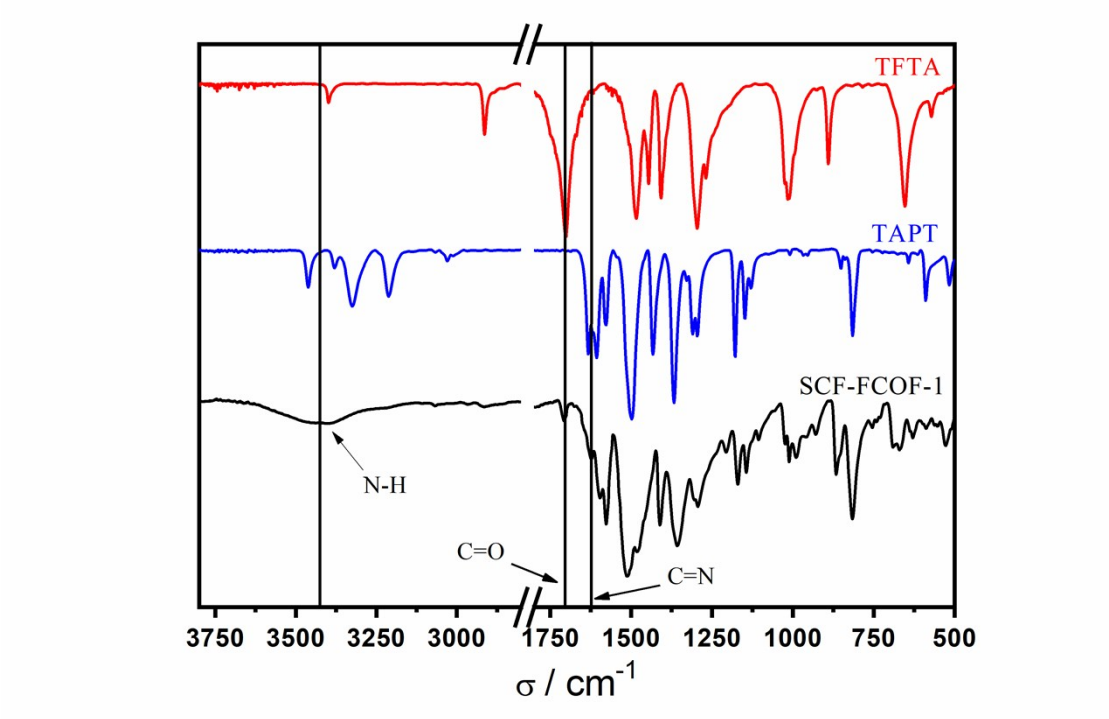


Figure S2. FT-IR spectra of monomers TFTA (red), TAPT (blue) and SCF-FCOF-1 (black).

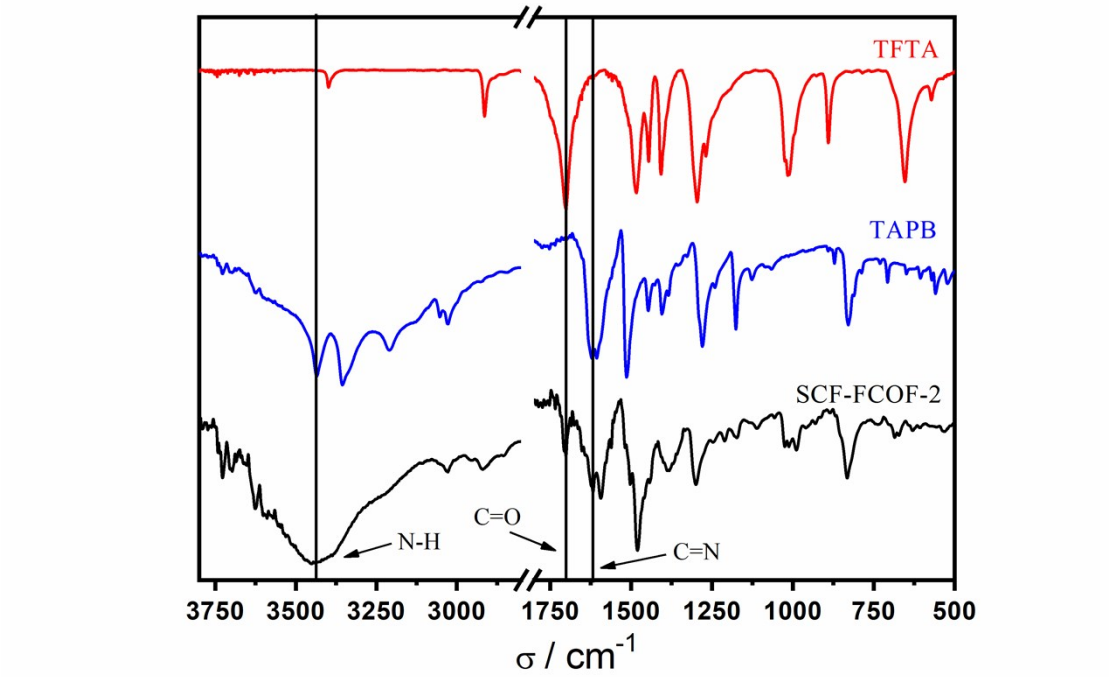


Figure S3. FT-IR spectra of monomers TFTA (red), TAPB (blue) and SCF-FCOF-2 (black).

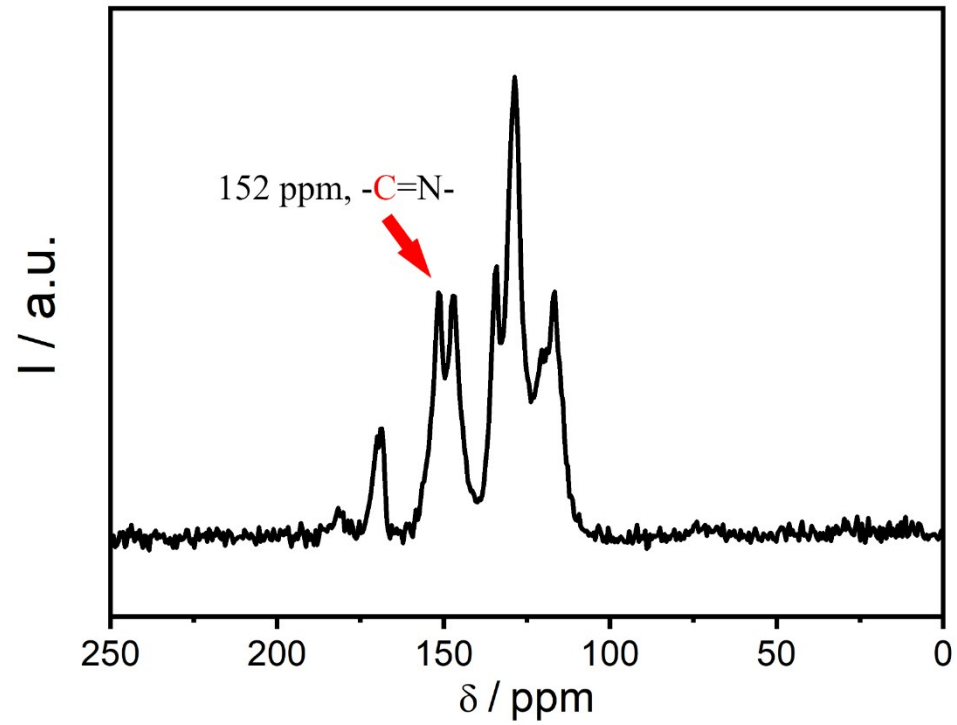


Figure S4. ^{13}C CP/MAS NMR spectrum of SCF-FCOF-1.

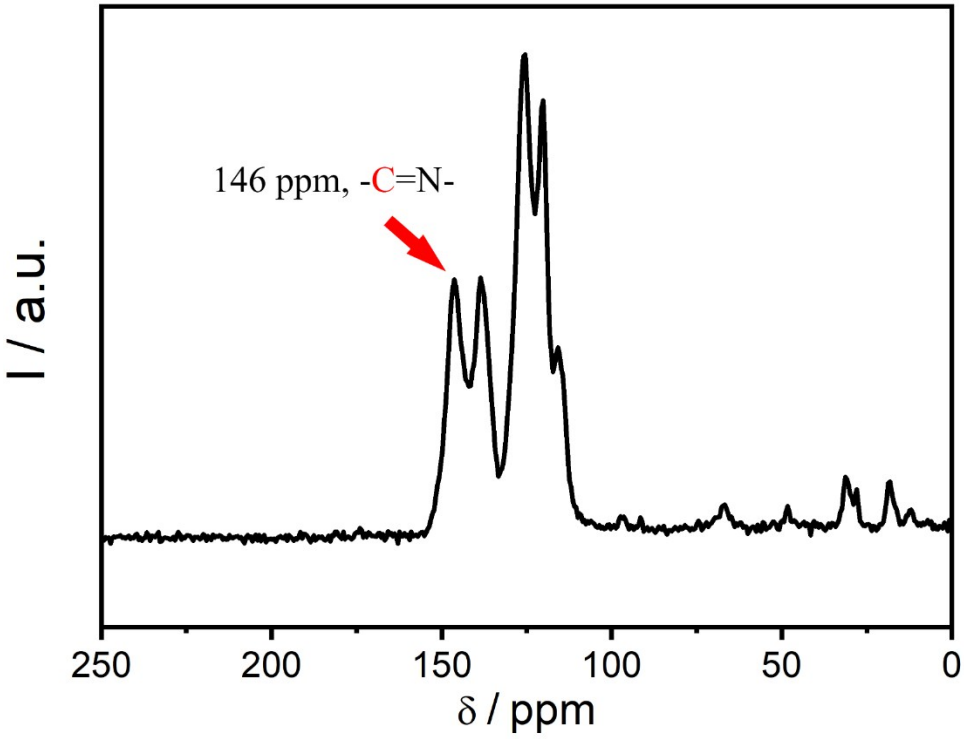


Figure S5. ^{13}C CP/MAS NMR spectrum of SCF-FCOF-2.

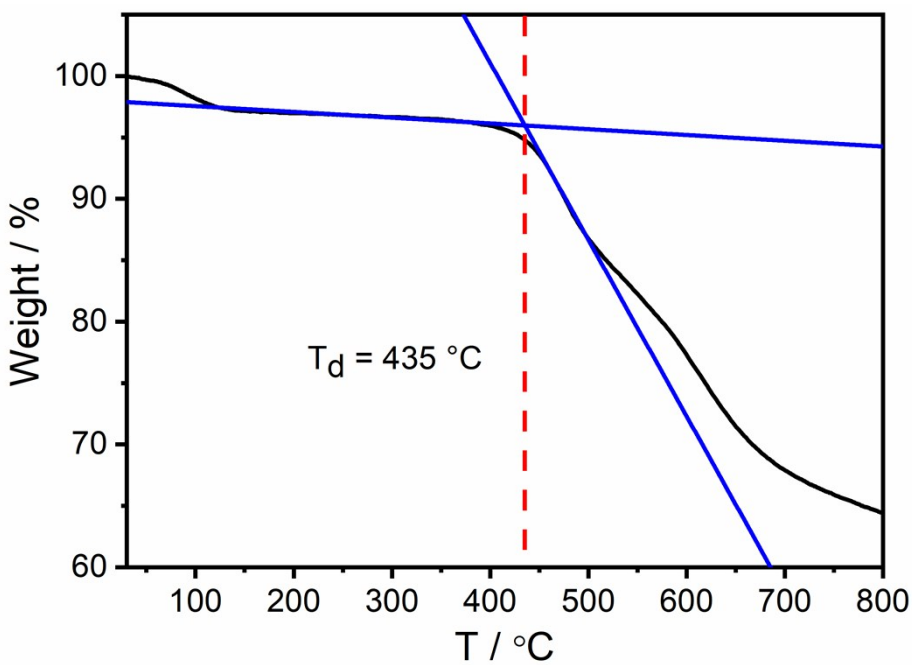


Figure S6. TGA of SCF-FCOF-1 in N_2 atmosphere (black). The decomposition temperature (T_d) was calculated from the intersection of the baseline and the tangent line (blue) in the TGA curves.

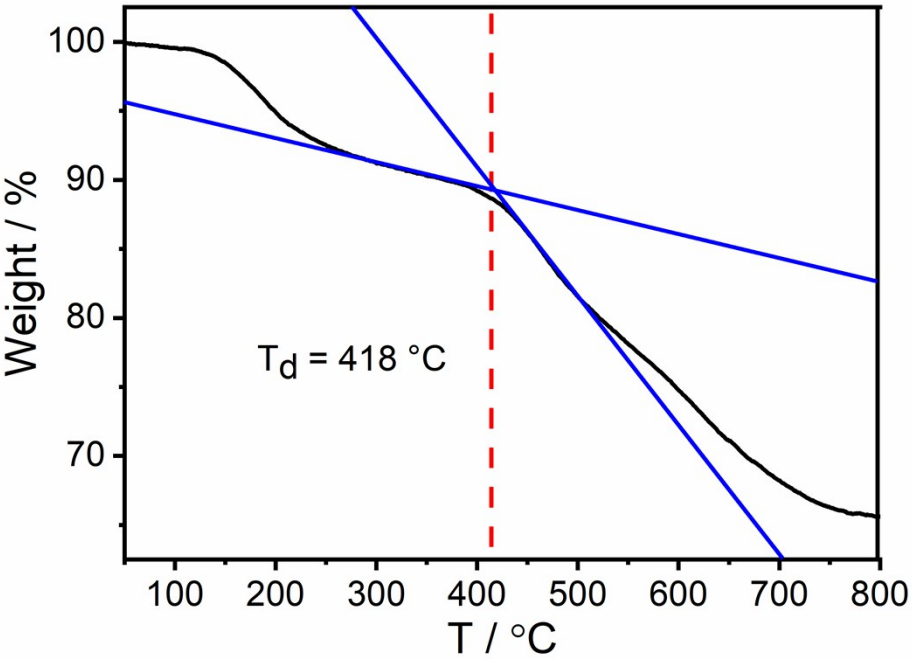


Figure S7. TGA of SCF-FCOF-2 in N_2 atmosphere (black). The decomposition temperature (T_d) was calculated from the intersection of the baseline and the tangent line (blue) in the TGA curves.

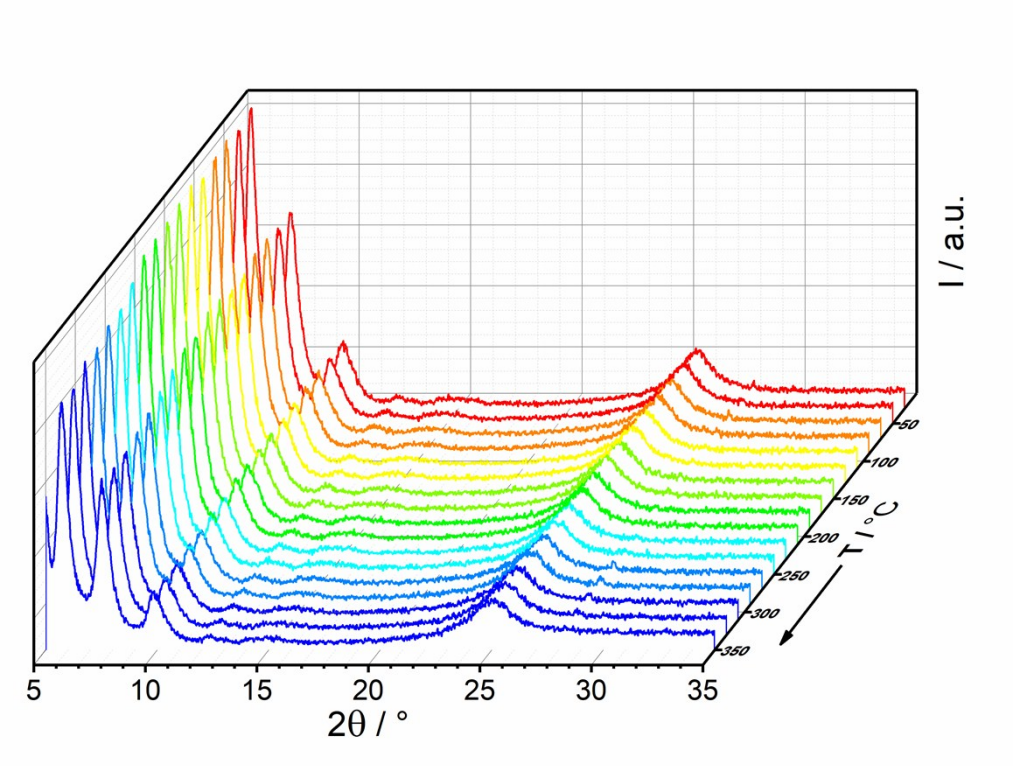


Figure S8. In-situ PXRD patterns for SCF-FCOF-1 range from 30 °C to 350 °C under vacuum.

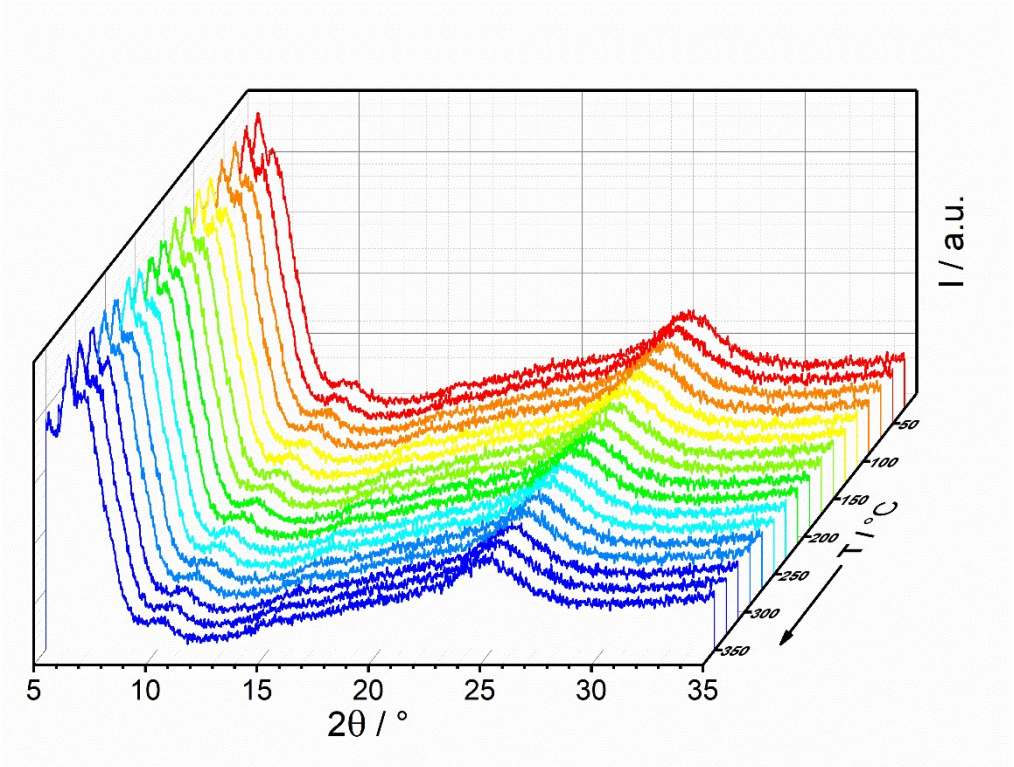


Figure S9. In-situ PXRD patterns for SCF-FCOF-2 range from 30 °C to 350 °C under vacuum.

Table S1. Fractional atomistic coordinates for the unit cell for SCF-FCOF-1 with eclipsed (AA) stacking mode optimized using the Forcite module.

