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Electronic Supplementary Information

Molecular simulation-based Deep Neural Network model for deciphering the adsorption of 5-Fluorouracil in COFs

Khushboo Yadava*[a], Ashutosh Yadav*[b]

[a]Department of Nano Science and Materials, School of Basic and Applied Science, Central University of Jammu, Rahya Jammu & Kashmir, India 181443.

[b]Department of Chemical Engineering, IIT Jammu, Jammu & Kashmir, India 181221.

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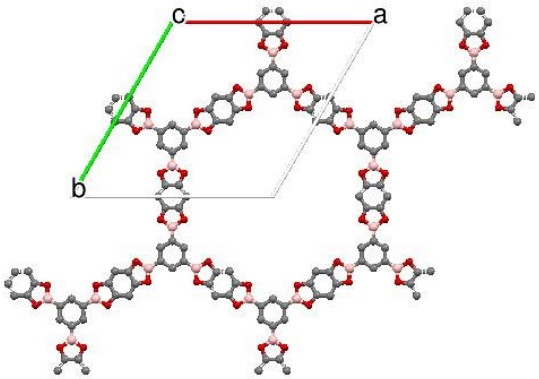
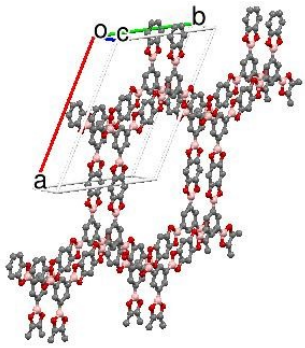
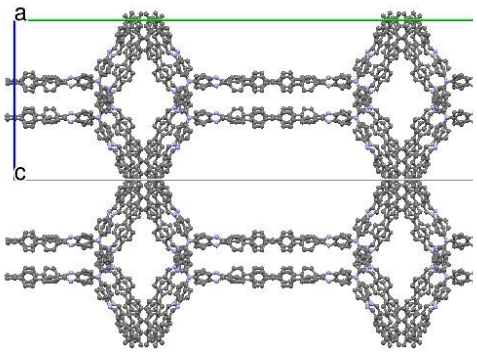
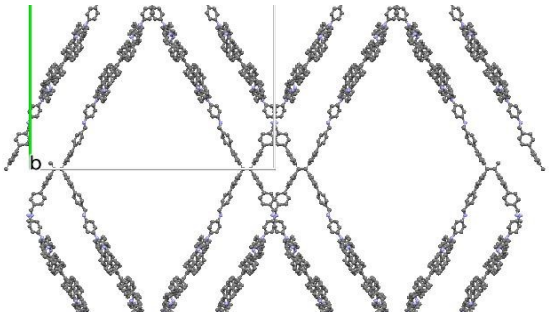
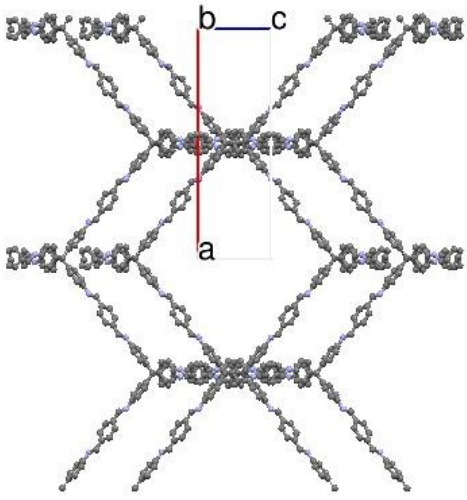
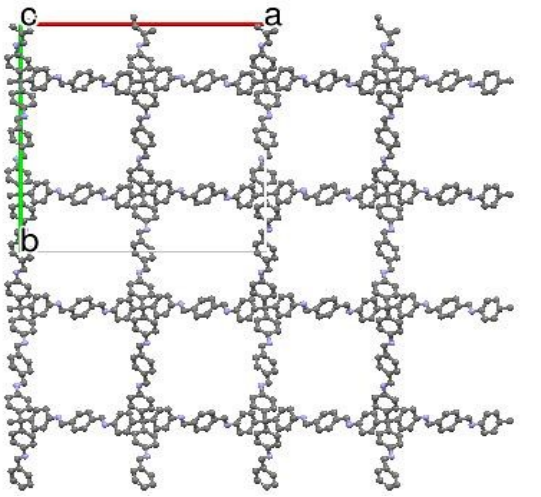
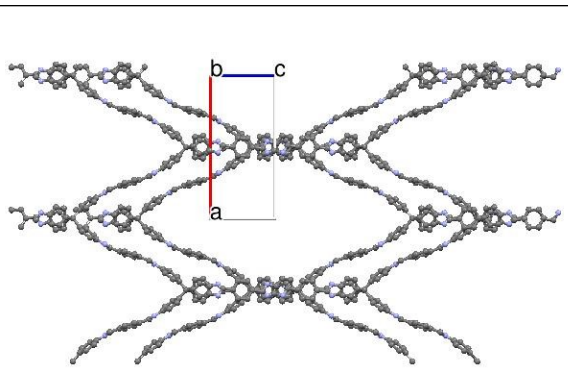
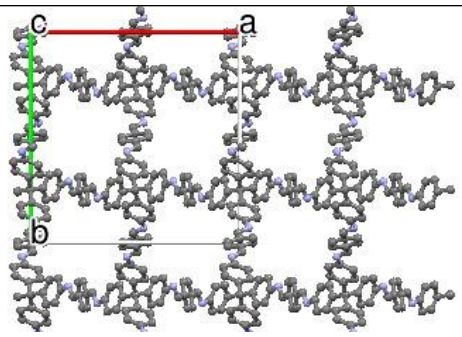
1.		
	COF-102 along c axis	**COF-102 perspective view**
		
