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Supplemental Information

Orderly Porous Covalent Organic Frameworks-based Materials: Superior Adsorbents for Pollutants Removal from Aqueous Solutions

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Supplementary Information for

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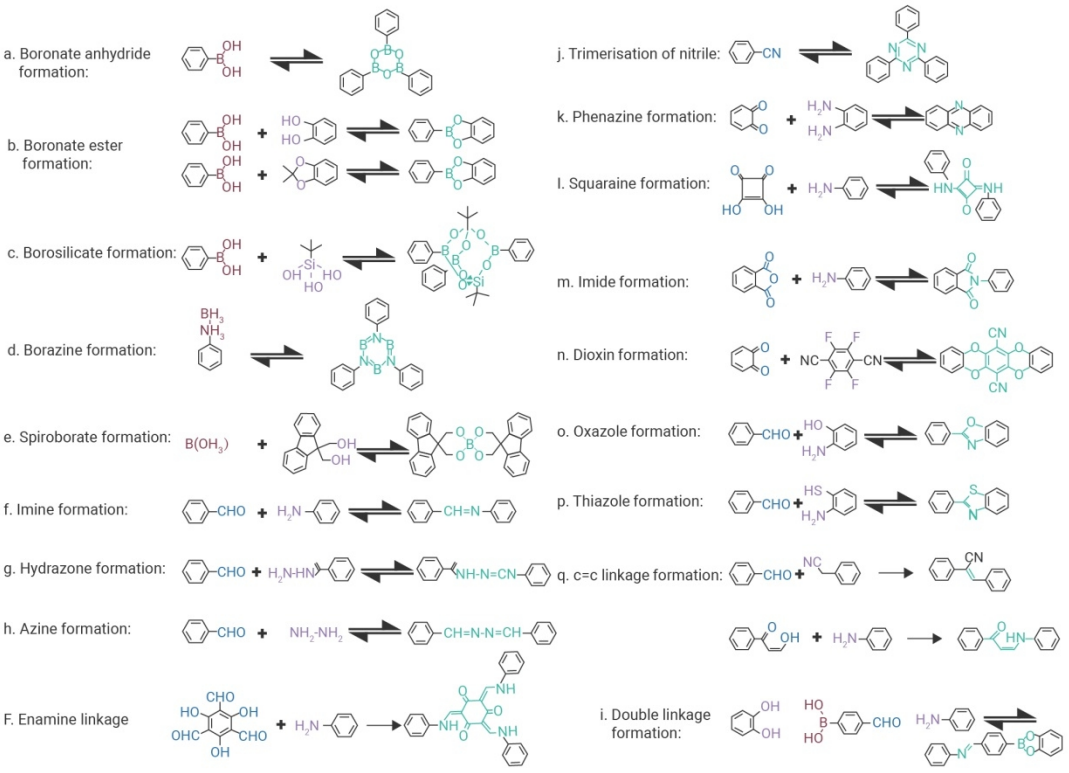

Fig. S1. Various linkages of COF formation[1].

Table S1 The typical kinetic and thermodynamic models commonly used to describe the adsorption process by COF-based materials.

	Equation	Parameters	Ref
Isotherm models			
Langmuir model	$C_e/q_e=1/(K_Lq_m)+C_e/q_m$ $R_L=1/(1+K_LC_0)$	C_e(mg·L^{-1}) equilibrium concentration; q_e(mg·g^{-1}) adsorption capacity at equilibrium time; K_L(L·mg^{-1}) the Langmuir constant; q_m(mg·g^{-1}) the maximum adsorption capacity; R_L the dimensionless parameter; C_0(mg·L^{-1}) highest concentration of the adsorbates;	2, 3
Freundlich model	$lnq_e = lnK_F + lnC_e/n$	K_F (mg·L^{-1}) the Freundlich constant; n-a constant describing the adsorption density;	2
Dubinin-Radushkevich	$lnq_e=lnq_m-K\varepsilon^2$ $E_D=1/(2K)^{½}$	K(mol^2/J^2) a constant; ε-the Polanyi potential; E_D (KJ·mol^{-1})	4
Temkin	$q_e=(R*T/b_T)lnK_T +$ $(R*T/b_T)lnC_e$	K_T(L·g^{-1}) Temkin constant; R(J/mol·K) constant 8.314; b_T(KJ·mol^{-1}) Temkin constant related to the heat of adsorption	5
Sips model	$q_e=q_m(KC_e)^n/[1+(kC_e)^n]$	k((mg·L^{-1})$^{-n}$) the constant of the sips models; n-the index of heterogeneity	6
Kinetic models			
Pseudo first-order model	$ln[(q_e-q_t)/q_e]=-K_1q_et$	q_t(mg·g^{-1}) the adsorption capacity at the time t; K_1(min^{-1}) pseudo-first-order rate constant of the adsorption;	5
Pseudo second-order model	$t/q_t=t/q_m+1/(K_2q_e^2)$	K_2 (g·mg^{-1}·min^{-1}) pseudo-second-order rate constant of the adsorption	5