SCF-FCOF-1 with eclipsed (AA) stacking mode				Space group symmetry: 1 P1 a = b = 37.492 Å c = 3.446 Å α = β = 90° γ = 120°			
Atom	x (Å)	y (Å)	z (Å)	Atom	x (Å)	y (Å)	z (Å)
C1	0.02784	0.48541	0.50000	F19	0.05391	0.47014	0.50000
C2	0.04288	0.52821	0.50000	F20	0.02787	0.58337	0.50000
C3	0.01454	0.54237	0.50000	C21	0.51459	0.54243	0.50000
C4	0.08758	0.55857	0.50000	C22	0.47179	0.51468	0.50000
N5	0.11476	0.54673	0.50000	C23	0.45763	0.47217	0.50000
C6	0.15886	0.57243	0.50000	C24	0.44143	0.52901	0.50000
C7	0.18252	0.55307	0.50000	N25	0.45327	0.56803	0.50000
C8	0.24580	0.61944	0.50000	C26	0.42757	0.58643	0.50000
C9	0.22208	0.63895	0.50000	C27	0.44693	0.62945	0.50000
C10	0.17908	0.61579	0.50000	C28	0.38056	0.62636	0.50000
C11	0.29139	0.64404	0.50000	C29	0.36105	0.58313	0.50000
C12	0.22549	0.57619	0.50000	C30	0.38421	0.56329	0.50000
N13	0.31417	0.62504	0.50000	C31	0.35596	0.64735	0.50000
H14	0.09700	0.59088	0.50000	C32	0.42381	0.64930	0.50000
H15	0.16748	0.51977	0.50000	N33	0.37496	0.68912	0.50000
H16	0.23671	0.67221	0.50000	H34	0.40912	0.50612	0.50000
H17	0.16235	0.63228	0.50000	H35	0.48023	0.64771	0.50000
H18	0.24272	0.56009	0.50000	H36	0.32779	0.56449	0.50000
H37	0.36772	0.53007	0.50000	F79	0.94609	0.52986	0.50000
H38	0.43991	0.68263	0.50000	F80	0.97213	0.41663	0.50000
F39	0.52986	0.58377	0.50000	C81	0.48541	0.45757	0.50000
F40	0.41663	0.44450	0.50000	C82	0.52821	0.48532	0.50000
C41	0.45757	0.97216	0.50000	C83	0.54237	0.52783	0.50000
C42	0.48532	0.95712	0.50000	C84	0.55857	0.47099	0.50000
C43	0.52783	0.98546	0.50000	N85	0.54673	0.43197	0.50000
C44	0.47099	0.91242	0.50000	C86	0.57243	0.41357	0.50000
N45	0.43197	0.88524	0.50000	C87	0.55307	0.37055	0.50000
C46	0.41357	0.84114	0.50000	C88	0.61944	0.37364	0.50000
C47	0.37055	0.81748	0.50000	C89	0.63895	0.41687	0.50000
C48	0.37364	0.75420	0.50000	C90	0.61579	0.43671	0.50000
C49	0.41687	0.77792	0.50000	C91	0.64404	0.35265	0.50000
C50	0.43671	0.82092	0.50000	C92	0.57619	0.35070	0.50000
C51	0.35265	0.70861	0.50000	N93	0.62504	0.31088	0.50000
C52	0.35070	0.77451	0.50000	H94	0.59088	0.49388	0.50000
N53	0.31088	0.68584	0.50000	H95	0.51977	0.35229	0.50000
H54	0.49388	0.90300	0.50000	H96	0.67221	0.43551	0.50000

H55	0.35229	0.83252	0.50000	H97	0.63228	0.46993	0.50000
H56	0.43551	0.76329	0.50000	H98	0.56009	0.31737	0.50000
H57	0.46993	0.83765	0.50000	F99	0.47014	0.41623	0.50000
H58	0.31737	0.75728	0.50000	F100	0.58337	0.55550	0.50000
F59	0.41623	0.94609	0.50000	C101	0.54243	0.02784	0.50000
F60	0.55550	0.97213	0.50000	C102	0.51468	0.04288	0.50000
C61	0.97216	0.51459	0.50000	C103	0.47217	0.01454	0.50000
C62	0.95712	0.47179	0.50000	C104	0.52901	0.08758	0.50000
C63	0.98546	0.45763	0.50000	N105	0.56803	0.11476	0.50000
C64	0.91242	0.44143	0.50000	C106	0.58643	0.15886	0.50000
N65	0.88524	0.45327	0.50000	C107	0.62945	0.18252	0.50000
C66	0.84114	0.42757	0.50000	C108	0.62636	0.24580	0.50000
C67	0.81748	0.44693	0.50000	C109	0.58313	0.22208	0.50000
C68	0.75420	0.38056	0.50000	C110	0.56329	0.17908	0.50000
C69	0.77792	0.36105	0.50000	C111	0.64735	0.29139	0.50000
C70	0.82092	0.38421	0.50000	C112	0.64930	0.22549	0.50000
C71	0.70861	0.35596	0.50000	N113	0.68912	0.31416	0.50000
C72	0.77451	0.42381	0.50000	H114	0.50612	0.09700	0.50000
N73	0.68583	0.37496	0.50000	H115	0.64771	0.16748	0.50000
H74	0.90300	0.40912	0.50000	H116	0.56449	0.23671	0.50000
H75	0.83252	0.48023	0.50000	H117	0.53007	0.16235	0.50000
H76	0.76329	0.32779	0.50000	H118	0.68263	0.24272	0.50000
H77	0.83765	0.36772	0.50000	F119	0.58377	0.05391	0.50000
H78	0.75728	0.43991	0.50000	F120	0.44450	0.02787	0.50000

Table S2. Fractional atomistic coordinates for the unit cell for SCF-FCOF-1 with staggered (AB) stacking mode optimized using the Forcite module.

SCF-FCOF-1 with staggered (AB) stacking mode				Space group symmetry: 1 P1 a = b = 37.506 Å c = 6.160 Å α = β = 90° γ = 120°			
Atom	x (Å)	y (Å)	z (Å)	Atom	x (Å)	y (Å)	z (Å)
N1	0.35250	0.70829	0.75000	F37	0.91672	0.22200	0.25000
C2	0.84796	0.20897	0.25000	H38	0.90348	0.00553	0.75000
C3	0.80516	0.18124	0.25000	N39	0.97752	0.01913	0.75000
C4	0.79098	0.13872	0.25000	H40	0.98391	0.09045	0.75000
C5	0.77479	0.19559	0.25000	C41	0.79103	0.63898	0.25000
N6	0.78661	0.23461	0.25000	C42	0.81876	0.62391	0.25000
C7	0.76092	0.25303	0.25000	C43	0.86128	0.65225	0.25000
C8	0.78027	0.29604	0.25000	C44	0.80441	0.57919	0.25000
C9	0.71390	0.29299	0.25000	N45	0.76539	0.55200	0.25000
C10	0.69441	0.24976	0.25000	C46	0.74697	0.50789	0.25000

C11	0.71756	0.22991	0.25000	C47	0.70396	0.48422	0.25000
C12	0.68930	0.31400	0.25000	C48	0.70702	0.42091	0.25000
C13	0.75716	0.31590	0.25000	C49	0.75024	0.44464	0.25000
H14	0.74249	0.17270	0.25000	C50	0.77009	0.48765	0.25000
H15	0.81357	0.31431	0.25000	C51	0.68600	0.37529	0.25000
H16	0.66115	0.23112	0.25000	C52	0.68410	0.44125	0.25000
H17	0.70107	0.19669	0.25000	H53	0.82730	0.56977	0.25000
H18	0.77327	0.34923	0.25000	H54	0.68570	0.49925	0.25000
F19	0.86325	0.25031	0.25000	H55	0.76888	0.43002	0.25000
F20	0.74999	0.11107	0.25000	H56	0.80331	0.50437	0.25000
C21	0.81875	0.12410	0.25000	H57	0.65077	0.42403	0.25000
C22	0.86155	0.15184	0.25000	F58	0.74969	0.61293	0.25000
C23	0.87573	0.19435	0.25000	F59	0.88893	0.63891	0.25000
C24	0.89191	0.13749	0.25000	C60	0.87590	0.69464	0.25000
N25	0.88008	0.09847	0.25000	C61	0.84816	0.70970	0.25000
C26	0.90577	0.08007	0.25000	C62	0.80565	0.68137	0.25000
C27	0.88642	0.03705	0.25000	C63	0.86251	0.75442	0.25000
C28	0.95277	0.04021	0.25000	N64	0.90153	0.78160	0.25000
C29	0.97227	0.08340	0.25000	C65	0.91993	0.82569	0.25000
C30	0.94913	0.10323	0.25000	C66	0.96295	0.84936	0.25000
C31	0.97736	0.01927	0.25000	C67	0.95979	0.91256	0.25000
C32	0.90955	0.01724	0.25000	C68	0.91660	0.88886	0.25000
H33	0.92422	0.16037	0.25000	C69	0.89678	0.84590	0.25000
H34	0.85313	0.01874	0.25000	C70	0.98073	0.95807	0.25000
H35	0.96565	0.13644	0.25000	C71	0.98276	0.89230	0.25000
F36	0.80346	0.08277	0.25000	H72	0.83963	0.76384	0.25000
H73	0.98126	0.83438	0.25000	H117	0.16562	0.14687	0.25000
H74	0.86356	0.82920	0.25000	H118	0.17080	0.03435	0.25000
F75	0.91723	0.72069	0.25000	F119	0.27932	0.19654	0.25000
F76	0.77800	0.69472	0.25000	F120	0.30529	0.08328	0.25000
N77	0.29171	0.64422	0.75000	N121	0.64750	0.29171	0.25000
H78	0.99446	0.89796	0.75000	C122	0.15204	0.79103	0.75000
N79	0.98087	0.95840	0.75000	C123	0.19484	0.81876	0.75000
H80	0.90955	0.89347	0.75000	C124	0.20902	0.86128	0.75000
H81	0.10204	0.09651	0.75000	C125	0.22521	0.80441	0.75000
N82	0.04160	0.02247	0.75000	N126	0.21339	0.76539	0.75000
H83	0.10653	0.01609	0.75000	C127	0.23908	0.74697	0.75000
N84	0.35578	0.64749	0.75000	C128	0.21973	0.70396	0.75000
C85	0.36102	0.15204	0.25000	C129	0.28610	0.70701	0.75000
C86	0.37609	0.19484	0.25000	C130	0.30559	0.75024	0.75000
C87	0.34775	0.20902	0.25000	C131	0.28244	0.77009	0.75000
C88	0.42081	0.22521	0.25000	C132	0.31070	0.68600	0.75000
N89	0.44801	0.21339	0.25000	C133	0.24284	0.68410	0.75000
C90	0.49211	0.23908	0.25000	H134	0.25751	0.82730	0.75000

C91	0.51578	0.21973	0.25000	H135	0.18643	0.68569	0.75000
C92	0.57909	0.28610	0.25000	H136	0.33885	0.76888	0.75000
C93	0.55536	0.30559	0.25000	H137	0.29893	0.80331	0.75000
C94	0.51235	0.28244	0.25000	H138	0.22673	0.65077	0.75000
C95	0.62471	0.31070	0.25000	F139	0.13675	0.74969	0.75000
C96	0.55875	0.24284	0.25000	F140	0.25001	0.88893	0.75000
H97	0.43023	0.25752	0.25000	C141	0.18125	0.87590	0.75000
H98	0.50075	0.18643	0.25000	C142	0.13845	0.84816	0.75000
H99	0.56998	0.33885	0.25000	C143	0.12427	0.80565	0.75000
H100	0.49563	0.29893	0.25000	C144	0.10809	0.86251	0.75000
H101	0.57597	0.22673	0.25000	N145	0.11992	0.90153	0.75000
F102	0.38707	0.13675	0.25000	C146	0.09423	0.91993	0.75000
F103	0.36109	0.25001	0.25000	C147	0.11358	0.96295	0.75000
C104	0.30536	0.18125	0.25000	C148	0.04723	0.95979	0.75000
C105	0.29030	0.13845	0.25000	C149	0.02773	0.91660	0.75000
C106	0.31863	0.12427	0.25000	C150	0.05087	0.89677	0.75000
C107	0.24559	0.10809	0.25000	C151	0.02264	0.98073	0.75000
N108	0.21840	0.11993	0.25000	C152	0.09045	0.98276	0.75000
C109	0.17431	0.09423	0.25000	H153	0.07578	0.83963	0.75000
C110	0.15064	0.11358	0.25000	H154	0.14687	0.98126	0.75000
C111	0.08745	0.04723	0.25000	H155	0.03435	0.86356	0.75000
C112	0.11114	0.02773	0.25000	F156	0.19654	0.91723	0.75000
C113	0.15410	0.05087	0.25000	F157	0.08328	0.77800	0.75000
C114	0.04193	0.02264	0.25000	H158	0.09652	0.99447	0.25000
C115	0.10770	0.09045	0.25000	N159	0.02248	0.98087	0.25000
H116	0.23616	0.07578	0.25000	H160	0.01609	0.90955	0.25000
H161	0.00554	0.10204	0.25000	C201	0.63898	0.84796	0.75000
N162	0.01913	0.04160	0.25000	C202	0.62391	0.80516	0.75000
H163	0.09045	0.10653	0.25000	C203	0.65225	0.79098	0.75000
N164	0.70829	0.35578	0.25000	C204	0.57919	0.77479	0.75000
C165	0.20897	0.36102	0.75000	N205	0.55199	0.78661	0.75000
C166	0.18124	0.37609	0.75000	C206	0.50789	0.76092	0.75000
C167	0.13872	0.34775	0.75000	C207	0.48422	0.78027	0.75000
C168	0.19559	0.42081	0.75000	C208	0.42091	0.71390	0.75000
N169	0.23461	0.44800	0.75000	C209	0.44464	0.69441	0.75000
C170	0.25303	0.49211	0.75000	C210	0.48765	0.71756	0.75000
C171	0.29604	0.51578	0.75000	C211	0.37529	0.68930	0.75000
C172	0.29298	0.57909	0.75000	C212	0.44125	0.75716	0.75000
C173	0.24976	0.55536	0.75000	H213	0.56977	0.74248	0.75000
C174	0.22991	0.51235	0.75000	H214	0.49925	0.81357	0.75000
C175	0.31400	0.62471	0.75000	H215	0.43002	0.66115	0.75000
C176	0.31590	0.55875	0.75000	H216	0.50437	0.70107	0.75000
H177	0.17270	0.43023	0.75000	H217	0.42403	0.77327	0.75000
H178	0.31430	0.50075	0.75000	F218	0.61293	0.86325	0.75000

H179	0.23112	0.56998	0.75000	F219	0.63891	0.74999	0.75000
H180	0.19669	0.49563	0.75000	C220	0.69464	0.81875	0.75000
H181	0.34923	0.57597	0.75000	C221	0.70970	0.86155	0.75000
F182	0.25031	0.38707	0.75000	C222	0.68137	0.87573	0.75000
F183	0.11107	0.36109	0.75000	C223	0.75441	0.89191	0.75000
C184	0.12410	0.30536	0.75000	N224	0.78160	0.88007	0.75000
C185	0.15184	0.29030	0.75000	C225	0.82569	0.90577	0.75000
C186	0.19435	0.31863	0.75000	C226	0.84936	0.88642	0.75000
C187	0.13749	0.24558	0.75000	C227	0.91255	0.95277	0.75000
N188	0.09847	0.21840	0.75000	C228	0.88886	0.97227	0.75000
C189	0.08007	0.17431	0.75000	C229	0.84590	0.94913	0.75000
C190	0.03705	0.15064	0.75000	C230	0.95807	0.97736	0.75000
C191	0.04021	0.08744	0.75000	C231	0.89230	0.90955	0.75000
C192	0.08340	0.11114	0.75000	H232	0.76384	0.92422	0.75000
C193	0.10322	0.15410	0.75000	H233	0.83438	0.85313	0.75000
C194	0.01927	0.04193	0.75000	H234	0.82920	0.96565	0.75000
C195	0.01724	0.10770	0.75000	F235	0.72068	0.80346	0.75000
H196	0.16037	0.23616	0.75000	F236	0.69471	0.91672	0.75000
H197	0.01874	0.16562	0.75000	N237	0.64422	0.35251	0.25000
H198	0.13644	0.17080	0.75000	H238	0.89796	0.90349	0.25000
F199	0.08277	0.27931	0.75000	N239	0.95840	0.97753	0.25000
F200	0.22200	0.30528	0.75000	H240	0.89347	0.98391	0.25000

Table S3. Fractional atomistic coordinates for the unit cell for SCF-FCOF-1 with 1.0-Å serrated stacking mode optimized using the Forcite module.

SCF-FCOF-1 with 1.0-Å serrated stacking mode				Space group symmetry: 1 P1 a = 37.474 Å b = 37.498 Å c = 6.796 Å α = β = 90° γ = 119.97°			
Atom	x (Å)	y (Å)	z (Å)	Atom	x (Å)	y (Å)	z (Å)
C1	0.51805	0.02639	0.25000	F37	0.43554	0.40141	0.25000
C2	0.54843	0.07107	0.25000	C38	0.96217	0.44189	0.25000
N3	0.53660	0.09826	0.25000	C39	0.94704	0.46958	0.25000
C4	0.56231	0.14234	0.25000	C40	0.97532	0.51209	0.25000
C5	0.54297	0.16603	0.25000	C41	0.90230	0.45513	0.25000
C6	0.60937	0.22927	0.25000	N42	0.87525	0.41609	0.25000
C7	0.62886	0.20551	0.25000	C43	0.83113	0.39748	0.25000
C8	0.60568	0.16252	0.25000	C44	0.80767	0.35446	0.25000
C9	0.63399	0.27486	0.25000	C45	0.74417	0.35717	0.25000
C10	0.56611	0.20898	0.25000	C46	0.76770	0.40040	0.25000
N11	0.61500	0.29767	0.25000	C47	0.81071	0.42042	0.25000
H12	0.58074	0.08045	0.25000	C48	0.69859	0.33608	0.25000
H13	0.50967	0.15103	0.25000	C49	0.76467	0.33441	0.25000
H14	0.66213	0.22011	0.25000	N50	0.67582	0.29432	0.25000
H15	0.62217	0.14578	0.25000	H51	0.89274	0.47792	0.25000
H16	0.55002	0.22624	0.25000	H52	0.82288	0.33635	0.25000
F17	0.45998	0.03746	0.25000	H53	0.75293	0.41892	0.25000
C18	0.53356	0.49923	0.25000	H54	0.82729	0.45363	0.25000
C19	0.50575	0.45646	0.25000	H55	0.74757	0.30109	0.25000
C20	0.46325	0.44237	0.25000	F56	0.93618	0.40056	0.25000
C21	0.51996	0.42600	0.25000	F57	0.96189	0.53969	0.25000
N22	0.55895	0.43766	0.25000	C58	0.50444	0.95568	0.25000
C23	0.57711	0.41173	0.25000	C59	0.46163	0.94068	0.25000
C24	0.62011	0.43081	0.25000	C60	0.44746	0.96903	0.25000
C25	0.61655	0.36423	0.25000	C61	0.43126	0.89601	0.25000
C26	0.57334	0.34498	0.25000	N62	0.44314	0.86885	0.25000
C27	0.55374	0.36838	0.25000	C63	0.41748	0.82478	0.25000
C28	0.63735	0.33946	0.25000	C64	0.43688	0.80116	0.25000
C29	0.63972	0.40747	0.25000	C65	0.37054	0.73792	0.25000
N30	0.67910	0.35837	0.25000	C66	0.35098	0.76159	0.25000
H31	0.49698	0.39375	0.25000	C67	0.37411	0.80456	0.25000
H32	0.63854	0.46408	0.25000	C68	0.34600	0.69238	0.25000
H33	0.55456	0.31174	0.25000	C69	0.41381	0.75822	0.25000
H34	0.52052	0.35207	0.25000	N70	0.36504	0.66965	0.25000
H35	0.67305	0.42339	0.25000	H71	0.39895	0.88660	0.25000
F36	0.57489	0.51442	0.25000	H72	0.47019	0.81621	0.25000