	COF-103 along a axis	**COF-103 along b axis**
		
	COF-105 along b axis	**COF-105_along c axis**

		
	COF-108_along b axis	**COF-108_along c axis**

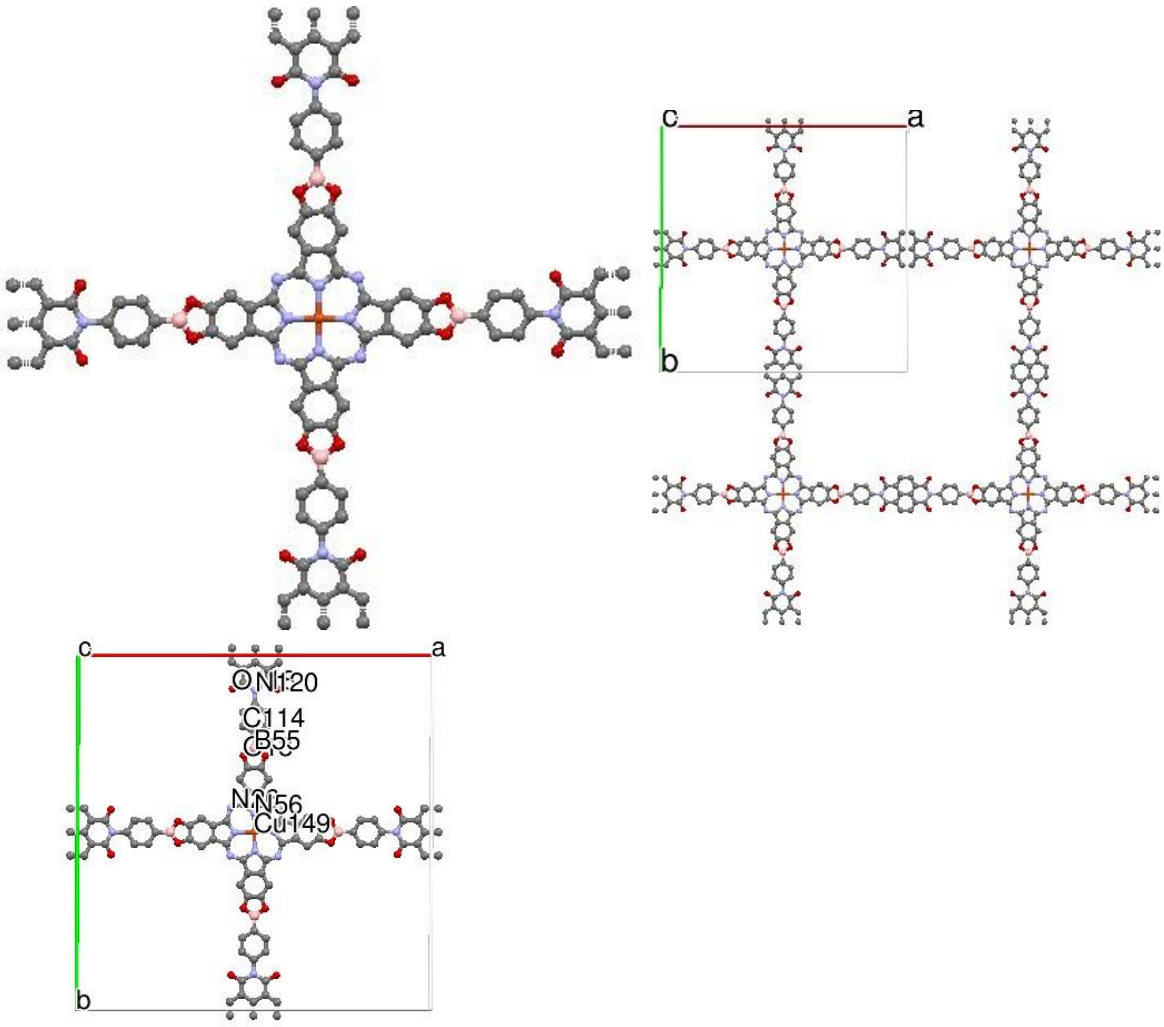


Figure S2. Crystallographic structures of COFs studied in Table 5 of main manuscript: COF-206

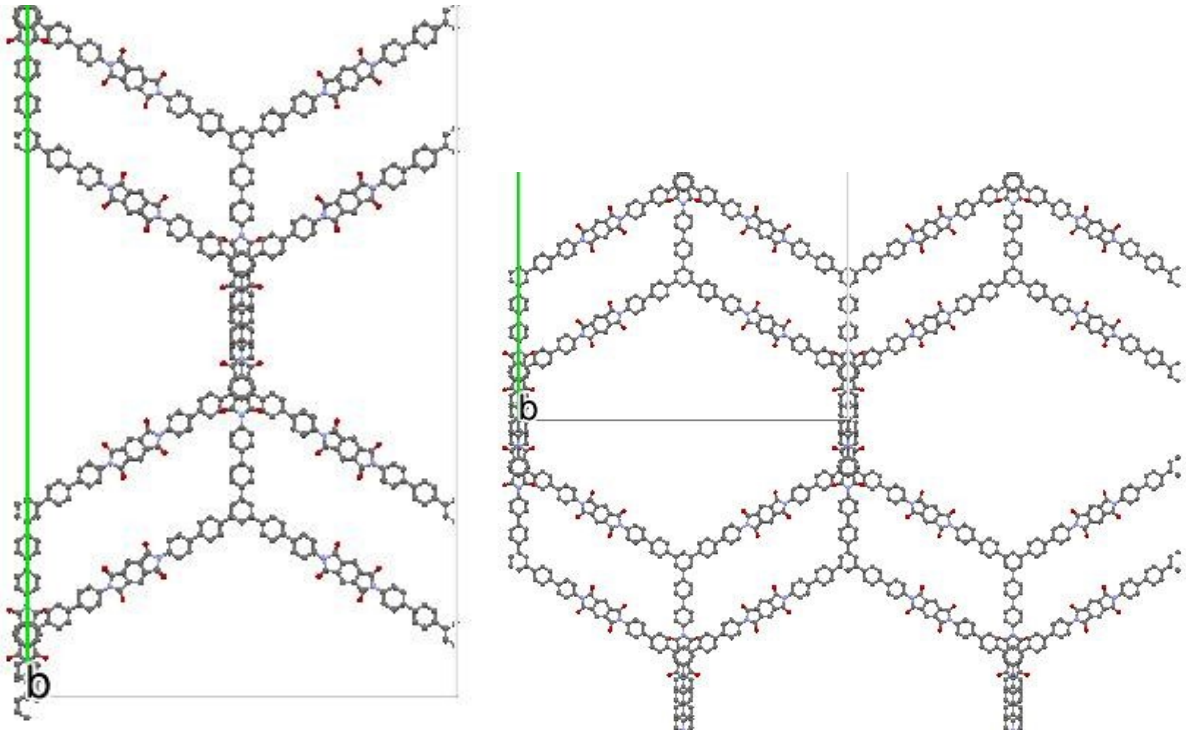


Figure S3. Crystallographic structures of COFs studied in Table 4 of main manuscript COF- 362

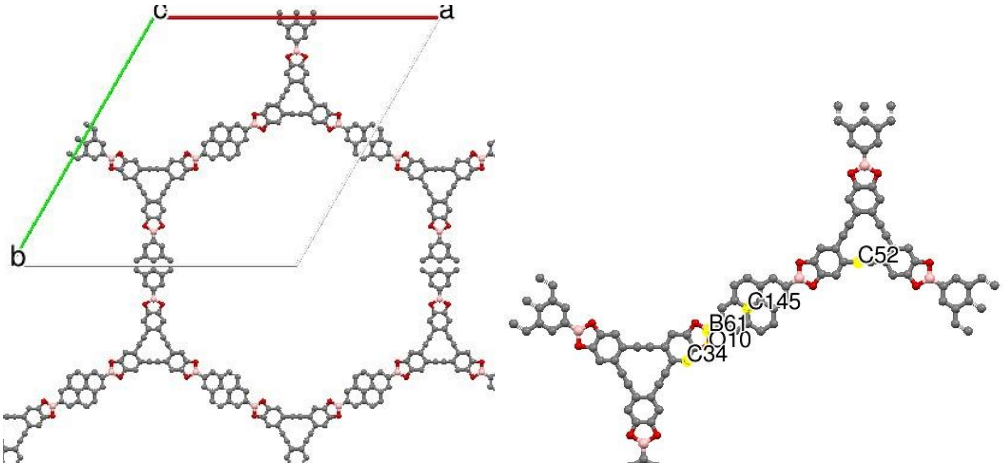


Figure S4. Crystallographic structures of COFs studied in Table 4 of main manuscript. COF-398