H73	0.31771	0.74695	0.25000	C117	1.00456	0.45654	0.25000
H74	0.35759	0.82128	0.25000	C118	0.47525	1.01138	0.25000
H75	0.42994	0.74100	0.25000	C119	0.53222	0.99804	0.25000
F76	0.51971	0.92961	0.25000	F120	0.57323	1.01135	0.25000
F77	0.40646	0.95572	0.25000	C121	0.52475	-0.01138	0.75000
C78	0.44868	0.47018	0.25000	C122	0.46778	0.00196	0.75000
C79	0.47646	0.51295	0.25000	F123	0.42677	-0.01135	0.75000
C80	0.51898	0.52706	0.25000	C124	-0.00456	0.54346	0.75000
C81	0.46208	0.54329	0.25000	C125	0.48195	0.97361	0.75000
N82	0.42302	0.53136	0.25000	C126	0.45157	0.92893	0.75000
C83	0.40440	0.55686	0.25000	N127	0.46340	0.90174	0.75000
C84	0.36136	0.53731	0.25000	C128	0.43769	0.85766	0.75000
C85	0.36400	0.60346	0.25000	C129	0.45703	0.83397	0.75000
C86	0.40727	0.62315	0.25000	C130	0.39063	0.77073	0.75000
C87	0.42734	0.60020	0.25000	C131	0.37114	0.79449	0.75000
C88	0.34281	0.62789	0.25000	C132	0.39432	0.83748	0.75000
C89	0.34127	0.56023	0.25000	C133	0.36601	0.72514	0.75000
N90	0.30100	0.60884	0.25000	C134	0.43389	0.79102	0.75000
H91	0.48492	0.57560	0.25000	N135	0.38500	0.70233	0.75000
H92	0.34325	0.50402	0.25000	H136	0.41926	0.91955	0.75000
H93	0.42577	0.65641	0.25000	H137	0.49033	0.84897	0.75000
H94	0.46057	0.61681	0.25000	H138	0.33787	0.77989	0.75000
H95	0.30793	0.54400	0.25000	H139	0.37783	0.85422	0.75000
F96	0.40734	0.45494	0.25000	H140	0.44998	0.77376	0.75000
F97	0.54666	0.56803	0.25000	F141	0.54002	0.96254	0.75000
C98	0.01773	0.52675	0.25000	C142	0.46644	0.50077	0.75000
C99	0.03285	0.49904	0.25000	C143	0.49425	0.54354	0.75000
C100	0.07756	0.51335	0.25000	C144	0.53675	0.55763	0.75000
N101	0.10478	0.55235	0.25000	C145	0.48004	0.57400	0.75000
C102	0.14888	0.57060	0.25000	N146	0.44105	0.56234	0.75000
C103	0.17265	0.61359	0.25000	C147	0.42289	0.58827	0.75000
C104	0.23585	0.61024	0.25000	C148	0.37989	0.56919	0.75000
C105	0.21203	0.56705	0.25000	C149	0.38345	0.63577	0.75000
C106	0.16901	0.54735	0.25000	C150	0.42666	0.65502	0.75000
C107	0.28146	0.63113	0.25000	C151	0.44626	0.63162	0.75000
C108	0.21562	0.63329	0.25000	C152	0.36265	0.66054	0.75000
N109	0.30421	0.67288	0.25000	C153	0.36028	0.59253	0.75000
H110	0.08695	0.49045	0.25000	N154	0.32090	0.64163	0.75000
H111	0.15771	0.63194	0.25000	H155	0.50302	0.60625	0.75000
H112	0.22658	0.54834	0.25000	H156	0.36146	0.53592	0.75000
H113	0.15221	0.51415	0.25000	H157	0.44544	0.68826	0.75000
H114	0.23293	0.66661	0.25000	H158	0.47948	0.64793	0.75000
F115	0.04376	0.56807	0.25000	H159	0.32695	0.57661	0.75000
F116	0.01796	0.42893	0.25000	F160	0.42511	0.48558	0.75000

F161	0.56446	0.59859	0.75000	F201	0.59354	0.04428	0.75000
C162	0.03783	0.55811	0.75000	C202	0.55132	0.52982	0.75000
C163	0.05296	0.53042	0.75000	C203	0.52354	0.48705	0.75000
C164	0.02468	0.48791	0.75000	C204	0.48102	0.47294	0.75000
C165	0.09770	0.54487	0.75000	C205	0.53792	0.45671	0.75000
N166	0.12475	0.58391	0.75000	N206	0.57698	0.46864	0.75000
C167	0.16887	0.60252	0.75000	C207	0.59560	0.44314	0.75000
C168	0.19233	0.64554	0.75000	C208	0.63864	0.46269	0.75000
C169	0.25583	0.64283	0.75000	C209	0.63600	0.39654	0.75000
C170	0.23230	0.59960	0.75000	C210	0.59273	0.37685	0.75000
C171	0.18929	0.57958	0.75000	C211	0.57266	0.39980	0.75000
C172	0.30141	0.66392	0.75000	C212	0.65719	0.37211	0.75000
C173	0.23533	0.66559	0.75000	C213	0.65873	0.43977	0.75000
N174	0.32418	0.70568	0.75000	N214	0.69900	0.39116	0.75000
H175	0.10726	0.52208	0.75000	H215	0.51508	0.42440	0.75000
H176	0.17712	0.66365	0.75000	H216	0.65675	0.49598	0.75000
H177	0.24707	0.58108	0.75000	H217	0.57423	0.34359	0.75000
H178	0.17271	0.54637	0.75000	H218	0.53943	0.38319	0.75000
H179	0.25243	0.69891	0.75000	H219	0.69207	0.45600	0.75000
F180	0.06382	0.59944	0.75000	F220	0.59266	0.54506	0.75000
F181	0.03811	0.46031	0.75000	F221	0.45334	0.43197	0.75000
C182	0.49556	0.04432	0.75000	C222	0.98227	0.47325	0.75000
C183	0.53837	0.05932	0.75000	C223	0.96715	0.50096	0.75000
C184	0.55254	0.03097	0.75000	C224	0.92244	0.48665	0.75000
C185	0.56874	0.10399	0.75000	N225	0.89522	0.44765	0.75000
N186	0.55686	0.13115	0.75000	C226	0.85112	0.42940	0.75000
C187	0.58252	0.17522	0.75000	C227	0.82735	0.38641	0.75000
C188	0.56312	0.19884	0.75000	C228	0.76415	0.38976	0.75000
C189	0.62946	0.26208	0.75000	C229	0.78797	0.43295	0.75000
C190	0.64902	0.23841	0.75000	C230	0.83099	0.45265	0.75000
C191	0.62589	0.19544	0.75000	C231	0.71854	0.36887	0.75000
C192	0.65400	0.30762	0.75000	C232	0.78438	0.36671	0.75000
C193	0.58619	0.24178	0.75000	N233	0.69579	0.32712	0.75000
N194	0.63496	0.33035	0.75000	H234	0.91305	0.50955	0.75000
H195	0.60105	0.11340	0.75000	H235	0.84229	0.36806	0.75000
H196	0.52981	0.18379	0.75000	H236	0.77342	0.45166	0.75000
H197	0.68229	0.25305	0.75000	H237	0.84779	0.48585	0.75000
H198	0.64241	0.17872	0.75000	H238	0.76707	0.33339	0.75000
H199	0.57006	0.25900	0.75000	F239	0.95624	0.43193	0.75000
F200	0.48029	0.07039	0.75000	F240	0.98204	0.57107	0.75000

Table S4. Fractional atomistic coordinates for the unit cell for SCF-FCOF-2 with eclipsed (AA) stacking mode optimized using the Forcite module.

SCF-FCOF-2 with eclipsed (AA) stacking mode				Space group symmetry: 1 P1 a = 37.881 Å b = 37.017 Å c = 3.629 Å α =89.98° β = 106.49° γ = 119.28°			
Atom	x (Å)	y (Å)	z (Å)	Atom	x (Å)	y (Å)	z (Å)
C1	0.02769	0.48804	0.52816	H37	0.32885	0.56641	0.34150
C2	0.04293	0.53118	0.52323	H38	0.37003	0.53229	0.37228
C3	0.01509	0.54633	0.50822	H39	0.44259	0.67865	1.05029
C4	0.08744	0.56090	0.53640	F40	0.53526	0.58407	0.85175
N5	0.11307	0.54763	0.51961	F41	0.41592	0.44239	0.47627
C6	0.15700	0.57300	0.53789	H42	0.40712	0.70518	0.58062
C7	0.17686	0.55292	0.43786	C43	0.45429	0.97002	0.28863
C8	0.24445	0.61944	0.59176	C44	0.48267	0.95470	0.39597
C9	0.22435	0.63943	0.69692	C45	0.52636	0.98231	0.45422
C10	0.18121	0.61659	0.66982	C46	0.46784	0.91051	0.45087
C11	0.29030	0.64395	0.60883	N47	0.42770	0.88378	0.39584
C12	0.21982	0.57576	0.45971	C48	0.40990	0.84047	0.44383
C13	0.31521	0.62481	0.66544	C49	0.36604	0.81306	0.26328
H14	0.09792	0.59392	0.55186	C50	0.37181	0.75455	0.51857
H15	0.15868	0.51936	0.33648	C51	0.41581	0.78250	0.70733
H16	0.24199	0.67262	0.81060	C52	0.43471	0.82492	0.66983
H17	0.16768	0.63317	0.76453	C53	0.35182	0.70932	0.56164
H18	0.23317	0.55905	0.36276	C54	0.34717	0.77055	0.29657
F19	0.05342	0.47192	0.54671	C55	0.30924	0.68639	0.56042
F20	0.02869	0.58771	0.50399	H56	0.49112	0.90057	0.52935
H21	0.30218	0.59293	0.72293	H57	0.34650	0.82459	0.08913
C22	0.51842	0.54215	0.75524	H58	0.43561	0.77192	0.89334
C23	0.47414	0.51377	0.66303	H59	0.46836	0.84541	0.82721
C24	0.45836	0.47067	0.56555	H60	0.31342	0.75026	0.14147
C25	0.44374	0.52809	0.65937	F61	0.41180	0.94460	0.22800
N26	0.45691	0.56763	0.74674	F62	0.55461	0.96862	0.55613
C27	0.43050	0.58550	0.73603	H63	0.29076	0.70171	0.51967
C28	0.45021	0.62701	0.91945	C64	0.97289	0.51911	0.49550
C29	0.38238	0.62526	0.69350	C65	0.95763	0.47596	0.49943
C30	0.36254	0.58350	0.51074	C66	0.98551	0.46084	0.51565
C31	0.38629	0.56381	0.53010	C67	0.91315	0.44613	0.48626
C32	0.35738	0.64670	0.65728	N68	0.88608	0.45857	0.46576
C33	0.42646	0.64670	0.90092	C69	0.84230	0.43250	0.45000
C34	0.37526	0.68879	0.60318	C70	0.81436	0.44754	0.31560
H35	0.41013	0.50478	0.58338	C71	0.75518	0.38324	0.40017
H36	0.48422	0.64419	1.07742	C72	0.78379	0.36870	0.54414

C73	0.82672	0.39284	0.56678	H100	0.67360	0.43105	0.82088
C74	0.70940	0.35752	0.38308	H101	0.63369	0.46471	0.85995
C75	0.77127	0.42317	0.28648	H102	0.55759	0.32266	0.07870
C76	0.68621	0.37684	0.42019	F103	0.46917	0.41419	0.46251
H77	0.90319	0.41329	0.48233	F104	0.58849	0.55588	0.83596
H78	0.82586	0.47801	0.22427	H105	0.59290	0.29081	0.41079
H79	0.77360	0.33918	0.65210	C106	0.54158	0.02435	0.41007
H80	0.84761	0.38076	0.68721	C107	0.51326	0.03976	0.30594
H81	0.75068	0.43561	0.16725	C108	0.46951	0.01206	0.24449
F82	0.94723	0.53526	0.48006	C109	0.52837	0.08432	0.26494
F83	0.97196	0.41948	0.52070	N110	0.56880	0.11140	0.33884
H84	0.70132	0.41056	0.45302	C111	0.58737	0.15544	0.31961
C85	0.48598	0.45613	0.55731	C112	0.63120	0.18186	0.51255
C86	0.53021	0.48455	0.64600	C113	0.62657	0.24292	0.32553
C87	0.54605	0.52760	0.74730	C114	0.58281	0.21620	0.12023
C88	0.56034	0.47030	0.63543	C115	0.56333	0.17287	0.11656
N89	0.54655	0.43132	0.51143	C116	0.64684	0.28918	0.34686
C90	0.57219	0.41336	0.48983	C117	0.65065	0.22516	0.51789
C91	0.55153	0.37287	0.27987	C118	0.68883	0.31347	0.33795
C92	0.61906	0.37388	0.44679	H119	0.50515	0.09434	0.18834
C93	0.63970	0.41451	0.66097	H120	0.65016	0.16890	0.66841
C94	0.61662	0.43405	0.68288	H121	0.56367	0.22877	-0.04071
C95	0.64364	0.35308	0.41767	H122	0.52978	0.15337	-0.04942
C96	0.57460	0.35342	0.25516	H123	0.68431	0.24482	0.68200
C97	0.62463	0.30929	0.38827	F124	0.58407	0.04973	0.47028
H98	0.59411	0.49336	0.72346	F125	0.44128	0.02578	0.14332
H99	0.51734	0.35648	0.13032	H126	0.70516	0.29771	0.28925

Table S5. Fractional atomistic coordinates for the unit cell for SCF-FCOF-2 with staggered (AB) stacking mode optimized using the Forcite module.

SCF-FCOF-2 with staggered (AB) stacking mode				Space group symmetry: 1 P1 a = 37.622 Å b = 37.857 Å c = 6.586 Å α = 90.24° β = 90.98° γ = 120.55°			
Atom	x (Å)	y (Å)	z (Å)	Atom	x (Å)	y (Å)	z (Å)
C1	0.34852	0.70793	0.74145	F37	0.91797	0.21957	0.32224
C2	0.85106	0.20964	0.26326	H38	0.36391	0.74104	0.73247
C3	0.80881	0.18383	0.21370	H39	0.95785	0.03265	0.73781
C4	0.79383	0.14201	0.17388	H40	0.90014	-0.00897	0.55620
C5	0.77984	0.19950	0.20253	C41	0.97613	0.01805	0.74330
N6	0.79140	0.23688	0.25769	H42	0.99303	0.09141	0.91974
C7	0.76619	0.25541	0.25345	C43	0.79292	0.63983	0.25025
C8	0.77916	0.29114	0.36953	C44	0.82047	0.62508	0.27177
C9	0.71938	0.29468	0.25233	C45	0.86285	0.65346	0.29953
C10	0.70663	0.25911	0.13361	C46	0.80595	0.58061	0.27040
C11	0.72984	0.23969	0.13323	N47	0.76799	0.55344	0.22172
C12	0.69476	0.31531	0.25178	C48	0.75059	0.50973	0.22293
C13	0.75597	0.31056	0.36996	C49	0.71507	0.48517	0.10411
H14	0.74823	0.17861	0.15434	C50	0.71218	0.42340	0.22977
H15	0.80722	0.30379	0.46154	C51	0.74776	0.44807	0.34986
H16	0.67907	0.24670	0.03799	C52	0.76675	0.49082	0.34713
H17	0.71956	0.21305	0.03577	C53	0.69126	0.37798	0.23753
H18	0.76640	0.33774	0.46408	C54	0.69615	0.44245	0.10616
F19	0.86714	0.25031	0.30080	H55	0.82795	0.57104	0.30628
F20	0.75334	0.11623	0.12538	H56	0.70204	0.49923	0.00917
C21	0.82021	0.12613	0.18469	H57	0.76030	0.43429	0.45001
C22	0.86242	0.15191	0.23505	H58	0.79322	0.50872	0.44667
C23	0.87747	0.19378	0.27377	H59	0.66903	0.42430	0.01047
C24	0.89129	0.13617	0.24879	F60	0.75169	0.61365	0.22493
N25	0.87879	0.09775	0.21377	F61	0.89026	0.64038	0.32215
C26	0.90387	0.07915	0.22553	C62	0.87755	0.69561	0.30435
C27	0.88947	0.04120	0.12845	C63	0.85003	0.71033	0.28230
C28	0.95098	0.04007	0.24018	C64	0.80761	0.68201	0.25677
C29	0.96487	0.07781	0.34144	C65	0.86474	0.75477	0.28618
C30	0.94161	0.09710	0.33516	N66	0.90327	0.78160	0.25581
C31	0.97623	0.01987	0.24497	C67	0.92125	0.82535	0.25524
C32	0.91274	0.02192	0.13471	C68	0.95908	0.84897	0.16076
H33	0.92345	0.15767	0.28437	C69	0.95996	0.91184	0.25253
H34	0.86021	0.02669	0.04563	C70	0.92206	0.88791	0.34938
H35	0.95309	0.12556	0.41919	C71	0.90295	0.84520	0.35158
F36	0.80417	0.08549	0.14591	C72	0.98058	0.95752	0.25185
C73	0.97812	0.89164	0.15785	C117	0.08989	0.05039	0.25668
H74	0.84242	0.76446	0.30488	C118	0.11406	0.03716	0.35977
H75	0.97375	0.83416	0.08752	C119	0.15713	0.06038	0.35812

H76	0.87443	0.82813	0.43228	C120	0.04384	0.02498	0.25430
F77	0.91866	0.72183	0.33466	C121	0.11027	0.08806	0.15519
F78	0.78025	0.69519	0.23613	H122	0.23841	0.08264	0.36107
C79	0.28560	0.64172	0.75740	H123	0.16822	0.14004	0.07341
H80	0.25227	0.62363	0.76604	H124	0.17412	0.04899	0.44140
H81	0.96550	0.92345	0.75386	F125	0.28311	0.19264	0.11638
H82	1.00643	0.90756	0.57222	F126	0.30737	0.09325	0.44371
C83	0.98041	0.95649	0.75181	C127	0.65148	0.29207	0.25855
H84	0.90683	0.90043	0.92599	C128	0.14894	0.79036	0.73674
H85	0.09273	0.09799	0.57335	C129	0.19119	0.81618	0.78630
C86	0.04286	0.02310	0.75369	C130	0.20617	0.85799	0.82612
H87	0.09916	0.00695	0.94555	C131	0.22016	0.80050	0.79747
C88	0.35202	0.64585	0.75806	N132	0.20860	0.76312	0.74231
H89	0.07615	0.04154	0.75677	C133	0.23381	0.74459	0.74655
H90	0.37011	0.63092	0.75746	C134	0.22084	0.70886	0.63047
C91	0.36382	0.15665	0.33919	C135	0.28062	0.70532	0.74767
C92	0.37942	0.19527	0.24825	C136	0.29337	0.74089	0.86639
C93	0.35141	0.20667	0.17448	C137	0.27016	0.76031	0.86677
C94	0.42434	0.22399	0.22701	C138	0.30524	0.68469	0.74822
N95	0.45131	0.21518	0.29793	C139	0.24403	0.68944	0.63004
C96	0.49541	0.24015	0.28337	H140	0.25177	0.82139	0.84566
C97	0.52007	0.23179	0.41267	H141	0.19278	0.69621	0.53846
C98	0.58226	0.28656	0.26268	H142	0.32093	0.75330	0.96201
C99	0.55756	0.29466	0.13100	H143	0.28044	0.78695	0.96423
C100	0.51453	0.27157	0.14017	H144	0.23360	0.66226	0.53592
C101	0.62789	0.31125	0.25363	F145	0.13286	0.74969	0.69920
C102	0.56308	0.25478	0.40314	F146	0.24667	0.88377	0.87462
H103	0.43436	0.25307	0.15472	C147	0.17979	0.87387	0.81531
H104	0.50584	0.20751	0.52252	C148	0.13758	0.84809	0.76495
H105	0.57158	0.31843	0.01849	C149	0.12253	0.80622	0.72623
H106	0.49664	0.27802	0.03254	C150	0.10871	0.86383	0.75121
H107	0.58139	0.24806	0.50732	N151	0.12121	0.90225	0.78623
F108	0.38952	0.14410	0.41210	C152	0.09613	0.92085	0.77447
F109	0.36529	0.24356	0.08531	C153	0.11053	0.95880	0.87155
C110	0.30883	0.18027	0.19104	C154	0.04902	0.95993	0.75982
C111	0.29324	0.14163	0.28192	C155	0.03513	0.92219	0.65856
C112	0.32124	0.13023	0.35549	C156	0.05839	0.90290	0.66484
C113	0.24831	0.11266	0.30082	C157	0.02377	0.98013	0.75503
N114	0.22140	0.12264	0.24308	C158	0.08726	0.97808	0.86529
C115	0.17719	0.09758	0.25259	H159	0.07655	0.84233	0.71563
C116	0.15333	0.11129	0.15383	H160	0.13979	0.97331	0.95437
H161	0.04691	0.87444	0.58081	C205	0.02188	0.10836	0.84215
F162	0.19583	0.91451	0.85409	H206	0.15758	0.23554	0.69512
F163	0.08203	0.78043	0.67776	H207	0.02625	0.16584	0.91248

H164	0.63609	0.25896	0.26753	H208	0.12557	0.17187	0.56772
H165	0.09986	1.00897	0.44380	F209	0.08134	0.27817	0.66534
C166	0.02387	0.98195	0.25670	F210	0.21975	0.30481	0.76387
H167	0.00697	0.90859	0.08026	C211	0.63618	0.84335	0.66081
H168	0.04215	0.96735	0.26219	C212	0.62058	0.80473	0.75175
H169	-0.00643	0.09244	0.42778	C213	0.64859	0.79333	0.82552
C170	0.01959	0.04351	0.24819	C214	0.57566	0.77601	0.77299
H171	0.09317	0.09957	0.07401	N215	0.54869	0.78482	0.70207
H172	0.03450	0.07655	0.24614	C216	0.50459	0.75985	0.71664
C173	0.71440	0.35828	0.24260	C217	0.47993	0.76821	0.58733
H174	0.74773	0.37637	0.23396	C218	0.41774	0.71344	0.73732
C175	0.20708	0.36017	0.74975	C219	0.44244	0.70534	0.86900
C176	0.17953	0.37492	0.72823	C220	0.48547	0.72843	0.85983
C177	0.13715	0.34654	0.70047	C221	0.37211	0.68875	0.74637
C178	0.19405	0.41939	0.72960	C222	0.43692	0.74522	0.59686
N179	0.23201	0.44656	0.77828	H223	0.56564	0.74693	0.84528
C180	0.24941	0.49027	0.77707	H224	0.49416	0.79249	0.47748
C181	0.28493	0.51483	0.89589	H225	0.42842	0.68157	0.98151
C182	0.28782	0.57660	0.77023	H226	0.50336	0.72198	0.96746
C183	0.25224	0.55193	0.65014	H227	0.41861	0.75194	0.49268
C184	0.23325	0.50918	0.65287	F228	0.61048	0.85590	0.58790
C185	0.30874	0.62202	0.76247	F229	0.63471	0.75644	0.91469
C186	0.30385	0.55755	0.89384	C230	0.69117	0.81973	0.80896
H187	0.17205	0.42896	0.69372	C231	0.70676	0.85837	0.71808
H188	0.29796	0.50077	0.99083	C232	0.67876	0.86977	0.64451
H189	0.23970	0.56571	0.54999	C233	0.75169	0.88734	0.69918
H190	0.20678	0.49128	0.55333	N234	0.77860	0.87736	0.75692
H191	0.33097	0.57570	0.98953	C235	0.82281	0.90242	0.74741
F192	0.24831	0.38635	0.77507	C236	0.84667	0.88871	0.84617
F193	0.10974	0.35962	0.67785	C237	0.91011	0.94961	0.74332
C194	0.12245	0.30439	0.69565	C238	0.88594	0.96284	0.64023
C195	0.14997	0.28967	0.71770	C239	0.84287	0.93962	0.64188
C196	0.19239	0.31799	0.74323	C240	0.95616	0.97502	0.74570
C197	0.13526	0.24523	0.71382	C241	0.88973	0.91194	0.84481
N198	0.09673	0.21840	0.74419	H242	0.76159	0.91736	0.63893
C199	0.07875	0.17465	0.74476	H243	0.83178	0.85996	0.92659
C200	0.04092	0.15103	0.83924	H244	0.82588	0.95101	0.55860
C201	0.04004	0.08816	0.74747	F245	0.71689	0.80736	0.88362
C202	0.07794	0.11209	0.65062	F246	0.69263	0.90675	0.55629
C203	0.09705	0.15480	0.64842	C247	0.64798	0.35415	0.24194
C204	0.01942	0.04248	0.74815	H248	0.92385	0.95846	0.24323
H249	0.62989	0.36908	0.24254	C251	0.95714	0.97690	0.24631
H250	0.90727	0.90201	0.42665	H252	0.90084	0.99305	0.05445

Table S6. Fractional atomistic coordinates for the unit cell for SCF-FCOF-2 with 1.0-Å serrated stacking mode optimized using the Forcite module.

SCF-FCOF-2 with 1.0-Å serrated stacking	Space group symmetry: 1 P1 a = 37.900 Å b = 37.573 Å c = 7.164 Å

mode				$\alpha = 81.83°$ $\beta = 101.20°$ $\gamma = 120.60°$			
Atom	x (Å)	y (Å)	z (Å)	Atom	x (Å)	y (Å)	z (Å)
C1	0.52704	0.04549	0.18743	F37	0.44578	0.41499	0.28215
C2	0.55667	0.09048	0.19695	C38	0.97383	0.46097	0.27861
N3	0.54399	0.11729	0.17386	C39	0.95908	0.48886	0.27275
C4	0.57014	0.16135	0.18450	C40	0.98755	0.53155	0.27166
C5	0.55388	0.18685	0.10009	C41	0.91450	0.47440	0.26688
C6	0.61861	0.24828	0.20660	N42	0.88789	0.43528	0.28785
C7	0.63471	0.22247	0.29310	C43	0.84401	0.41726	0.28323
C8	0.61084	0.17954	0.28218	C44	0.82189	0.37641	0.35485
C9	0.64379	0.29394	0.22555	C45	0.75722	0.37789	0.27133
C10	0.57787	0.22985	0.10910	C46	0.77947	0.41888	0.19773
C11	0.62495	0.31710	0.24197	C47	0.82239	0.43839	0.20318
H12	0.58945	0.10082	0.21872	C48	0.71143	0.35684	0.26316
H13	0.52257	0.17331	0.02482	C49	0.77907	0.35699	0.35078
H14	0.66534	0.23530	0.37520	C50	0.68692	0.31442	0.23085
H15	0.62395	0.16084	0.35616	H51	0.90465	0.49722	0.25055
H16	0.56453	0.24855	0.03762	H52	0.83807	0.35970	0.41628
F17	0.46764	0.05435	0.16375	H53	0.76361	0.43559	0.13111
C18	0.54170	0.51528	0.27747	H54	0.83807	0.46941	0.13973
C19	0.51493	0.47208	0.27870	H55	0.76320	0.32574	0.41232
C20	0.47251	0.45642	0.28088	F56	0.94755	0.41947	0.27761
C21	0.53021	0.44279	0.27857	F57	0.97447	0.55931	0.26649
N22	0.56890	0.45600	0.26938	C58	0.51539	0.97543	0.18946
C23	0.58758	0.43088	0.27133	C59	0.47227	0.95910	0.17332
C24	0.62713	0.44980	0.21867	C60	0.45692	0.98649	0.16407
C25	0.62802	0.38464	0.27718	C61	0.44285	0.91400	0.16659
C26	0.58856	0.36601	0.33480	N62	0.45607	0.88761	0.19281
C27	0.56848	0.38870	0.33103	C63	0.43078	0.84337	0.19096
C28	0.64861	0.35989	0.26995	C64	0.44834	0.81936	0.28098
C29	0.64693	0.42701	0.21884	C65	0.38330	0.75602	0.20124
C30	0.69202	0.37906	0.28587	C66	0.36616	0.78028	0.10434
H31	0.50821	0.41000	0.28240	C67	0.38955	0.82351	0.09991
H32	0.64227	0.48227	0.17249	C68	0.35780	0.71004	0.21980
H33	0.57327	0.33408	0.38794	C69	0.42486	0.77622	0.28821
H34	0.53871	0.37322	0.38063	C70	0.37596	0.68526	0.22627
H35	0.67651	0.44258	0.16711	H71	0.40999	0.90324	0.14695
F36	0.58293	0.53196	0.27572	H72	0.48010	0.83423	0.35099
H73	0.33480	0.76595	0.02984	H117	0.59168	0.30154	0.23248
H74	0.37549	0.84108	0.02206	H118	0.71102	0.41126	0.31931
H75	0.43901	0.75880	0.36739	H119	0.70140	0.29740	0.20563
F76	0.53178	0.95035	0.19757	H120	0.40756	0.69953	0.19828
F77	0.41558	0.97184	0.14968	H121	0.29547	0.59153	0.33415

C78	0.45703	0.48314	0.28166	H122	0.30134	0.70977	0.22633
C79	0.48381	0.52633	0.28062	C123	1.01608	0.47561	0.28383
C80	0.52623	0.54200	0.27822	C124	0.48392	1.02921	0.17114
C81	0.46857	0.55559	0.28207	C125	0.54236	1.01811	0.19660
N82	0.42957	0.54251	0.28226	F126	0.58371	1.03269	0.21187
C83	0.41154	0.56806	0.28395	C127	0.51370	-0.02794	0.68947
C84	0.36909	0.55155	0.22258	C128	0.45518	-0.01699	0.66454
C85	0.37348	0.61645	0.27498	F129	0.41384	-0.03169	0.65046
C86	0.41595	0.63250	0.34257	C130	-0.01399	0.52763	0.77278
C87	0.43485	0.60868	0.34655	C131	0.47057	0.95568	0.67356
C88	0.35357	0.64231	0.26504	C132	0.44121	0.91056	0.66683
C89	0.35025	0.57548	0.21618	N133	0.45449	0.88421	0.69336
C90	0.31204	0.62413	0.29318	C134	0.42925	0.83997	0.69178
H91	0.49053	0.58842	0.27733	C135	0.44688	0.81601	0.78194
H92	0.35071	0.52025	0.17492	C136	0.38183	0.75262	0.70337
H93	0.43462	0.66329	0.39560	C137	0.36462	0.77681	0.60629
H94	0.46737	0.62196	0.40238	C138	0.38799	0.82005	0.60111
H95	0.31766	0.56206	0.16073	C139	0.35636	0.70665	0.72225
F96	0.41582	0.46646	0.28368	C140	0.42343	0.77288	0.78969
F97	0.55294	0.58344	0.27680	C141	0.37451	0.68190	0.72811
C98	0.02983	0.54620	0.27705	H142	0.40834	0.89976	0.64701
C99	0.04457	0.51830	0.28315	H143	0.47866	0.83093	0.85156
C100	0.08908	0.53262	0.28796	H144	0.33323	0.76243	0.53216
N101	0.11649	0.57178	0.28580	H145	0.37388	0.83755	0.52312
C102	0.16020	0.58925	0.28675	H146	0.43763	0.75550	0.86886
C103	0.18646	0.63049	0.33356	F147	0.53013	0.94704	0.69721
C104	0.24671	0.62718	0.28508	C148	0.45578	0.47991	0.78192
C105	0.21992	0.58567	0.23635	C149	0.48253	0.52311	0.78080
C106	0.17733	0.56684	0.23853	C150	0.52496	0.53880	0.77878
C107	0.29208	0.64771	0.27342	C151	0.46725	0.55236	0.78171
C108	0.22918	0.64914	0.33547	N152	0.42820	0.53929	0.78039
C109	0.31562	0.69083	0.23828	C153	0.41016	0.56485	0.78163
H110	0.09848	0.50960	0.29688	C154	0.36775	0.54842	0.71914
H111	0.17378	0.64809	0.37225	C155	0.37200	0.61312	0.77400
H112	0.23133	0.56789	0.18829	C156	0.41445	0.62911	0.84226
H113	0.15805	0.53540	0.19450	C157	0.43339	0.60536	0.84560
H114	0.24821	0.68057	0.38000	C158	0.35207	0.63891	0.76550
F115	0.05609	0.58772	0.27655	C159	0.34887	0.57230	0.71334
F116	0.02912	0.44783	0.28864	C160	0.31046	0.62066	0.79281
H161	0.48924	0.58519	0.77783	H205	0.56291	0.24522	0.53562
H162	0.34943	0.51720	0.67042	F206	0.46581	0.05084	0.66446
H163	0.43303	0.65977	0.89678	F207	0.58197	0.02938	0.71164
H164	0.46585	0.61853	0.90267	C208	0.54048	0.51210	0.77831
H165	0.31631	0.55895	0.65718	C209	0.51373	0.46889	0.77961

F166	0.41456	0.46321	0.78378	C210	0.47129	0.45321	0.78145
F167	0.55166	0.58024	0.77727	C211	0.52907	0.43964	0.77973
C168	0.02825	0.54232	0.77720	N212	0.56785	0.45290	0.77289
C169	0.04302	0.51445	0.78305	C213	0.58658	0.42782	0.77500
C170	0.01457	0.47174	0.78437	C214	0.62617	0.44681	0.72298
C171	0.08752	0.52885	0.78692	C215	0.62680	0.38150	0.77835
N172	0.11478	0.56805	0.78312	C216	0.58740	0.36286	0.83655
C173	0.15847	0.58568	0.78327	C217	0.56743	0.38561	0.83415
C174	0.18463	0.62694	0.83001	C218	0.64719	0.35669	0.76904
C175	0.24506	0.62372	0.78330	C219	0.64588	0.42398	0.72198
C176	0.21832	0.58232	0.73279	C220	0.69059	0.37569	0.78630
C177	0.17569	0.56341	0.73446	H221	0.50704	0.40684	0.78170
C178	0.29054	0.64426	0.77380	H222	0.64143	0.47934	0.67818
C179	0.22738	0.64562	0.83307	H223	0.57207	0.33086	0.88866
C180	0.31418	0.68743	0.74067	H224	0.53770	0.37016	0.88404
H181	0.09706	0.50592	0.79651	H225	0.67551	0.43961	0.67066
H182	0.17184	0.64449	0.86826	F226	0.58170	0.52882	0.77659
H183	0.22980	0.56468	0.68418	F227	0.44460	0.41178	0.78272
H184	0.15643	0.53203	0.68951	C228	0.97233	0.45706	0.78015
H185	0.24631	0.67698	0.87843	C229	0.95758	0.48493	0.77469
F186	0.05446	0.58385	0.77602	C230	0.91305	0.47050	0.76992
F187	0.02763	0.44399	0.78864	N231	0.88645	0.43143	0.79271
C188	0.48214	0.02574	0.67160	C232	0.84260	0.41356	0.78854
C189	0.52526	0.04209	0.68765	C233	0.82033	0.37271	0.85990
C190	0.54062	0.01475	0.69659	C234	0.75577	0.37437	0.77458
C191	0.55486	0.08710	0.69714	C235	0.77820	0.41542	0.70220
N192	0.54218	0.11391	0.67413	C236	0.82112	0.43484	0.70862
C193	0.56834	0.15798	0.68460	C237	0.70994	0.35339	0.76411
C194	0.55213	0.18350	0.59965	C238	0.77747	0.35336	0.85474
C195	0.61692	0.24497	0.70558	C239	0.68536	0.31102	0.73091
C196	0.63292	0.21912	0.79304	H240	0.90325	0.49337	0.75266
C197	0.60902	0.17617	0.78248	H241	0.83639	0.35588	0.92138
C198	0.64218	0.29067	0.72390	H242	0.76247	0.43225	0.63531
C199	0.57618	0.22652	0.60793	H243	0.83686	0.46588	0.64564
C200	0.62340	0.31398	0.73897	H244	0.76145	0.32207	0.91559
H201	0.58765	0.09746	0.71875	F245	0.94606	0.41555	0.77974
H202	0.52083	0.16995	0.52431	F246	0.97293	0.55539	0.76781
H203	0.66352	0.23194	0.87547	H247	0.40612	0.69620	0.70022
H204	0.62207	0.15746	0.85701	H248	0.29379	0.58797	0.83192
H249	0.29998	0.70642	0.72946	H251	0.70964	0.40781	0.82104
H250	0.59011	0.29863	0.72762	H252	0.69984	0.29392	0.70678

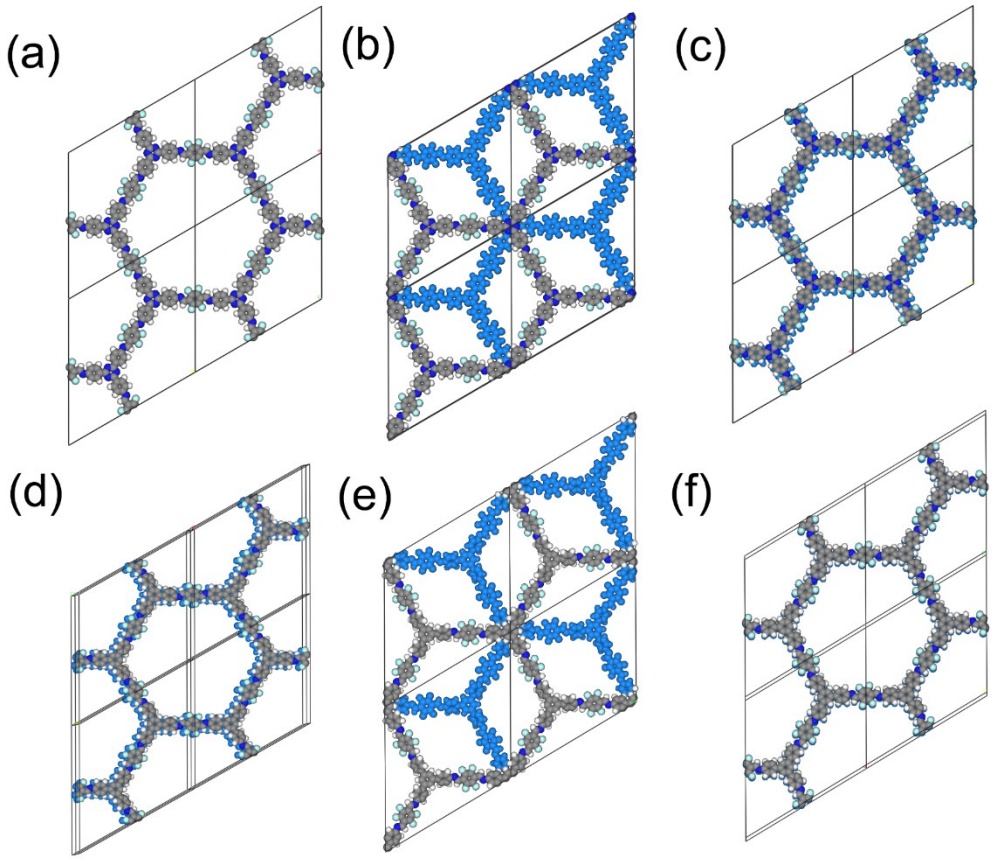


Figure S10. The possible structures of SCF-COF-1 and SCF-FCOF-2 based on hex topology: (a, d) eclipsed (AA) stacking mode, (b, e) staggered (AB) stacking mode, and (c, f) 1.0-Å serrated stacking mode.

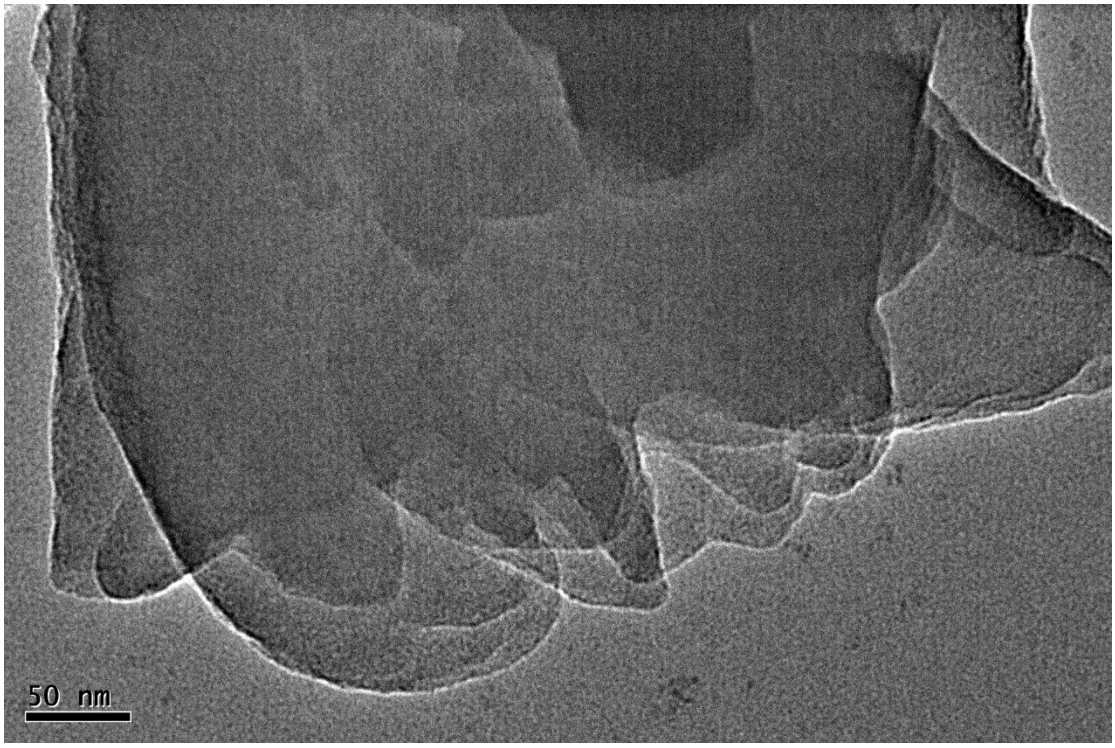


Figure S11. HRTEM image of SCF-FCOF-2(Scale bar, 50nm).

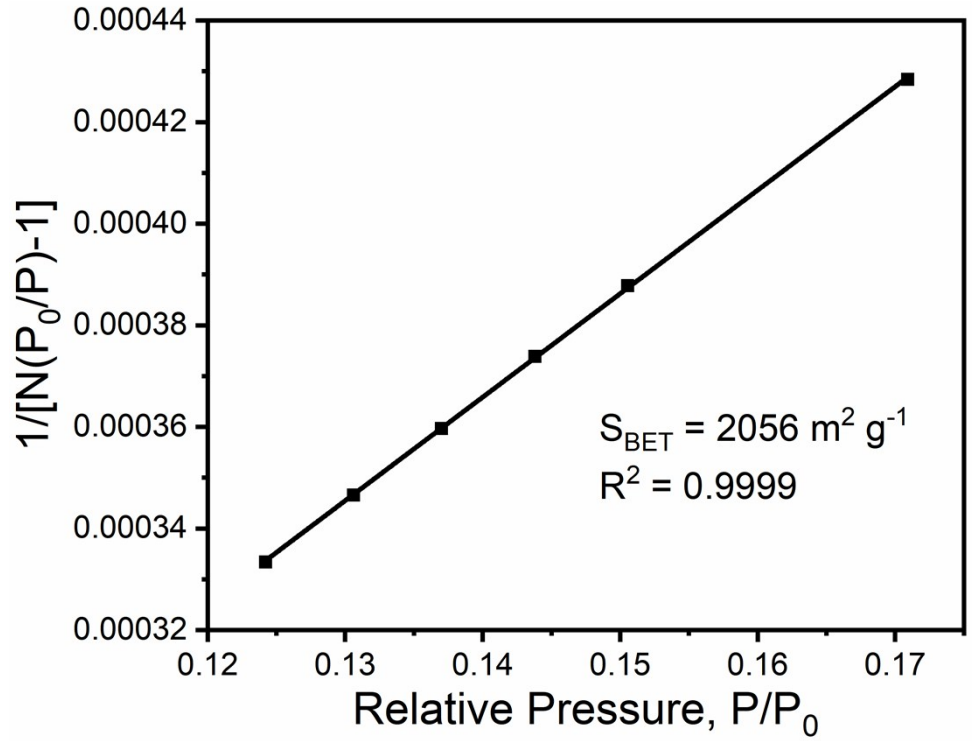


Figure S12. BET plot calculated from N_2 adsorption isotherms at 77 K for SCF-FCOF-.