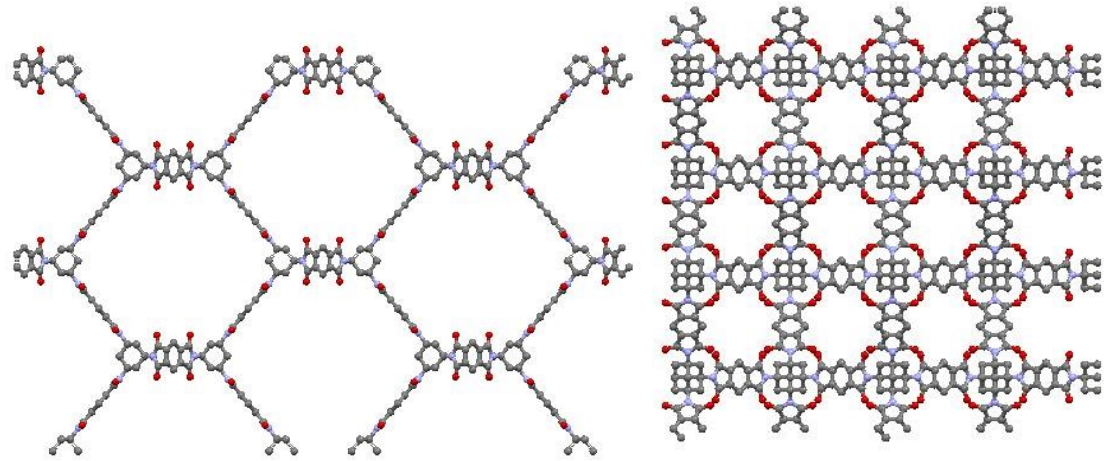
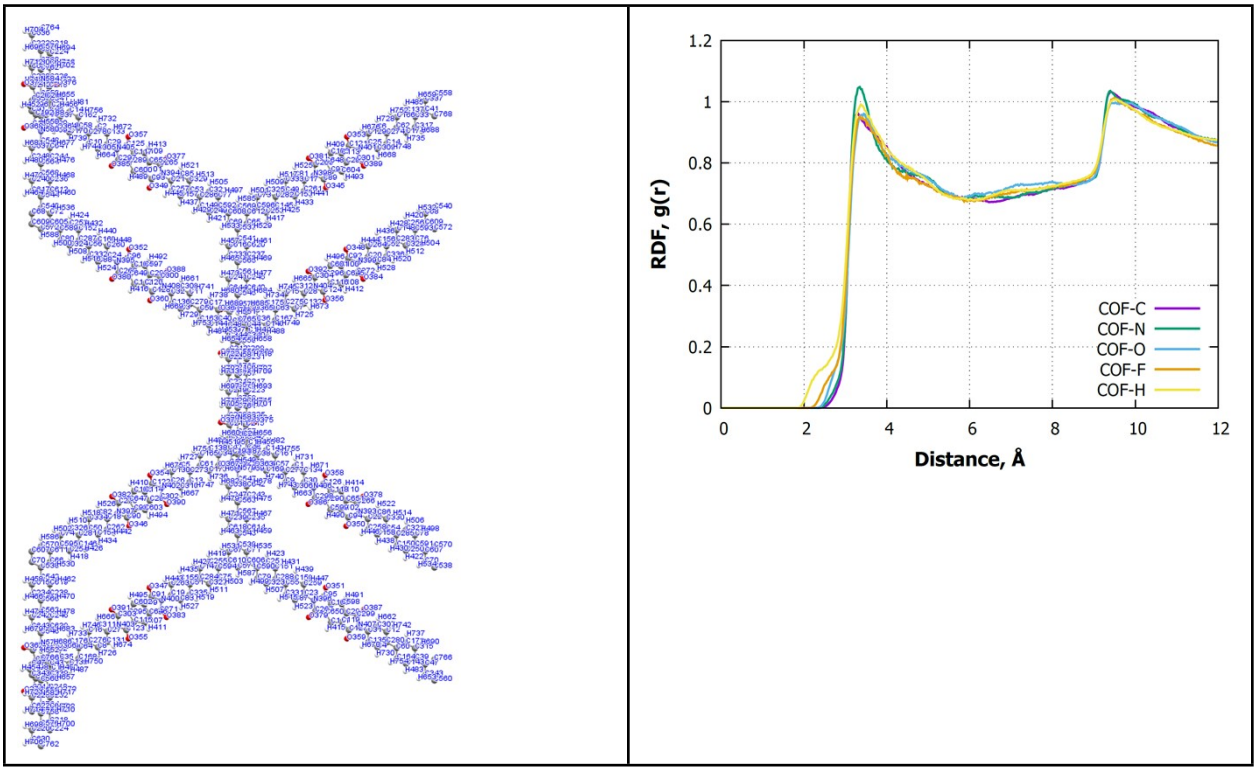