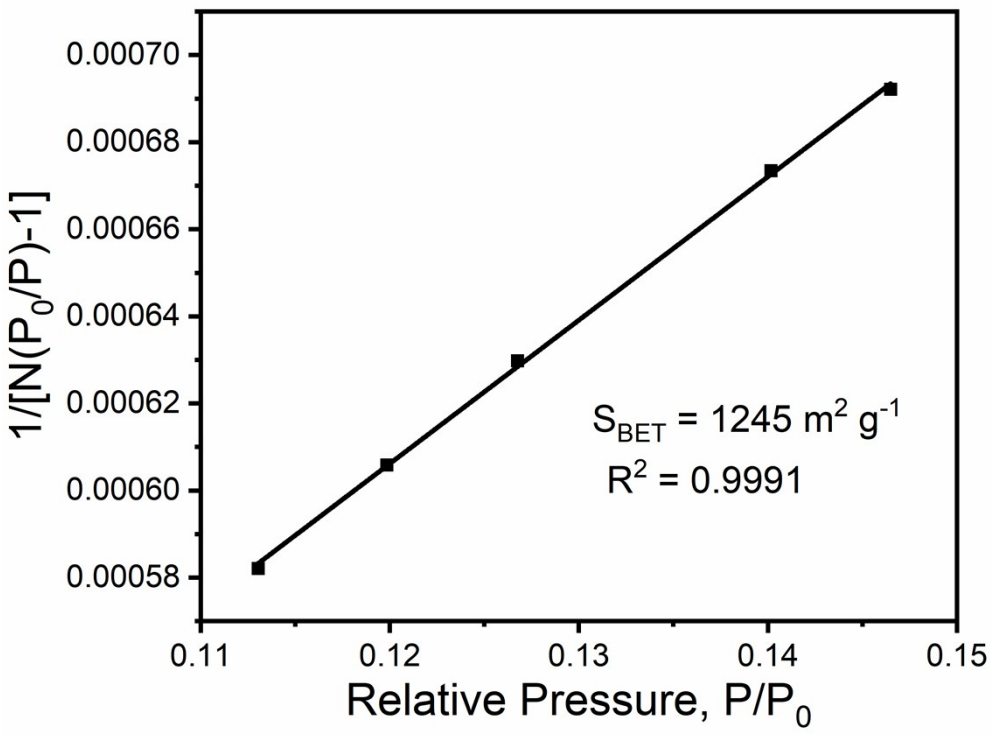


Figure S13. BET plot calculated from N_2 adsorption isotherms at 77 K for SCF-FCOF-2.

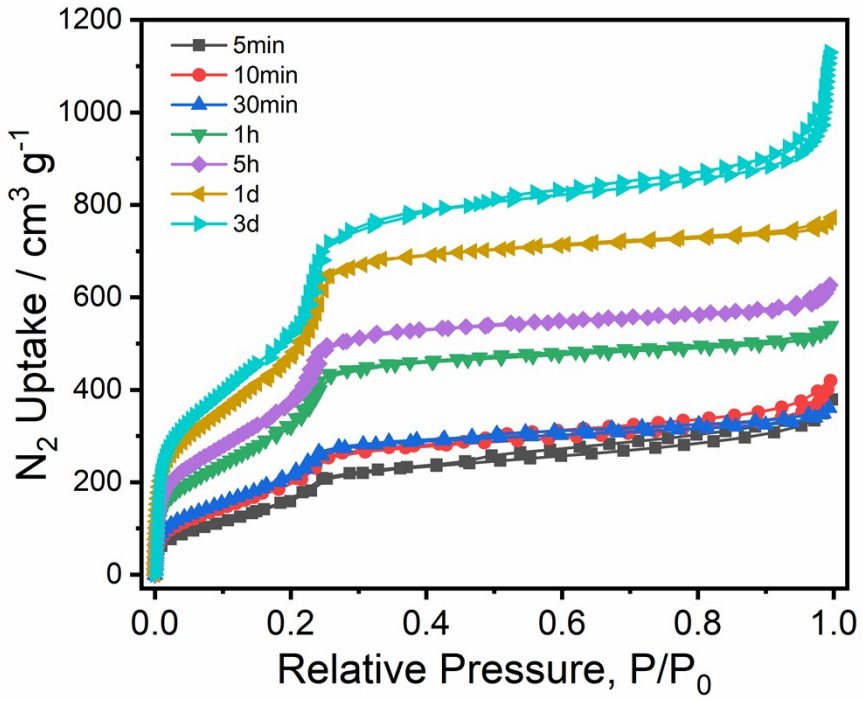


Figure S14. N_2 sorption isotherms for SCF-FCOF-1s synthesized for different reaction time intervals.

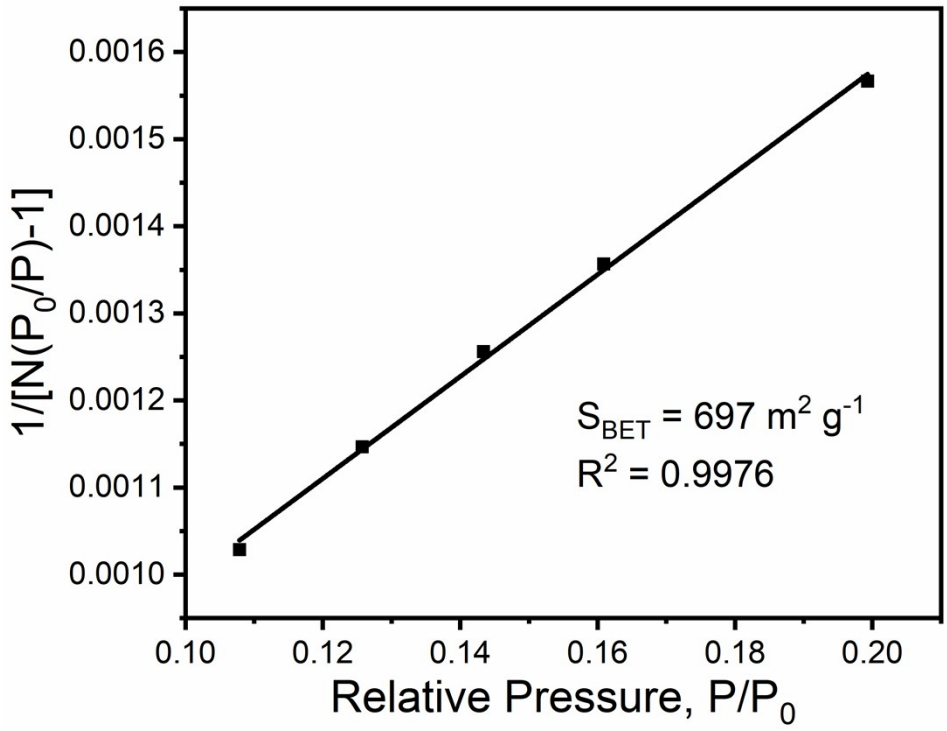


Figure S15. BET plot calculated from N_2 adsorption isotherms at 77 K for SCF-FCOF-1 synthesized for 5 min.

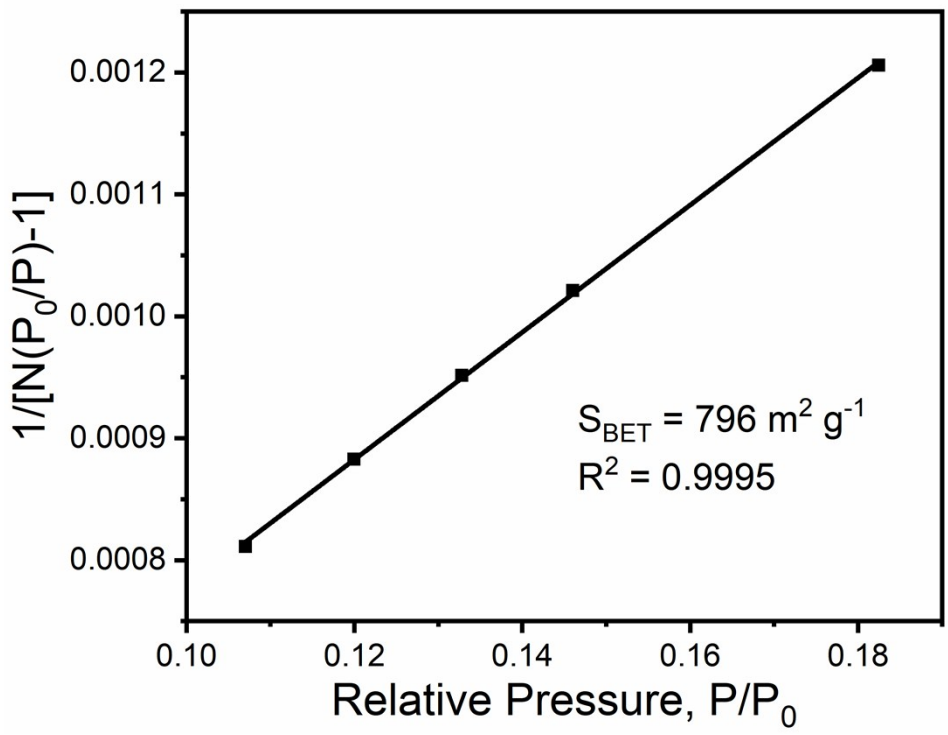


Figure S16. BET plot calculated from N_2 adsorption isotherms at 77 K for SCF-FCOF-1 synthesized for 10 min.

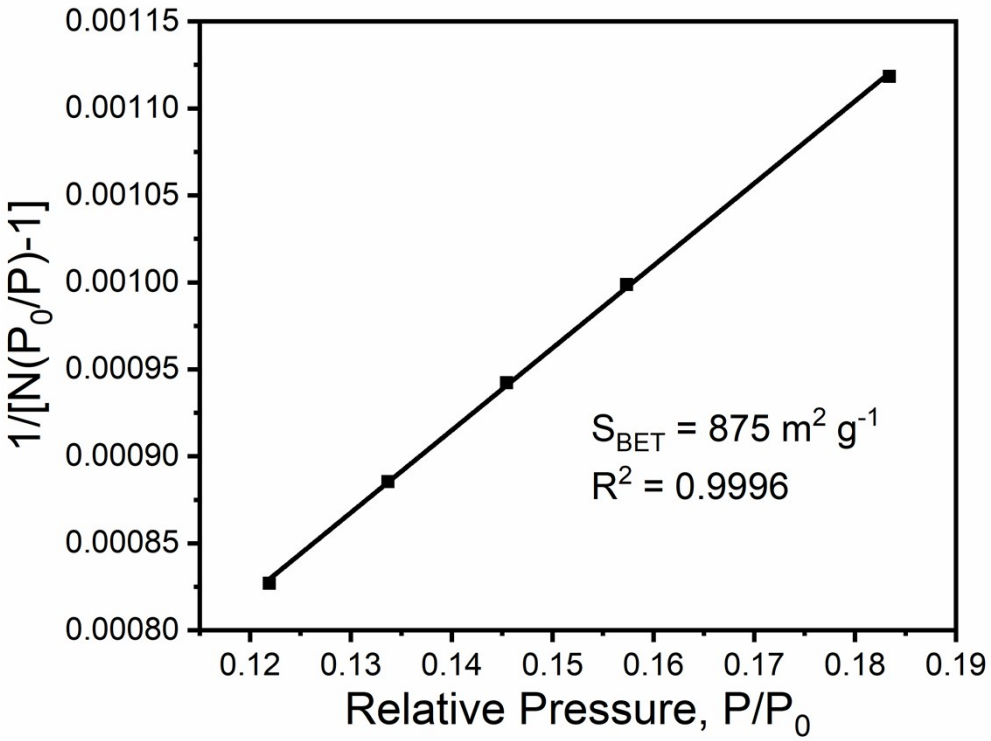


Figure S17. BET plot calculated from N_2 adsorption isotherms at 77 K for SCF-FCOF-1 synthesized for 30 min.

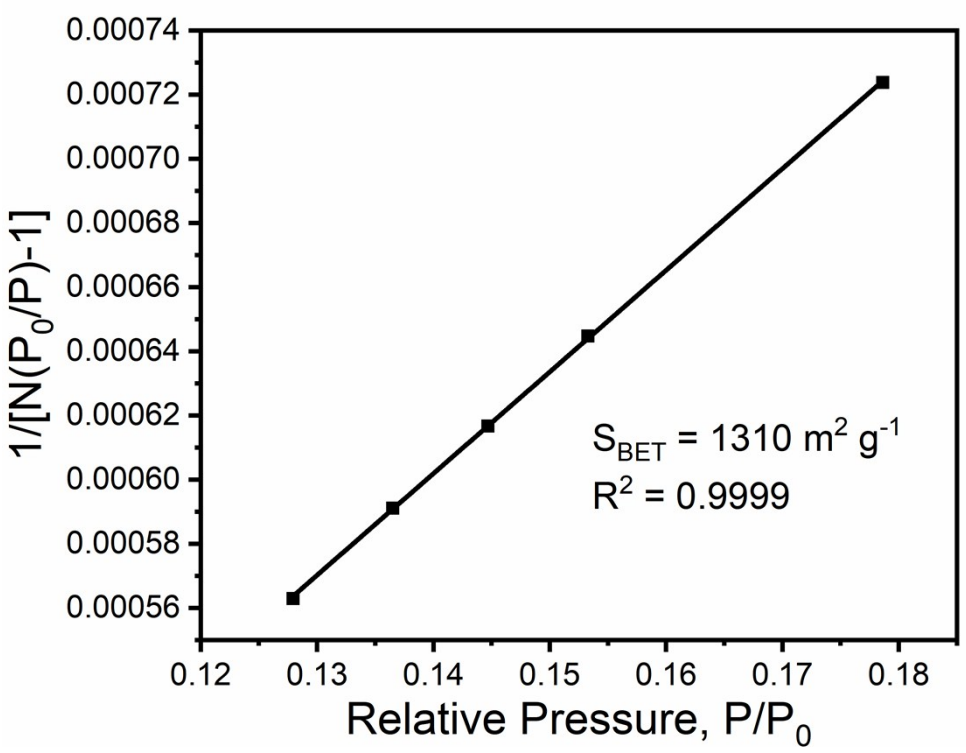


Figure S18. BET plot calculated from N_2 adsorption isotherms at 77 K for SCF-FCOF-1 synthesized for 1 h.

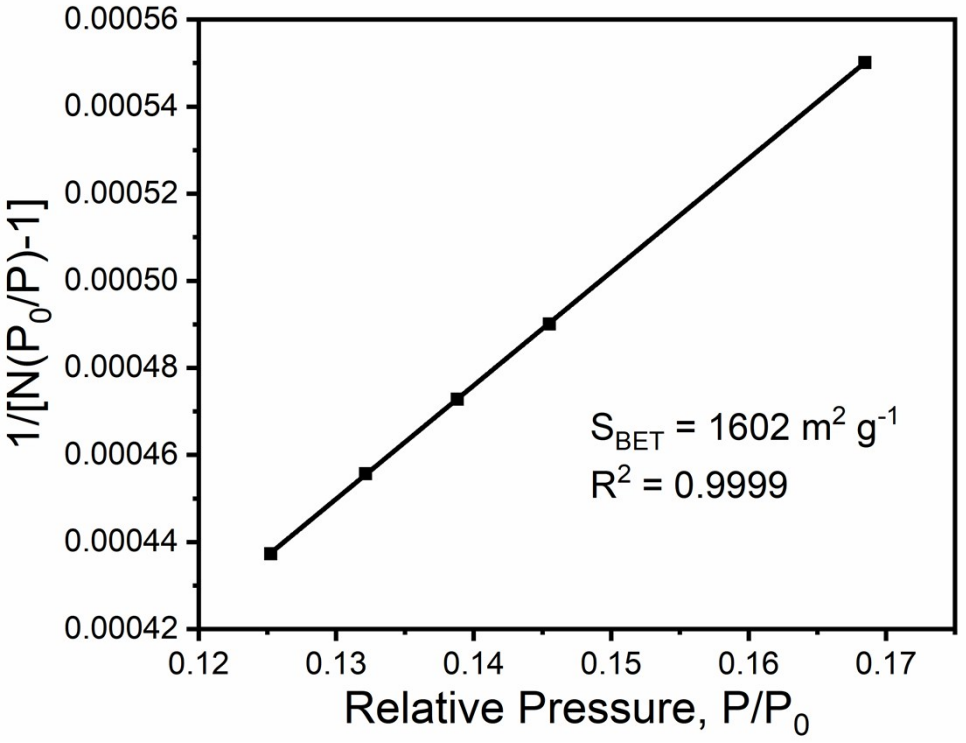


Figure S19. BET plot calculated from N_2 adsorption isotherms at 77 K for SCF-FCOF-1 synthesized for 5 h.

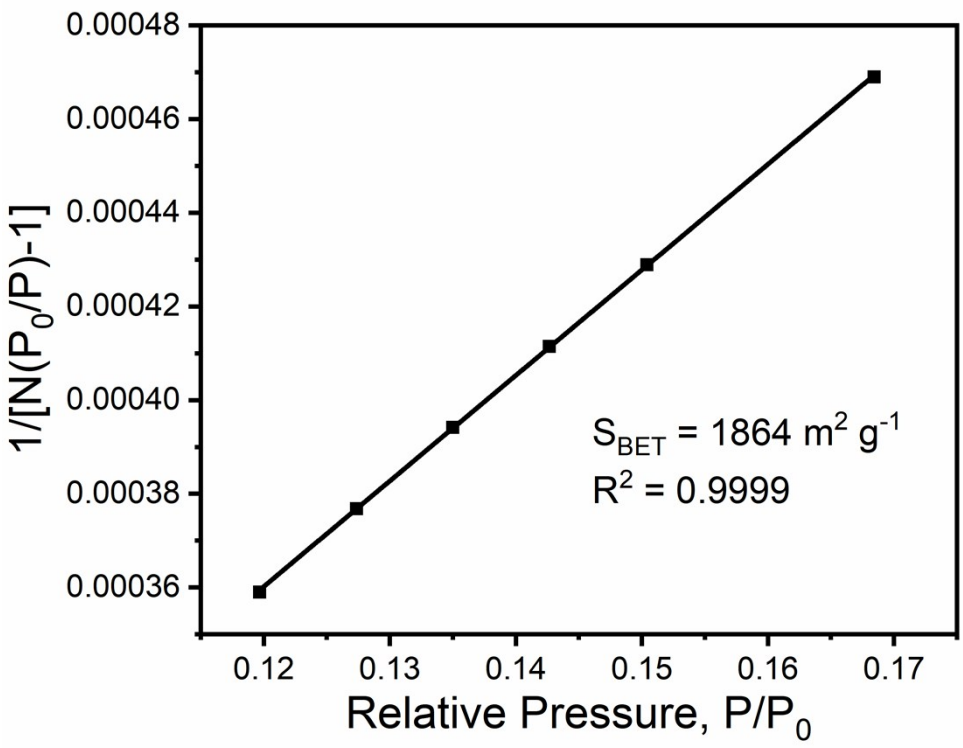


Figure S20. BET plot calculated from N_2 adsorption isotherms at 77 K for SCF-FCOF-1 synthesized for 1 d.

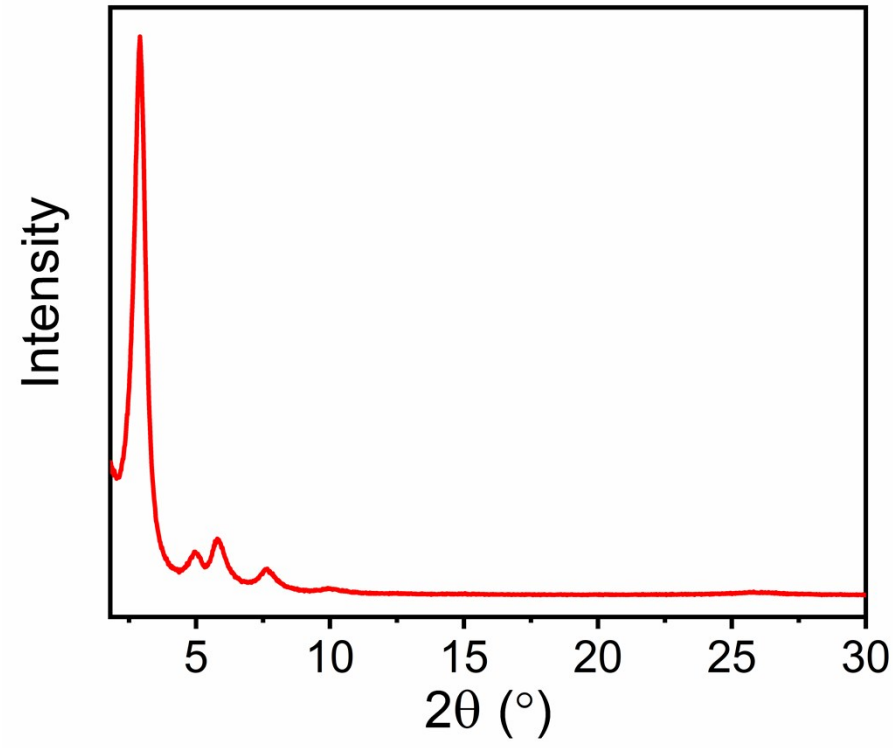


Figure S21. PXRD pattern for SCF-FCOF-1 prepared in 1-gram-scale.

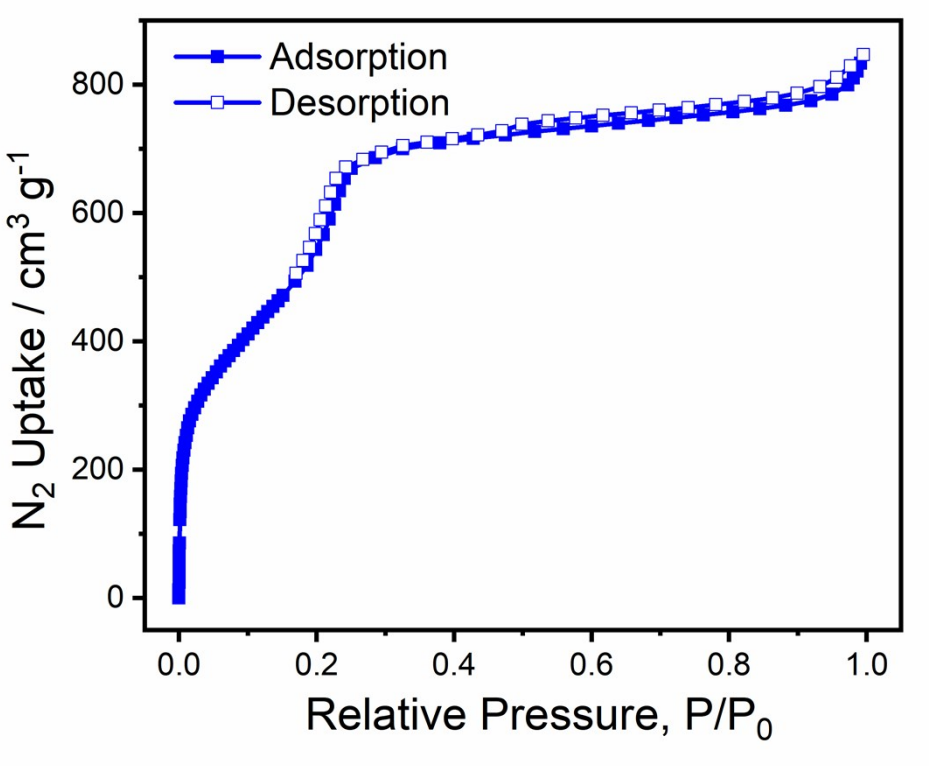


Figure S22. N_2 sorption isotherms for SCF-FCOF-1 prepared in 1-gram-scale.

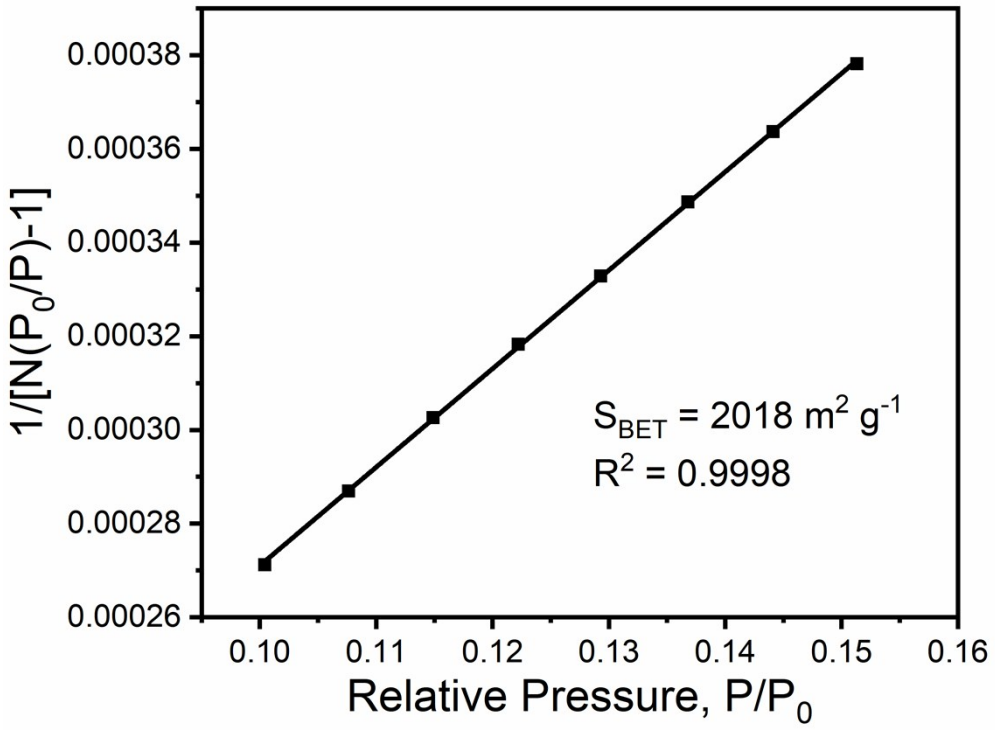
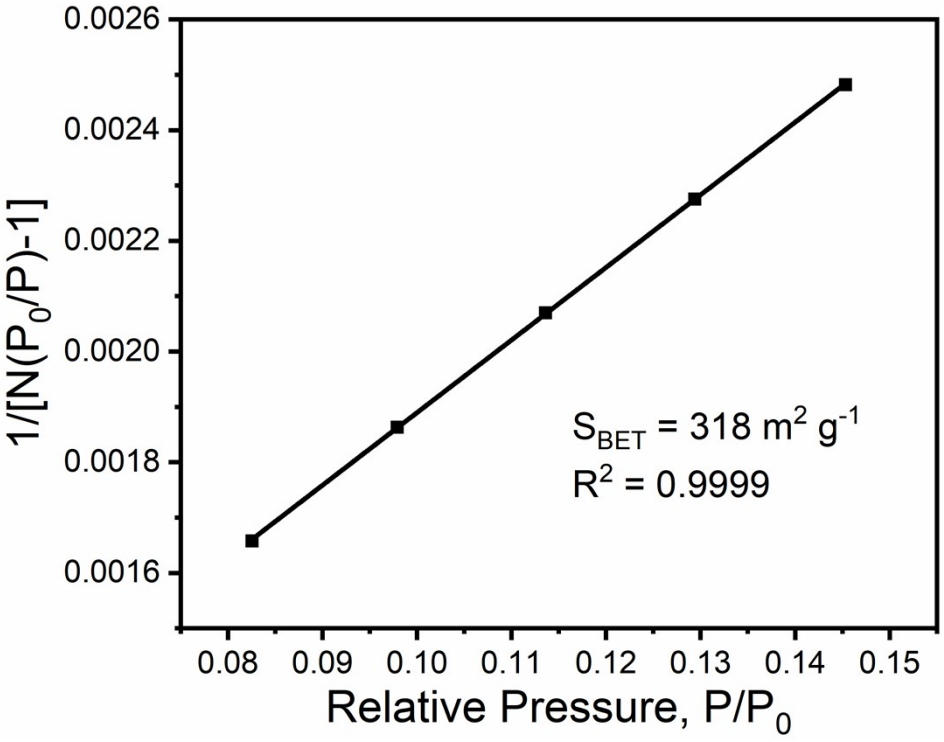


Figure S23. BET plot calculated from N_2 adsorption isotherms at 77 K for SCF-FCOF-1 prepared in 1-gram-scale.



~~**Figure S21.**~~ **Figure S24.** BET plot calculated from N_2 adsorption isotherms at 77 K for SCF-HCOF-1.

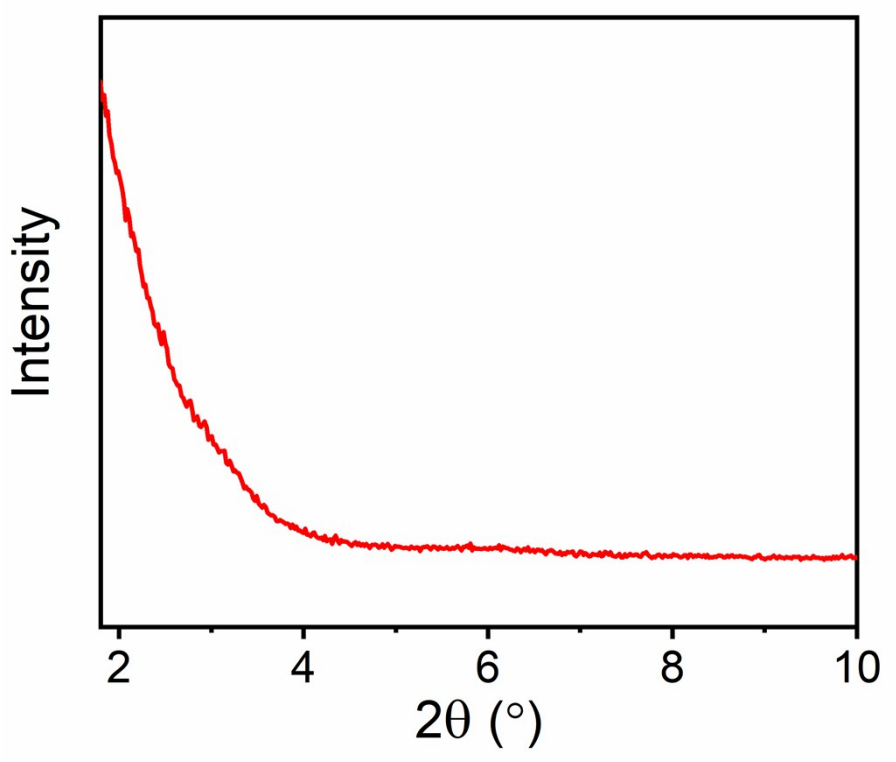


Figure S25. PXRD pattern for TFBDA-TFPT.

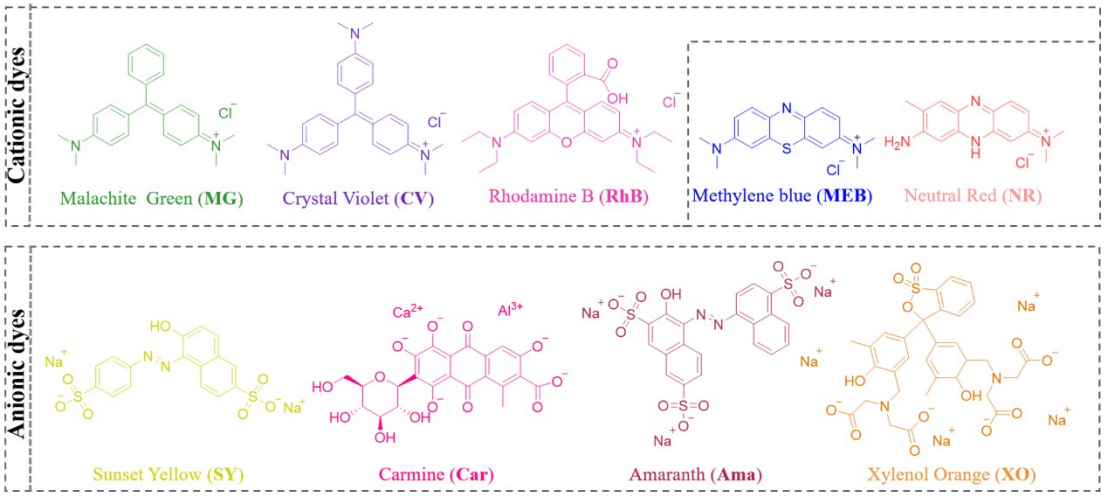


Figure S26. Molecular formulas of tested organic dyes.

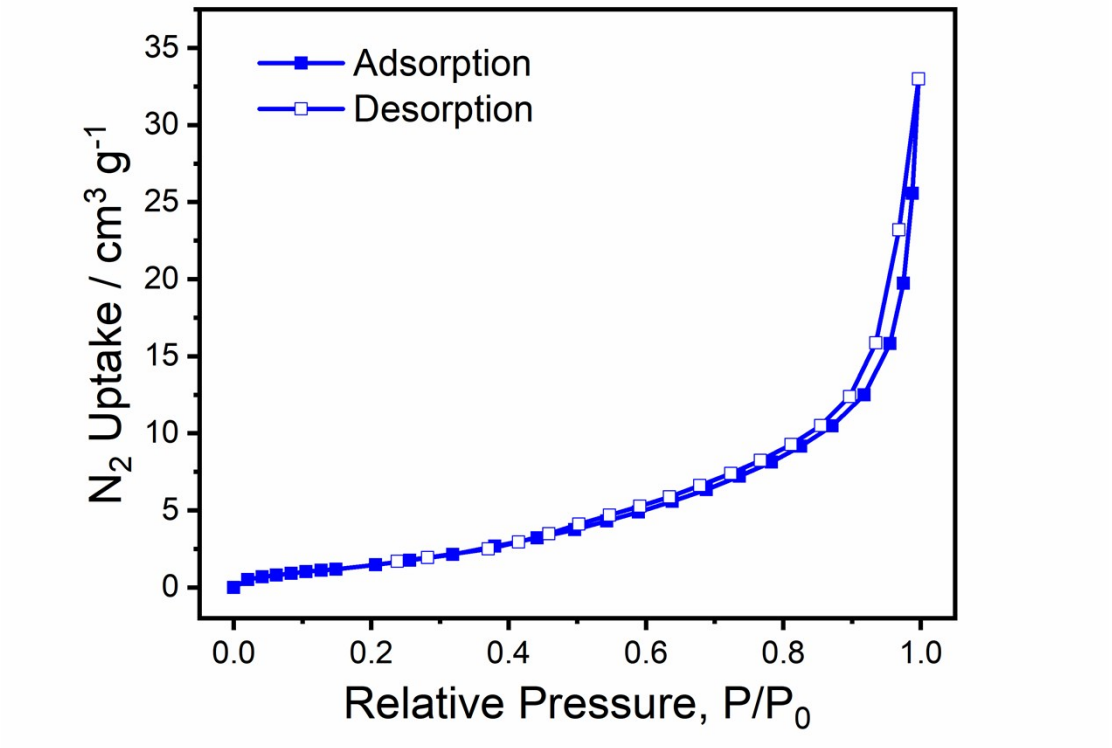


Figure S27. N_2 sorption isotherms for LS-SCF-FCOP.

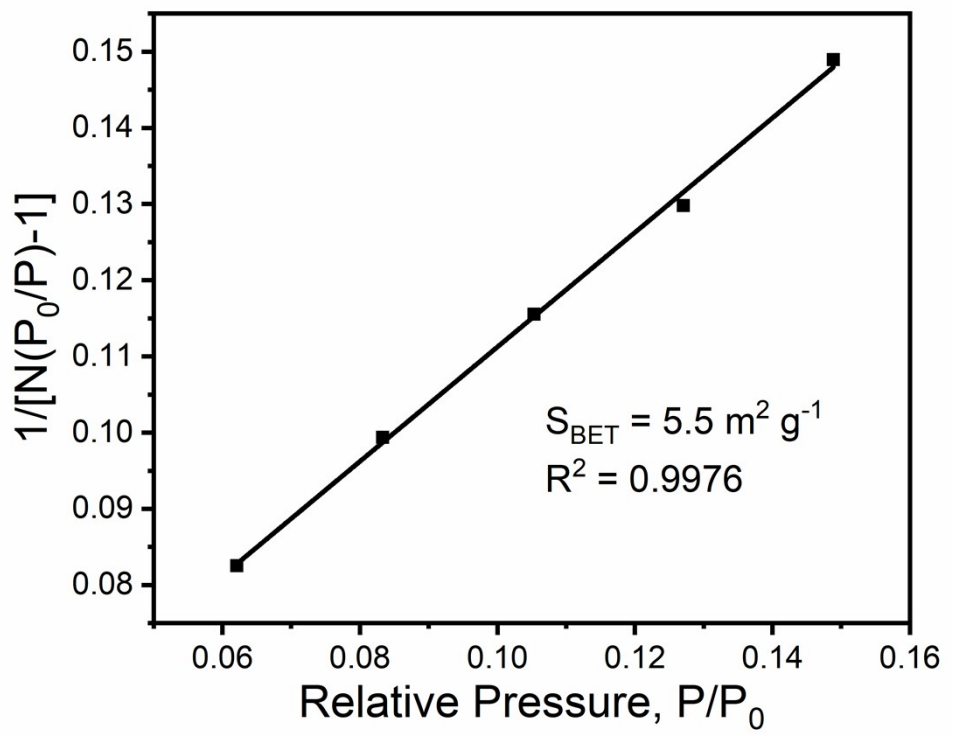


Figure S28. N_2 sorption isotherms for LS-SCF-FCOP.

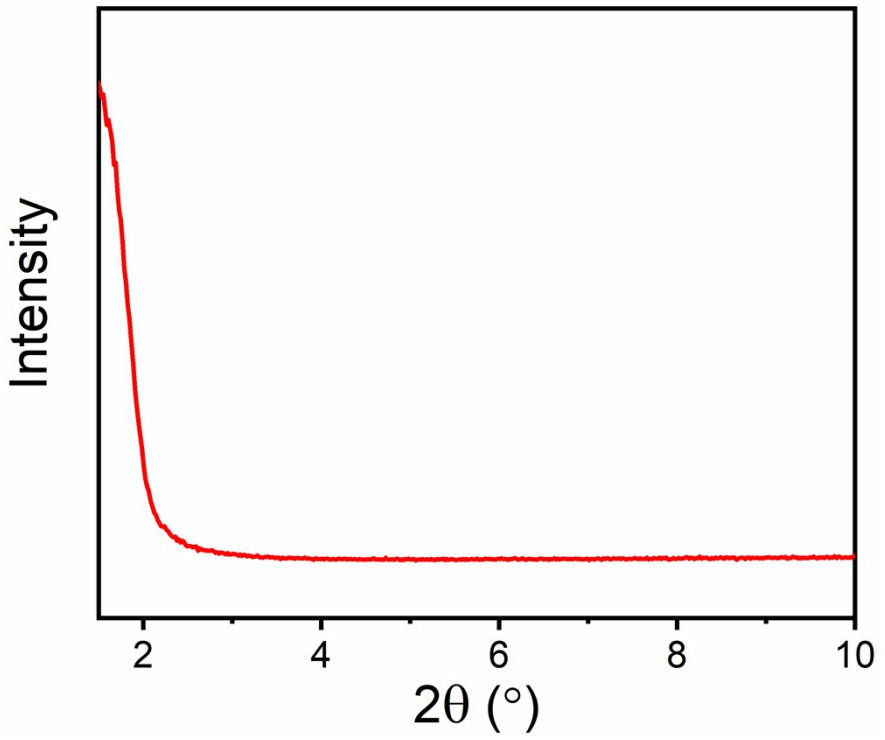


Figure S29. PXRD pattern for LS-SCF-FCOP.