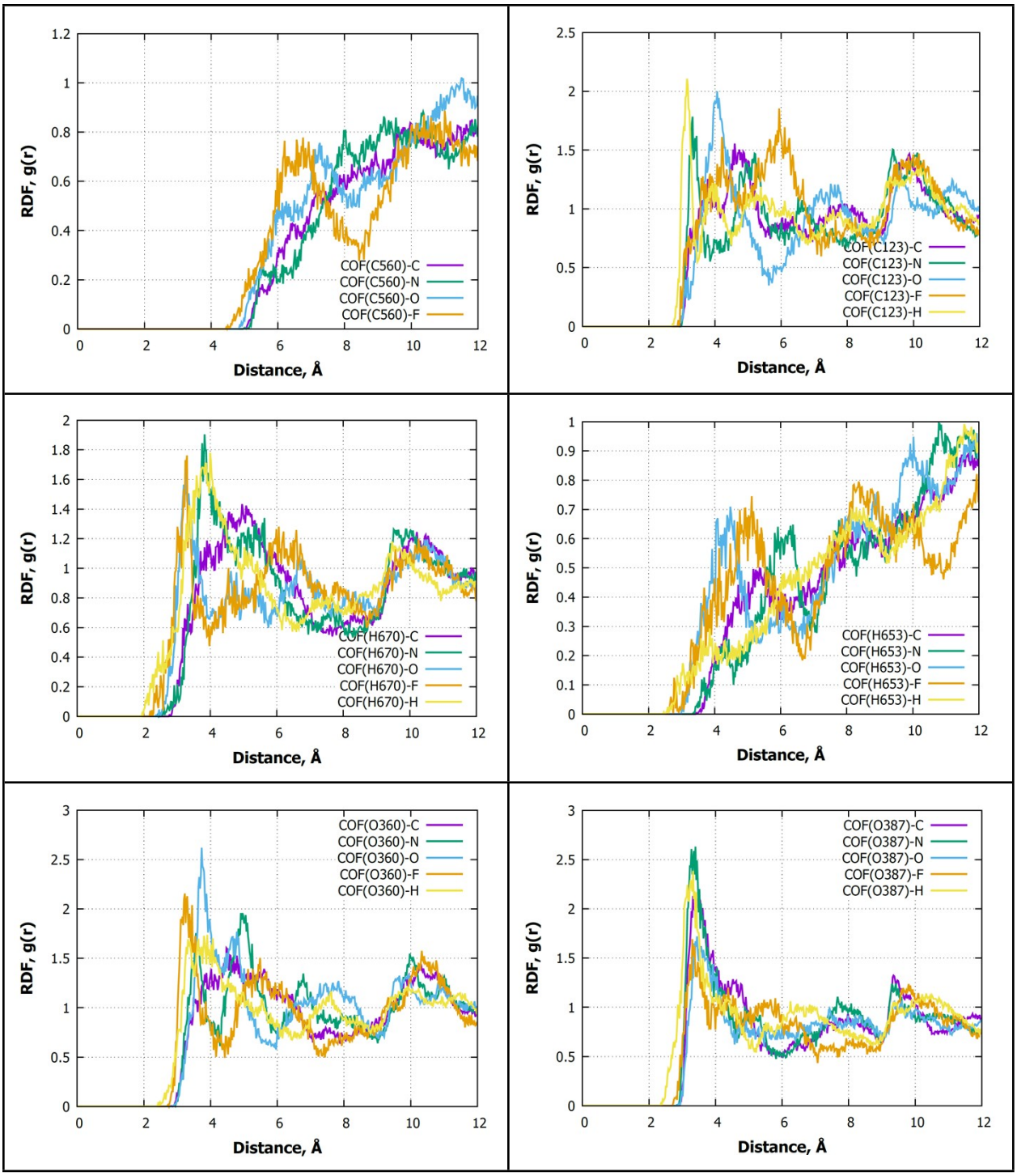
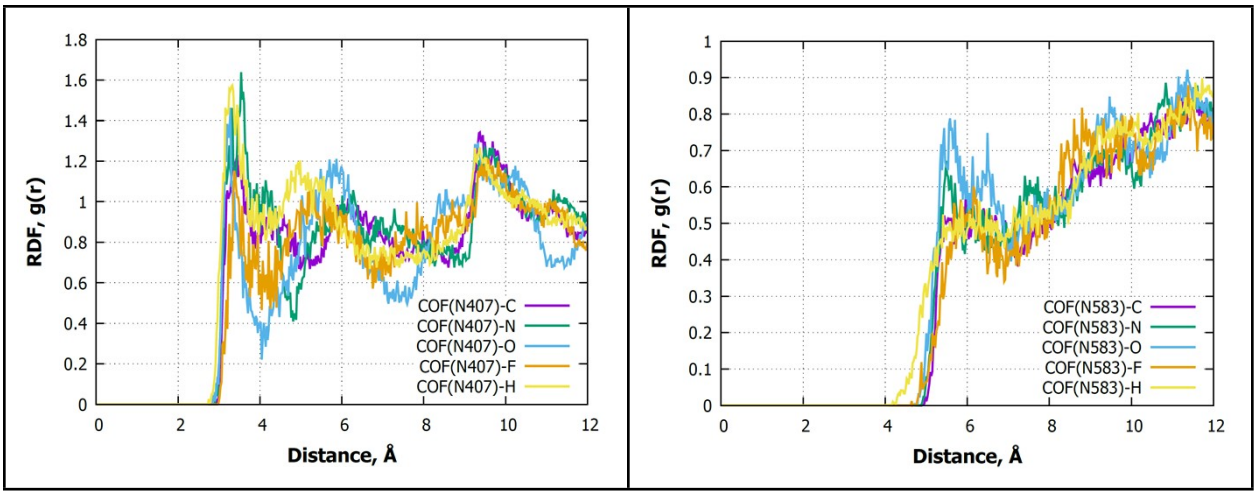


Figure S5. Crystallographic structures of COFs studied in Table 4 of main manuscript. COF-363




RDF, g(r)
Distance, Å
COF(C560)-C
COF(C560)-N
COF(C560)-O
COF(C560)-F
COF(C123)-C
COF(C123)-N
COF(C123)-O
COF(C123)-F
COF(C123)-H
COF(H670)-C
COF(H670)-N
COF(H670)-O
COF(H670)-F
COF(H670)-H
COF(H653)-C
COF(H653)-N
COF(H653)-O
COF(H653)-F
COF(H653)-H
COF(O360)-C
COF(O360)-N
COF(O360)-O
COF(O360)-F
COF(O360)-H
COF(O387)-C
COF(O387)-N
COF(O387)-O
COF(O387)-F
COF(O387)-H



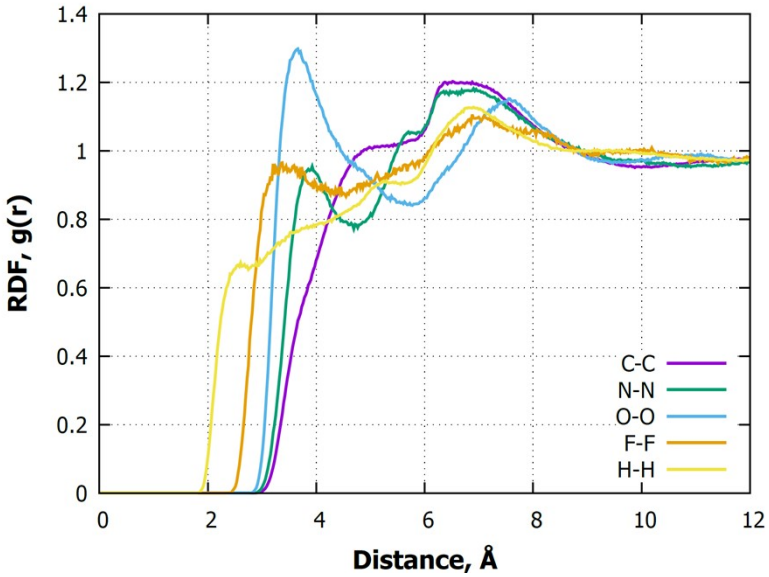
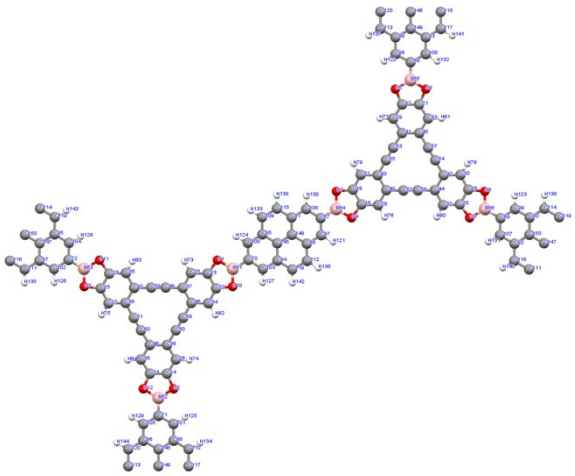
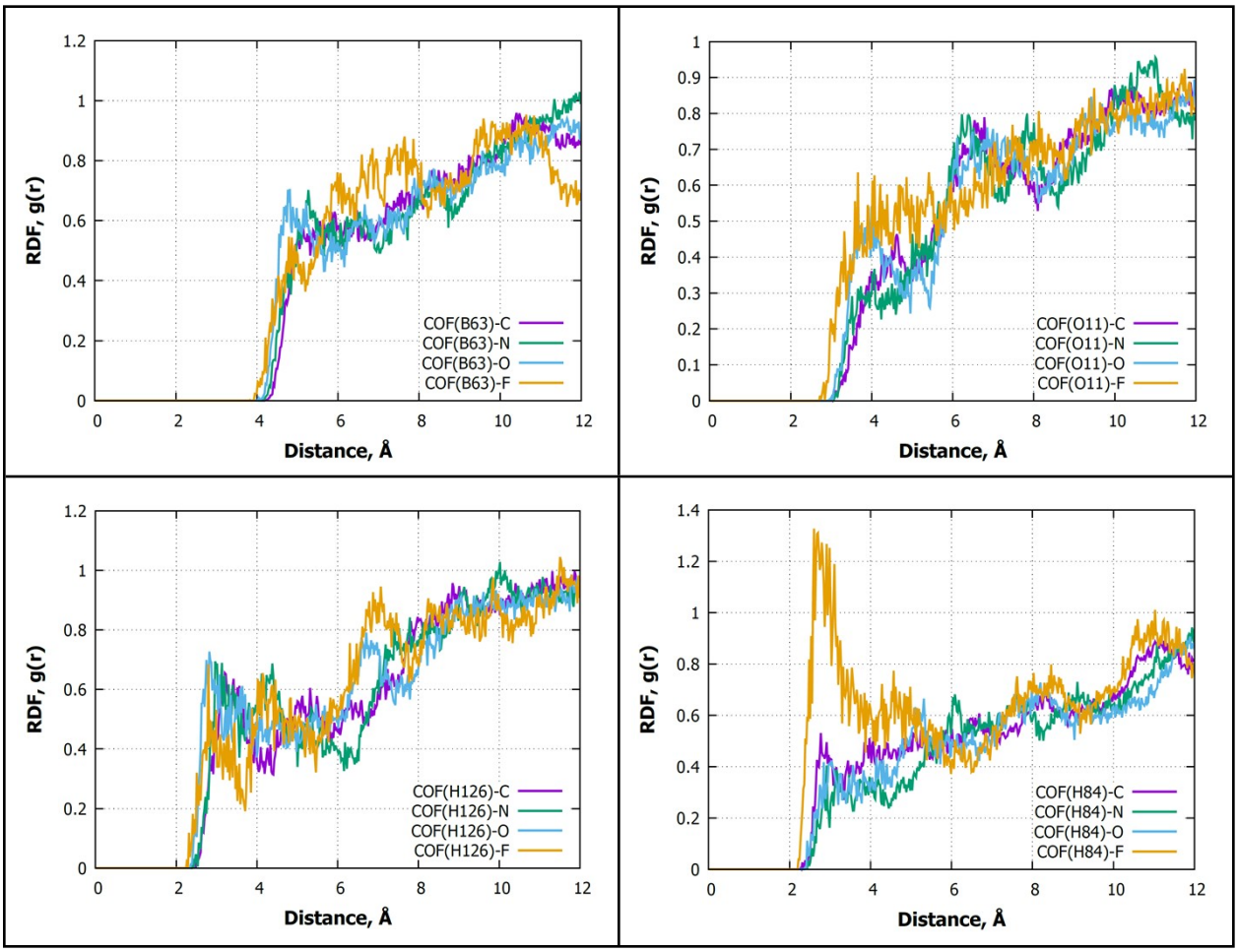


Figure S6. Radial Distribution Function (RDF) Analysis of selected atoms in COF-362 i.e. PI-COF-3




RDF, g(r)
Distance, Å
COF(B63)-C
COF(B63)-N
COF(B63)-O
COF(B63)-F
COF(O11)-C
COF(O11)-N
COF(O11)-O
COF(O11)-F
COF(H126)-C
COF(H126)-N
COF(H126)-O
COF(H126)-F
COF(H84)-C
COF(H84)-N
COF(H84)-O
COF(H84)-F