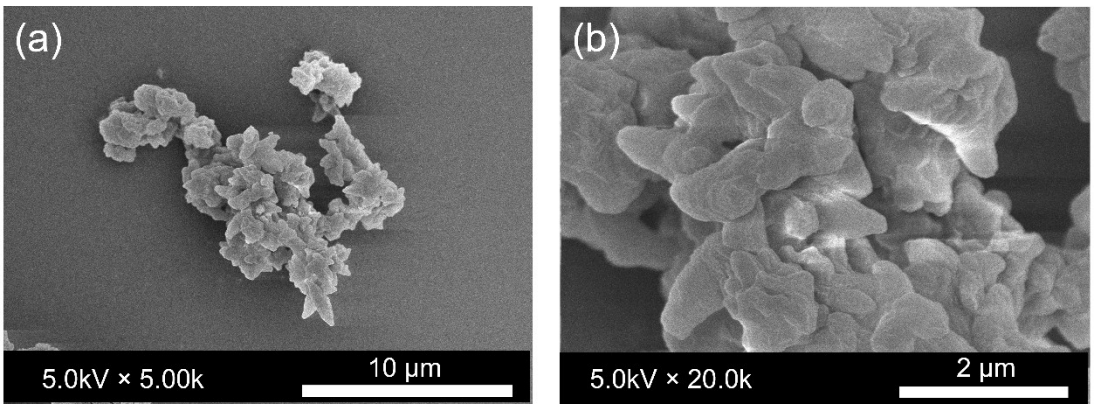


Figure S30. SEM images of SCF-HCOF-1. Magnification: (a) 5.00k (scale bar: 10µm); (b) 20.0k (scale bar: 2µm).

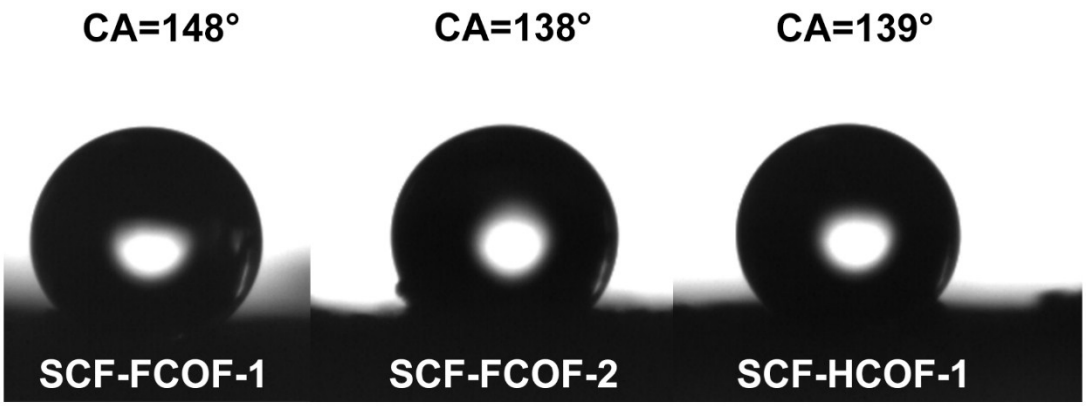


Figure S31. Water contact angles (CA) of water droplet on the pressed pellet of SCF-FCOF-1, SCF-FCOF-2 and SCF-HCOF-1.

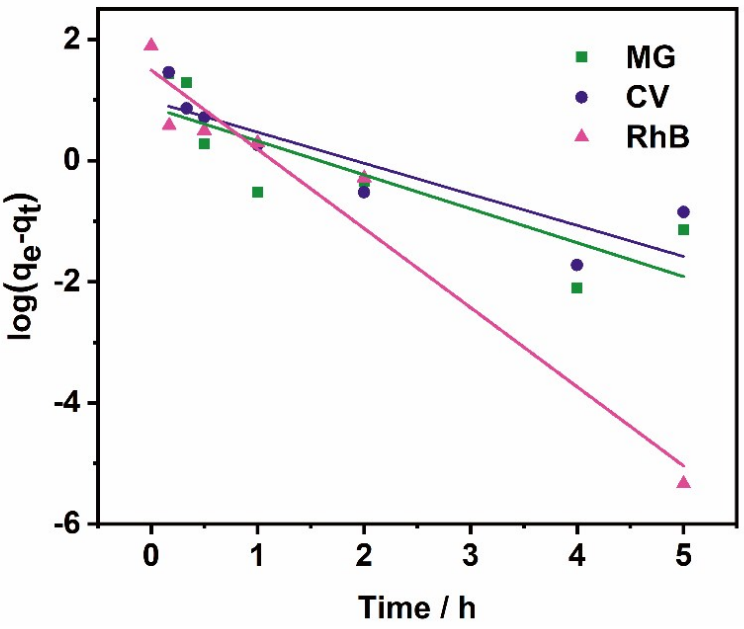


Figure S32. Pseudo-first-order plot for MG, CV and RhB uptake by SCF-FCOF-1.

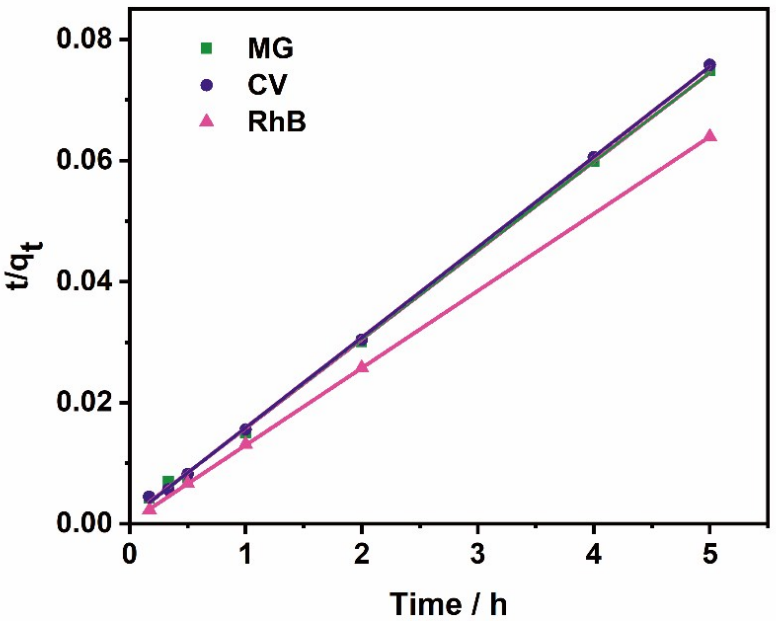


Figure S33. Pseudo-second-order plot for MG, CV and RhB uptake by SCF-FCOF-1.

Table S7. Kinetic parameters for MG, CV and RhB uptake by SCF-FCOF-1

Dyes	$q_{e,exp}$ (mg g^{-1})	Pseudo-First-Order Model			Pseudo-Second-Order Model		
		k_{obs} (min^{-1})	q_e (mg g^{-1})	R^2	k_{obs} (g mg^{-1} min^{-1})	q_e (mg g^{-1})	R^2
MG	66.84	1.29	7.64	0.6610	0.19	68.16	0.9993
CV	65.96	1.18	9.59	0.7484	0.23	67.07	0.9996
RhB	78.20	3.01	31.42	0.9390	0.63	78.49	1.0000

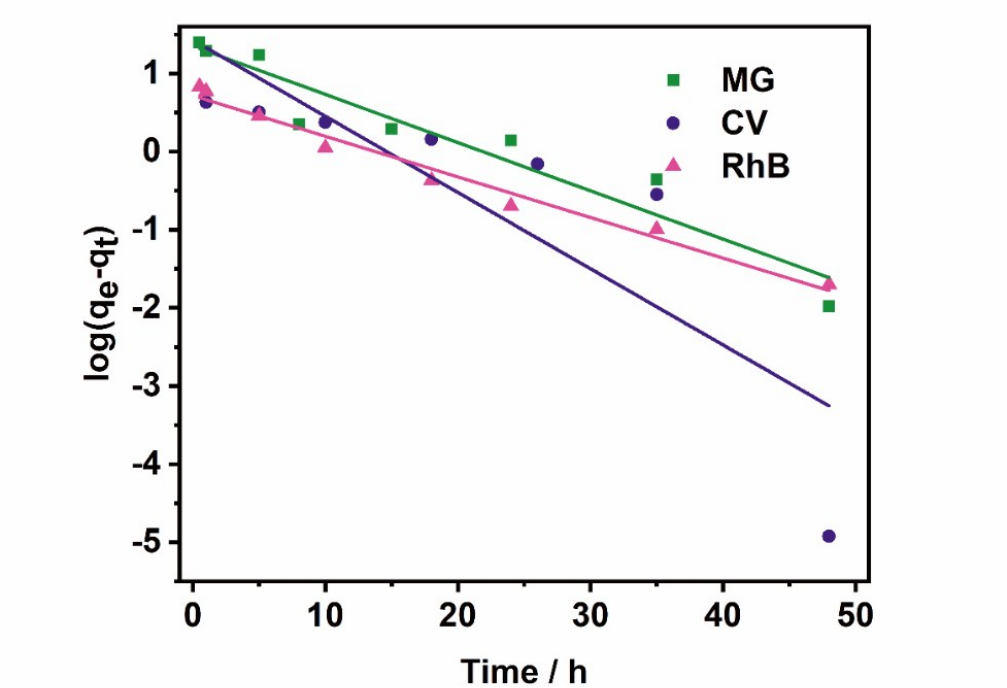


Figure S34. Pseudo-first-order plot for MG, CV and RhB uptake by SCF-HCOF-1.

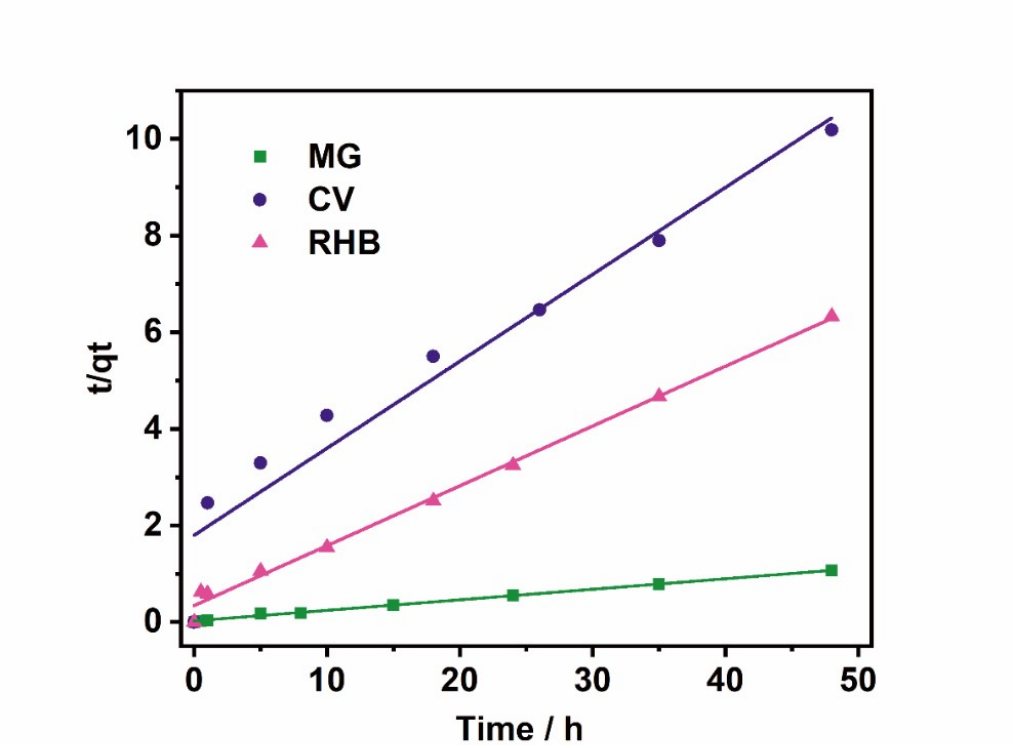


Figure S35. Pseudo-second-order plot for MG, CV and RhB uptake by SCF-HCOF-1.

Table S8. Kinetic parameters for MG, CV and RhB uptake by SCF-HCOF-1

Dyes	$q_{e,exp}$ (mg g^{-1})	Pseudo-First-Order Model			Pseudo-Second-Order Model		
		k_{obs} (min^{-1})	q_e (mg g^{-1})	R^2	k_{obs} (g mg^{-1} min^{-1})	q_e (mg g^{-1})	R^2
MG	45.089	0.14	22.26	0.9018	0.021	45.89	0.9968
CV	4.7122	0.22	26.68	0.6546	0.018	5.56	0.9259
RhB	7.5801	0.12	5.18	0.9754	0.045	8.08	0.9935

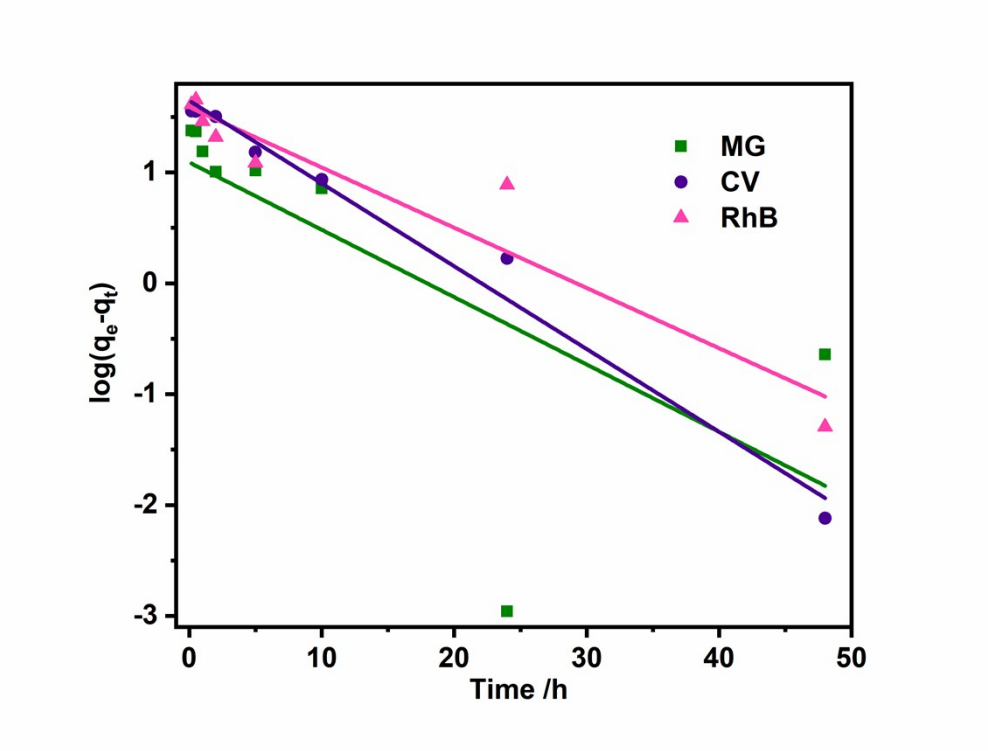


Figure S36. (a) Pseudo-first-order plot for MG, CV and RhB uptake by SCF-FCOF-2

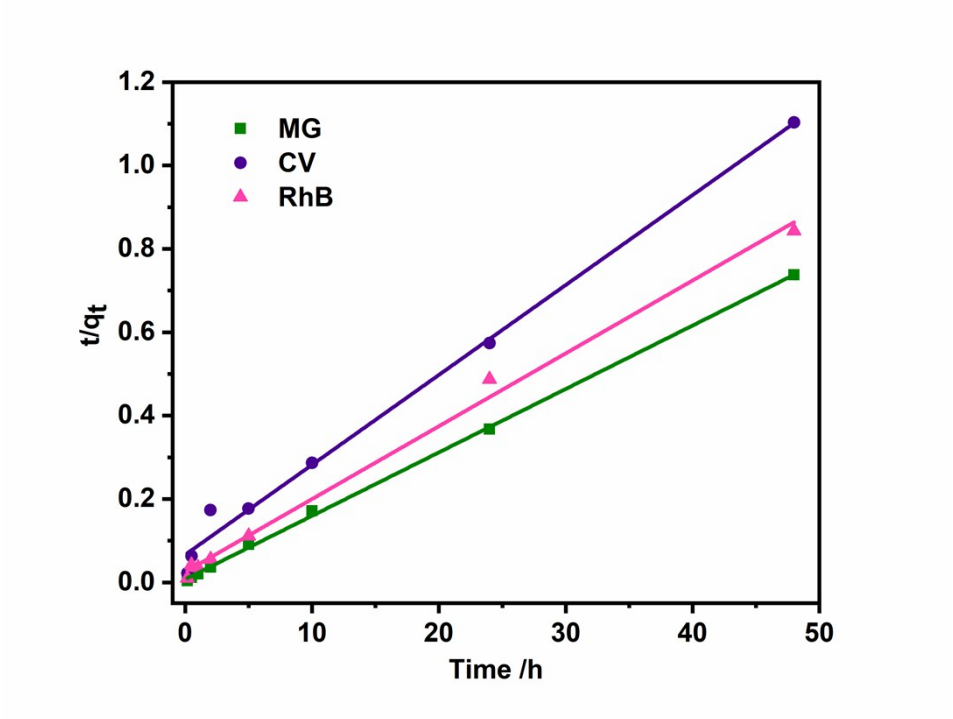


Figure S37. (a) Pseudo-second-order plot for MG, CV and RhB uptake by SCF-FCOF-2

Table S9. Kinetic parameters for MG, CV and RhB uptake by SCF-FCOF-2

Dyes	$q_{e,exp}$ (mg g^{-1})	Pseudo-First-Order Model			Pseudo-Second-Order Model		
		k_{obs} (min^{-1})	q_e (mg g^{-1})	R^2	k_{obs} (g mg^{-1} min^{-1})	q_e (mg g^{-1})	R^2
MG	65.32	0.14	12.31	0.3725	0.031	65.70	0.9993
CV	43.52	0.17	44.36	0.9784	0.0070	46.36	0.9907
RhB	56.95	0.12	38.73	0.8992	0.012	57.24	0.9946

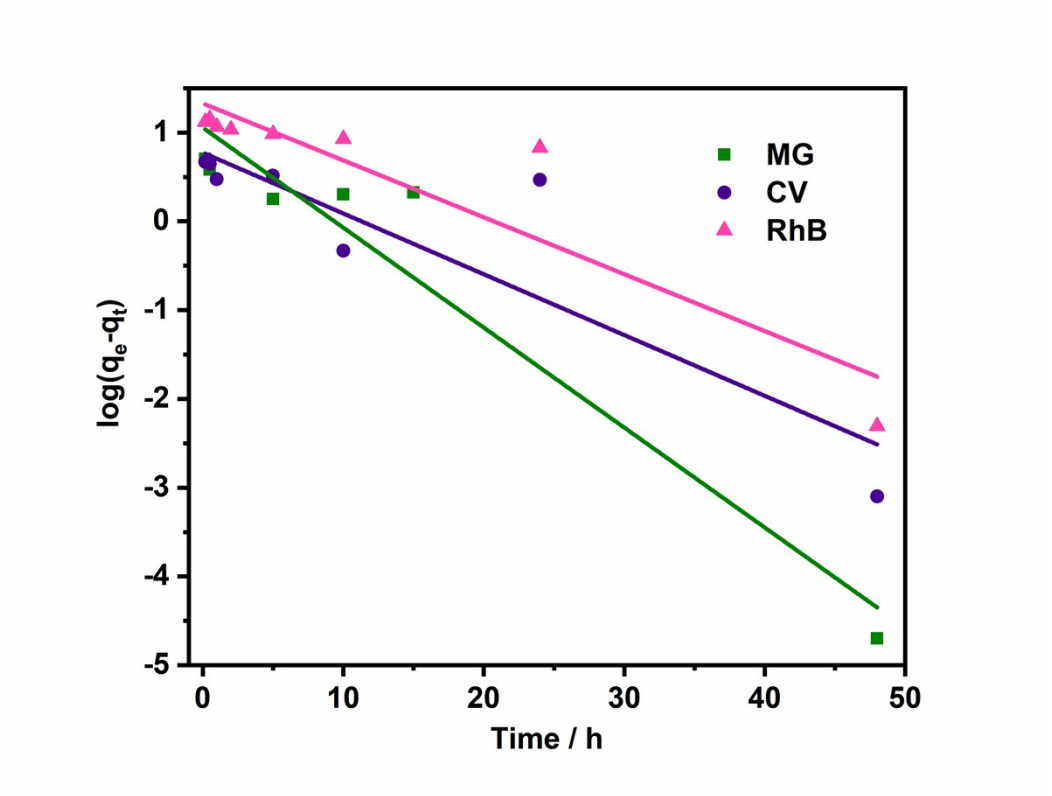


Figure S38. (a) Pseudo-first-order plot for MG, CV and RhB uptake by LS-SCF-COP

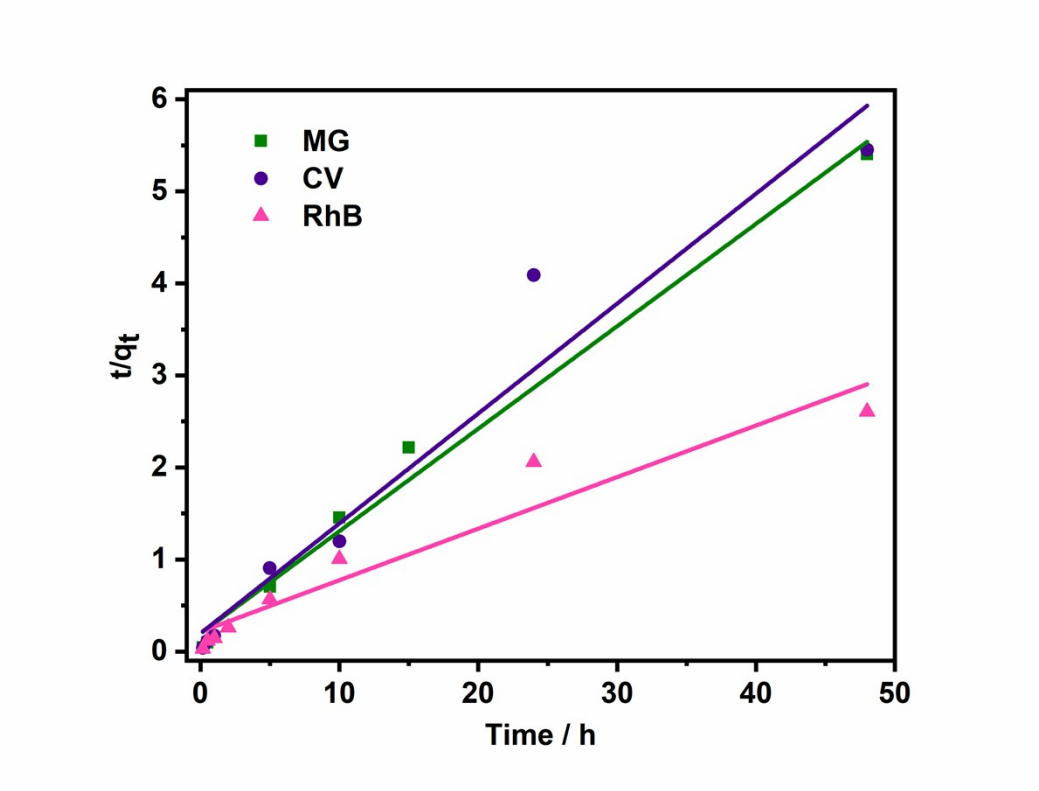


Figure S39. Pseudo-second-order plot for MG, CV and RhB uptake by LS-SCF-COP

Table S10. Kinetic parameters for MG, CV and RhB uptake by LS-SCF-COP

Dyes	$q_{e,exp}$ (mg g^{-1})	Pseudo-First-Order Model			Pseudo-Second-Order Model		
		k_{obs} (min^{-1})	q_e (mg g^{-1})	R^2	k_{obs} (g mg^{-1} min^{-1})	q_e (mg g^{-1})	R^2
MG	8.88	0.26	11.34	0.9138	0.064	8.98	0.9865
CV	8.81	0.16	5.93	0.7446	0.072	8.37	0.9404
RhB	18.42	0.15	21.27	0.8108	0.015	17.85	0.9184