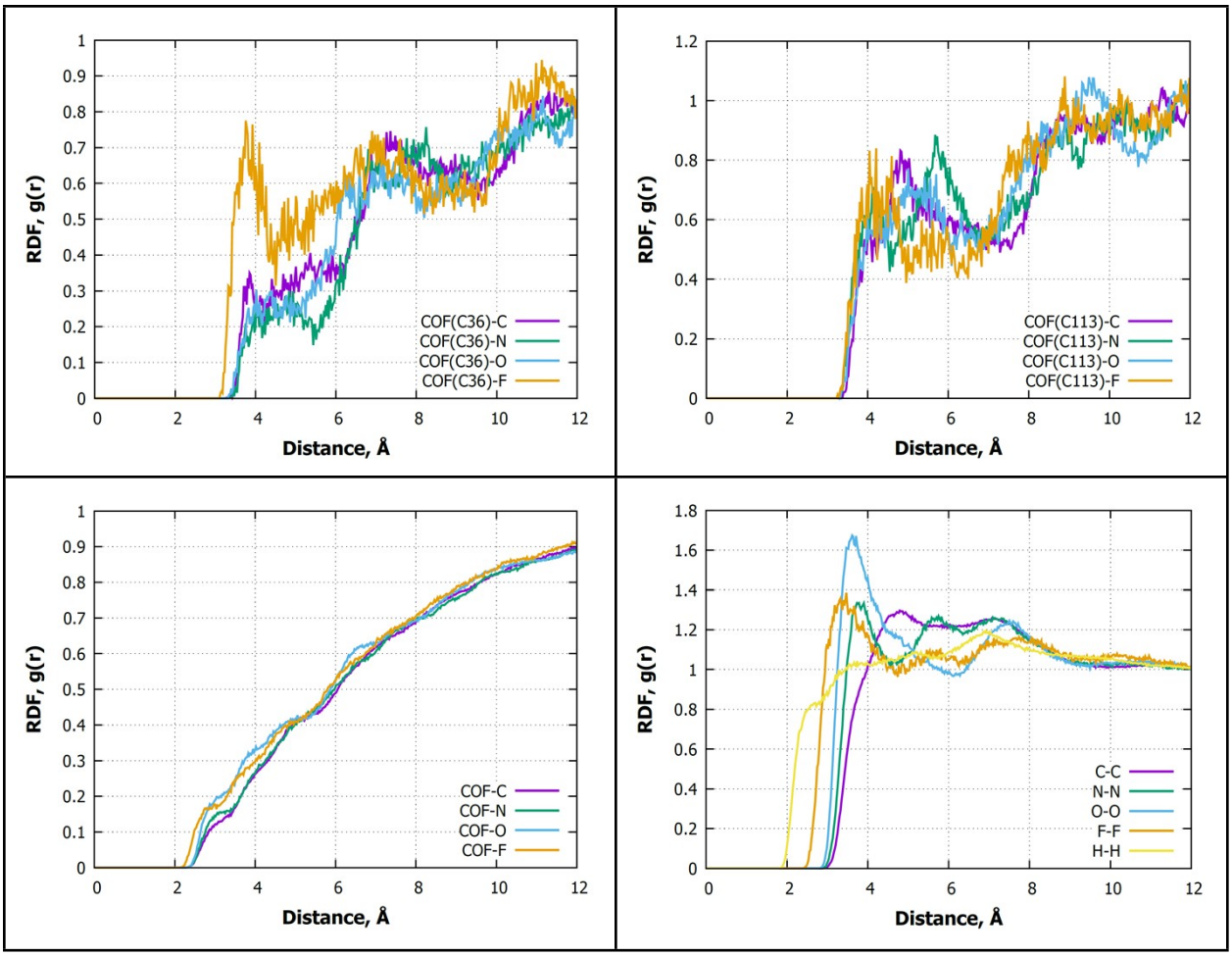
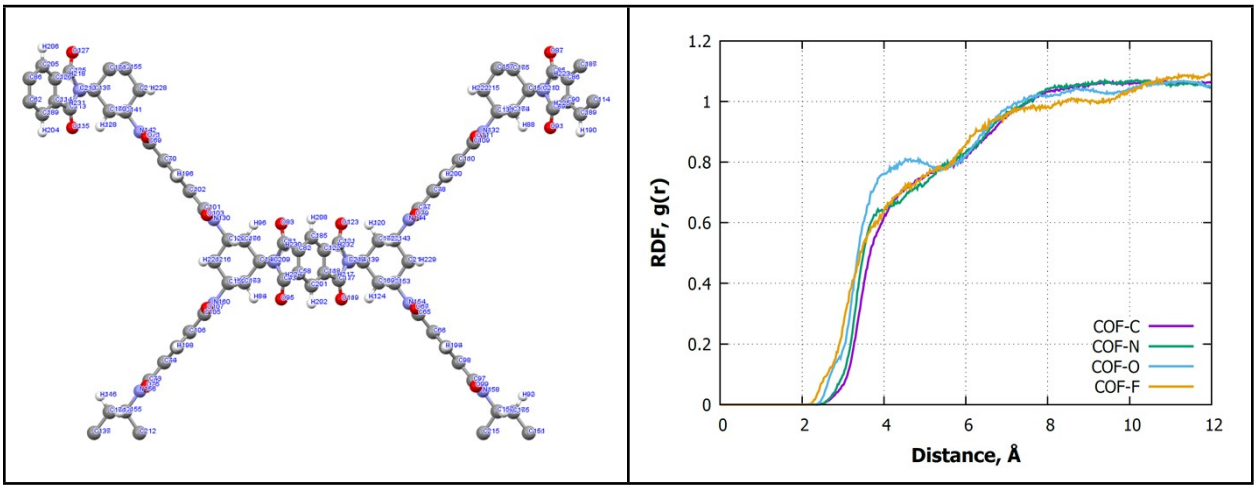
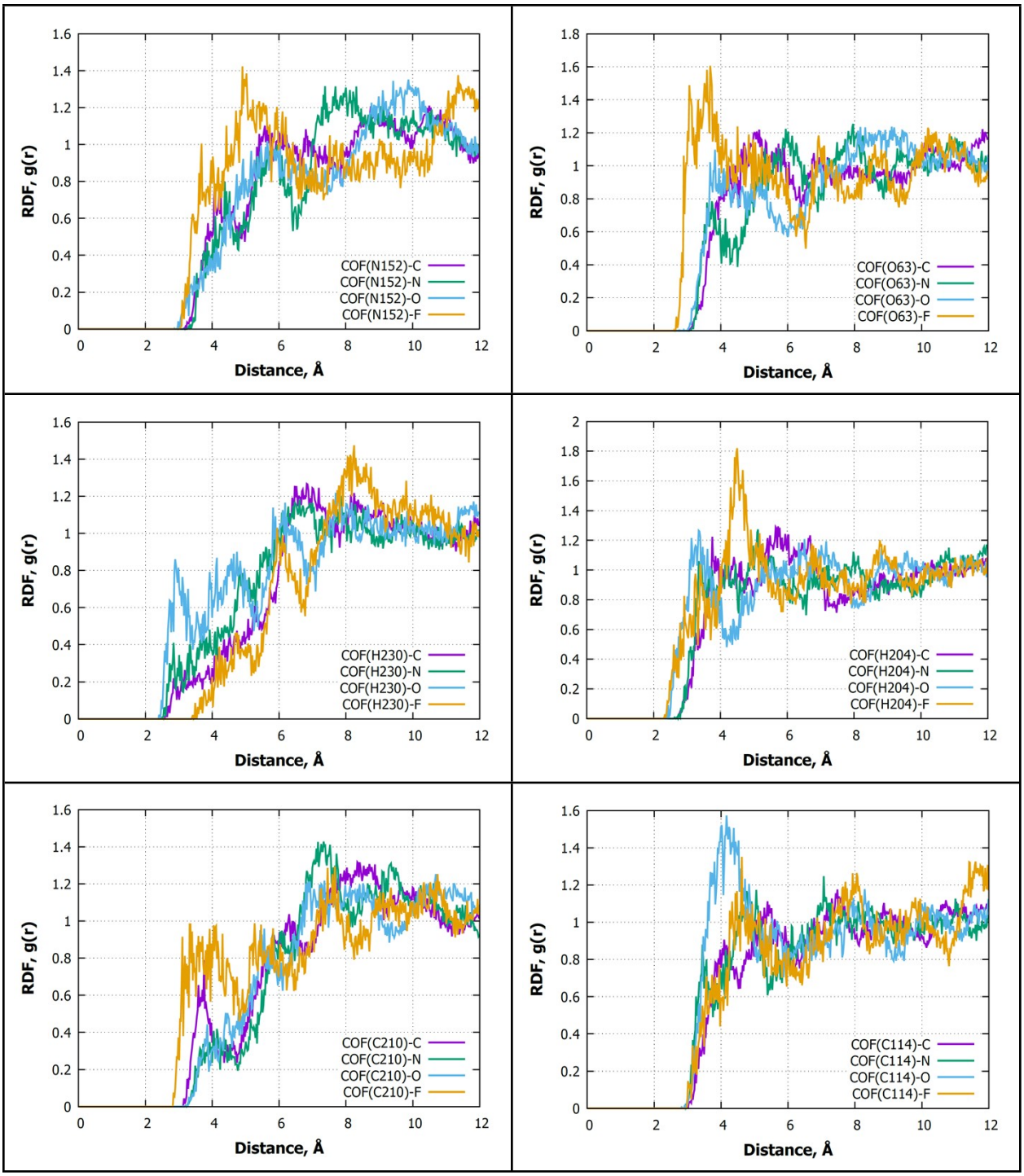