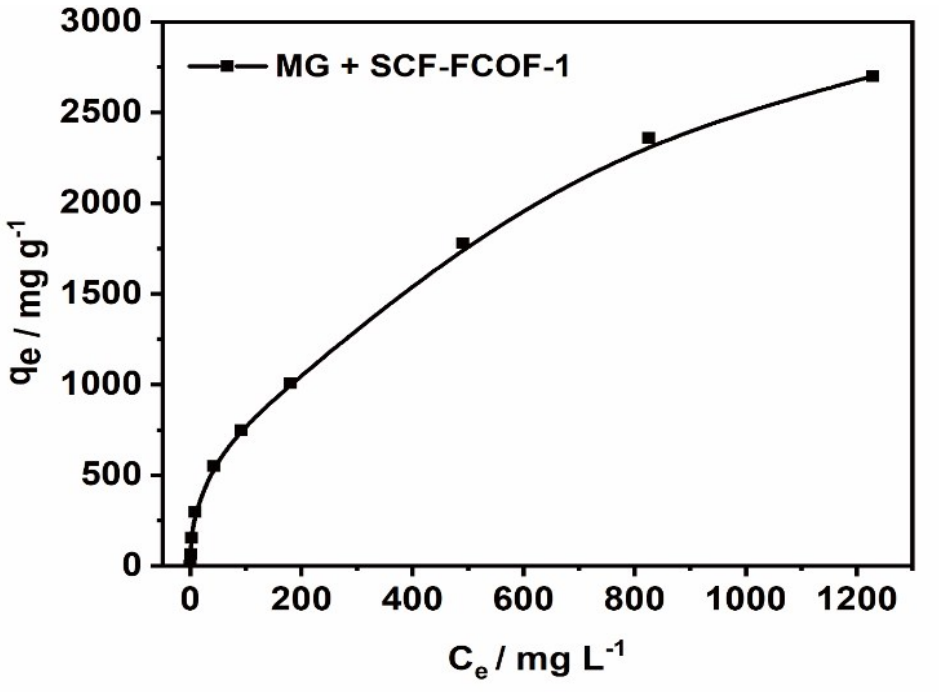


Figure S40. Adsorption isotherm of MG uptake by SCF-FCOF-1

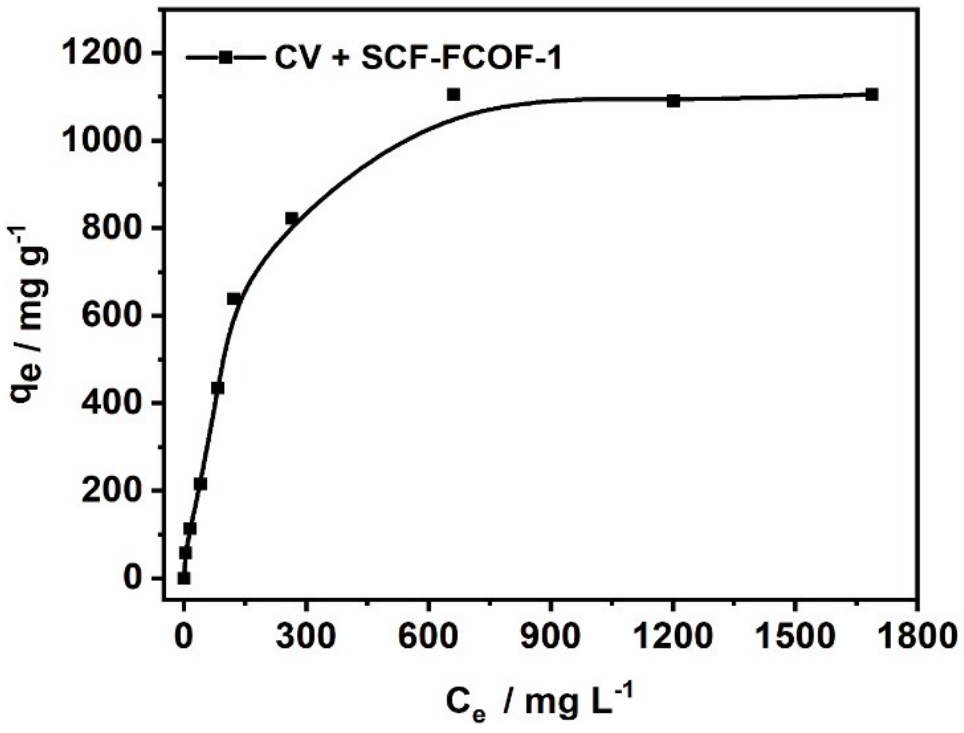


Figure S41. Adsorption isotherm of CV uptake by SCF-FCOF-1

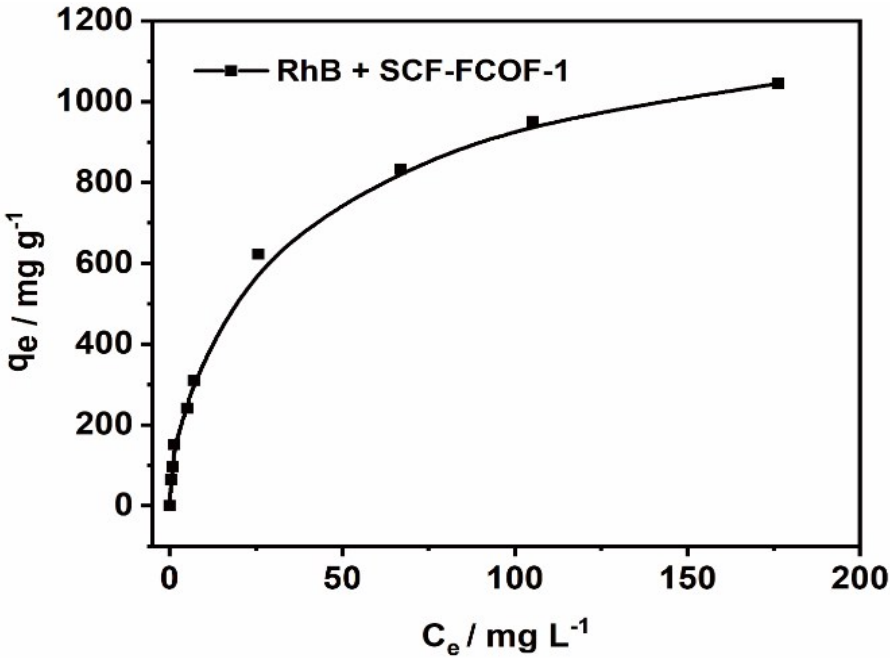


Figure S42. Adsorption isotherm of RhB uptake by SCF-FCOF-1

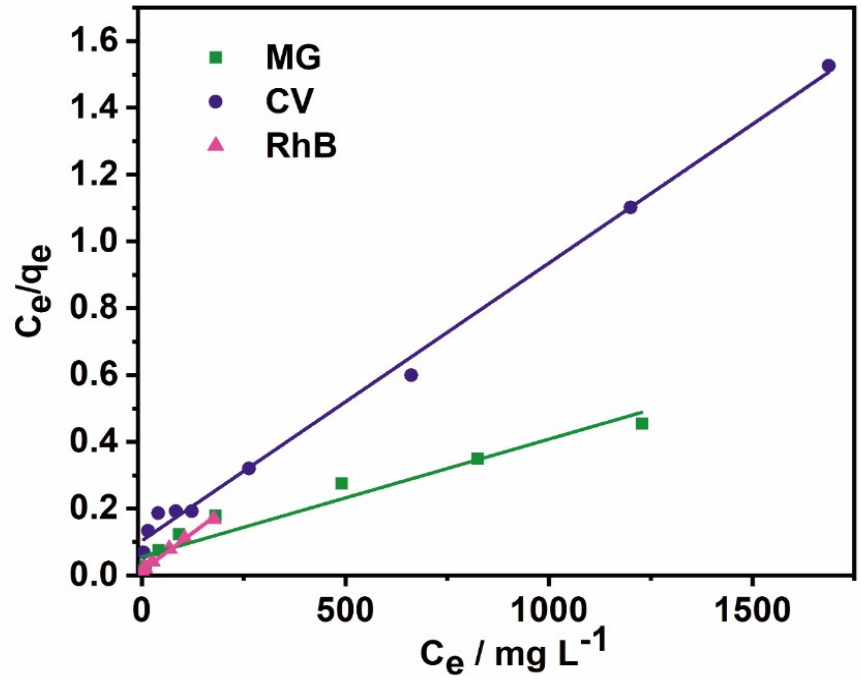


Figure S43. Langmuir adsorption isotherm plot for MG, CV and RhB uptake by SCF-FCOF-1.

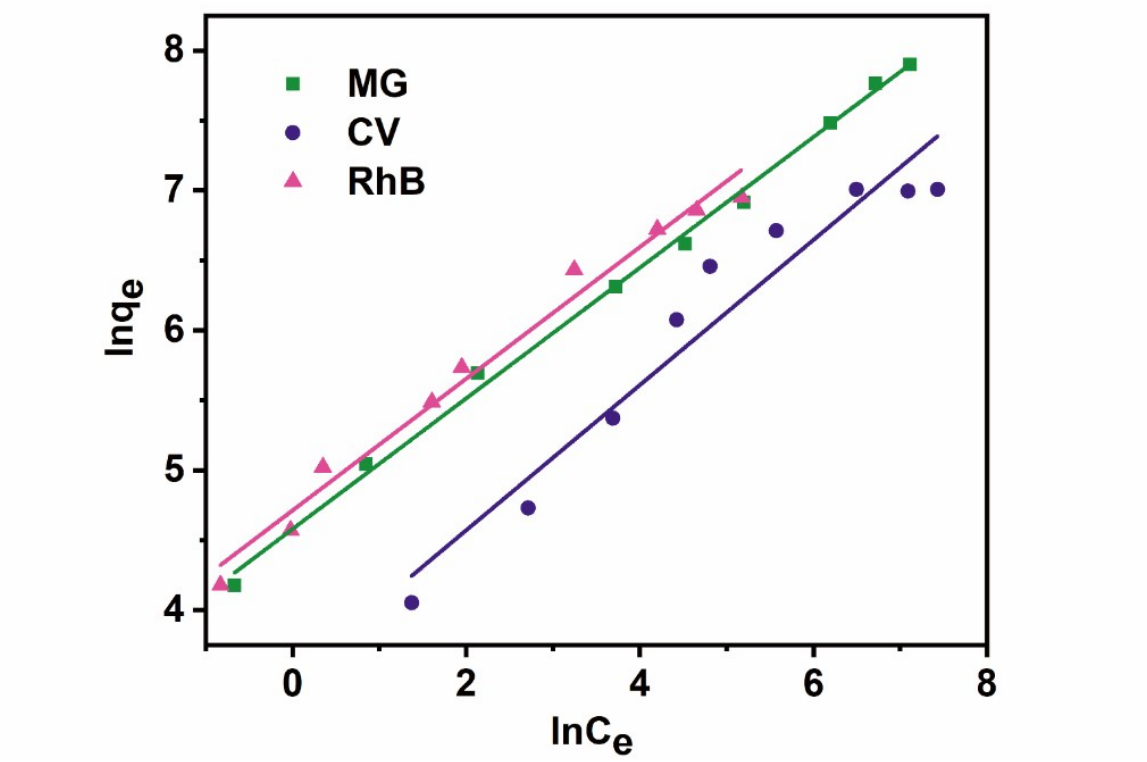


Figure S44. Freundlich adsorption isotherm plot for MG, CV and RhB uptake by SCF-FCOF-1.

Table S11. Adsorption isotherm parameters for MG, CV and RhB uptake by SCF-FCOF-1

Dyes	$q_{max,exp}$ (mg g^{-1})	Langmuir Model			Freundlich Model		
		K_L (L mg^{-1})	q_{max} (mg g^{-1})	R^2	K_F ($mg^{(1-1/n)}$ g^{-1} $L^{1/n}$)	n	R^2
MG	2701	0.006344	2841	0.9271	97.32	2.14	0.9962
CV	1106	0.008047	1203	0.9955	34.17	1.93	0.9257
RhB	1044	0.07018	1099	0.9913	111.2	2.12	0.9799

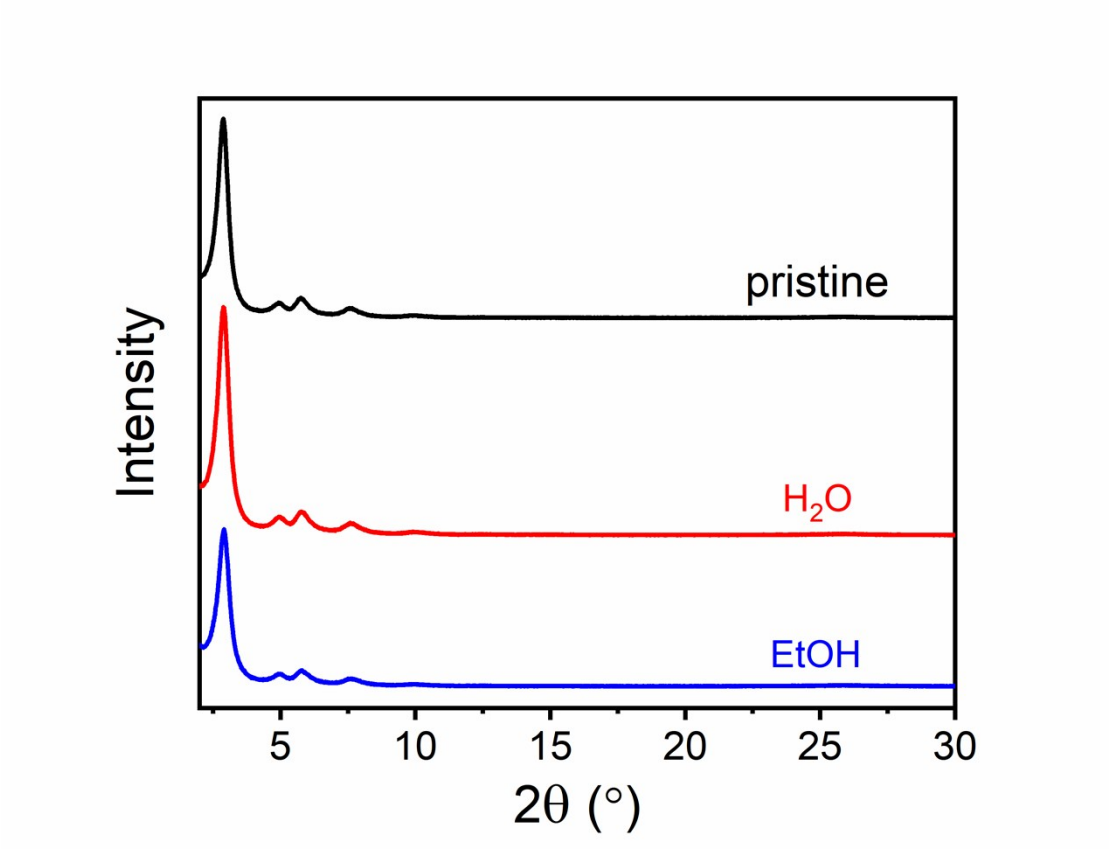


Figure S45. PXRD patterns after 12 h treatment of SCF-FCOF-1 in water and ethanol.

Table S12. The comparation of adsorption capacity between SCF-FCOF-1 with many other porous materials

Materials	$q_{MG,max}$	Materials	$q_{CV,max}$	Materials	$q_{RhB,max}$
SCF-FCOF-1 (This work)	2701	SCF-FCOF-1 (This work)	1106	SCF-FCOF-1 (This work)	1044
SCF-FCOF-2 (This work)	421.4	SCF-FCOF-2 (This work)	117.8	SCF-FCOF-2 (This work)	541.0
SCF-HCOF-1 (This work)	168.1	SCF-HCOF-1 (This work)	74.9	SCF-HCOF-1 (This work)	56.3
LS-SCF-FCOP (This work)	80.5	LS-SCF-FCOP (This work)	40.8	LS-SCF-FCOP (This work)	155.1

β–MCM-41 silica/RH composite[1]	285.0	DLP[2]	26.69	CMP[3]	535
PIL/POM[4]	1109	Sodium Alginate/ZnO/GO[5]	13.85	TS-COF-1[6]	625
BMCN1[7]	309.6	Carbon nanotubes[8]	580	β-CD COF[9]	3.8
rGO[10]	476.2	G-Fe[11]	909	TPT-TAPB-COF[12]	970
$CuFe_2O_4$/DC[13]	769.2	zeolite[14]	149.4	TPT-Azine-COF[12]	725
Si-POP-2[15]	662.0	CNF[16]	48	CTF[17]	229.9
MOG-PUF[18]	125.9	GHNFs[19]	134.6	Gg-cl(PAA-co-AAm)/Fe_3O_4 nanocomposites[20]	654.9
α-Bi_2O_3[21]	312.0	Organoclay[22]	148.9	Organoclay[22]	155.4
Activated Carbon[23]	245.3	Activated Carbon[24]	393.2	Actived Carbon[25]	423
PCNS[26]	1455	CuO/MCM-41[27]	52.90	rGO-AgarBs[28]	312.6
Graphene hydrogels[29]	740.7	CNR@TARH[30]	93.45	BOPs[31]	1388
3D ZnO[32]	2587	HPP-3[33]	700.0	HPP-3[33]	1544
Cu-MOFs/Fe_3O_4[34]	113.7	MOF[35]	713.5	H-UiO-66-17.3 nm MOF[36]	724.6
MIL-100(Fe)[37]	485	PCN-222(Fe)[38]	812	HKUST− Fe3O4[39]	57.2
MIL-53(Al)–NH_2[40]	164.9	Mn-MOF[41]	938	SCNU-Z1-Cl[42]	130

MIL101(Fe)@PDopa@Fe_3O_4[43]	833.3	Zn-MOF[44]	54.50	$MgFe_2O_4$@MOF[45]	219.1
MIL-101-SO_3H[46]	676	Sr-BTTC[47]	184	$P_2W_{18}O_{62}$@Fe_3O_4/MIL-101 (Cr)[48]	164

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