Figure S7. RDF analysis of selected atoms in COF-398




RDF, g(r)
Distance, Å
COF(N152)-C
COF(N152)-N
COF(N152)-O
COF(N152)-F
COF(O63)-C
COF(O63)-N
COF(O63)-O
COF(O63)-F
COF(H230)-C
COF(H230)-N
COF(H230)-O
COF(H230)-F
COF(H204)-C
COF(H204)-N
COF(H204)-O
COF(H204)-F
COF(C210)-C
COF(C210)-N
COF(C210)-O
COF(C210)-F
COF(C114)-C
COF(C114)-N
COF(C114)-O
COF(C114)-F

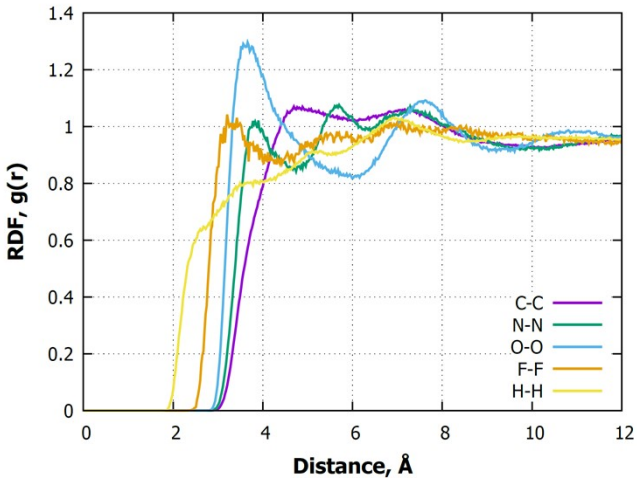


Figure S8. RDF analysis of selected atoms in COF-363

Table S1. Major RDF interactions (Angstroms) in four COFs belonging to Table 5 of main paper

COF code	**COF-363**	**COF-362**	**COF-206**	**COF-398**
host-adsorbate	COF_C 2.316 COF_O 2.316 COF_F 2.100 COF_N 2.34 COF_H 1.812	COF_C 2.292 COF_N 6 2.316 COF_F 2.100 COF_O 2.172 COF_H 1.740	COF_C 2.268 COF_F 2.100 COF_N 2.172 COF_H 1.812 COF_O 2.268	COF_C 2.196 COF_N 2.268 COF_O 2.244 COF_H 1.812 COF_F 2.100
adsorbate-adsorbate	F_F 2.364 O_O 2.748 N_N 2.844 C_C 2.772 H_H 1.764	F_F 2.388 O_O 2.676 C_C 2.748 H_H 1.764 N_N 2.772	F_F 2.388 O_O 2.748 N_N 2.796 H_H 1.764 C_C 2.700	C_C 2.796 N_N 2.820 F_F 2.412 O_O 2.748 H_H 1.788