Intraparticle diffusion model	$q_t=K_i t^{1/2}+C$	K_i(mg·g^{-1}·min$^{-1/2}$) the intraparticle diffusion rate constant; C the intercept related to the boundary thickness	4
Elovich model	$q_t=\ln(\alpha\beta)/\beta+\ln(t)/\beta$	α-the initial adsorption rate; β-the desorption constant	4
Thermodynamic model	$K_0 = q_e/C_e$ $\Delta G = -RT \ln K_0$ $\ln K_0 = \Delta S/R-\Delta H/(RT)$	entropy change (ΔS, J·mol^{-1} K^{-1}); free energy change (ΔG, kJ·mol^{-1}); enthalpy change (ΔH, kJ·mol^{-1}); the thermodynamic equilibrium constant (K^0); the universal gas constant (R 8.314 J·mol^{-1} K^{-1})	7

Table S2 Abbreviations.

(CP/MAS) NMRs	The solid-state 13C cross-polarization magic-angle-spinning (CP/MAS) NMR spectroscopy
$[NH_4^+]$ $[COF\text{-}SO_3^-]$	SO_3^--anchored COF
$[P(O_2Ph)_3]^-$	Hexa-coordinated phosphorus moieties
2D	Two-dimensional
3D	Three-dimensional
3D ionic COFs	Tetrakis (4-formylphenyl) methane + diimidium bromide
ACOF	Azine-linked COF
ACs	Activated carbons
Ag NPs@COF	Ag nanoparticles@COF
Ag NPs@COF-LZU1	COF-supported Ag NPs material
BD	benzidine
BD-(CF3)2	3,3'-bis(trifluoromethyl)benzidine
BFBP2 +·$2Cl^-$	1,1-bis(4-formylphenyl)-4,4'-bipyridinium dichloride
BG	brilliant green
BIPY	bipyridine
BPA	Bisphenol A
CMPs	Conjugated microporous polymers
CNFs	Carbon nanofibers
CNTs	Carbon nanotubes
COF1	1,3,5-triaminobenzene (TAB) + 2,3-dihydroxyterephthalaldehyde (2,3-Dha)
COF-102	tetra-boronic acid + allyl-functionalized truncating
COF-103	tetra(4-(dihydroxy)borylphenyl) silane
COF2	1,3,5-triaminobenzene (TAB) + 2,5-dihydroxyterephthalaldehyde (2,5-Dha)
COF-366-Co	5,10,15,20-tetrakis(4-aminophenyl) porphinato] cobalt [Co(TAP)] + 1,4-benzenedi carboxaldehyde
COF-BTA-DHBZ	3,3′-dihydroxybenzidine (DHBZ) + [1,1′-biphenyl]-3,3′,5,5′-tetracarbaldehyde (BTA)
COF-COOH	carboxyl-containing COF
COF-ETTA-2,3-Dha	4,4′,4″,4‴-(ethene-1,1,2,2-tetrayl)tetraaniline (ETTA) + 2,3-dihydroxybenzene-1,4-dicarbaldehyde (2,3-Dha))
COF-LZU8	Thioether-functionalized hydrazone-linked COF
COF-LZU8	Thioether-functionalized hydrazone-linked COF
COFs	Covalent organic frameworks
COF-SH	Sulfhydryl functionalized COF
COF-S-SH	Sulfur-based chelating-group-laced COF
COF-S-SH	Thiol-functionalized COF
COF-TE	Amide-rich layered COF (1,3,5-trimesoyl chloride + p-Phenylenediamine)

COF-TP	Amide-rich layered COF (1,3,5-trimesoyl chloride + p-Phenylenediamine)
COF-TpPa-1	COF-2,4,6-Triformylphloroglucinol pPhenylenediamine
COF-TpPa-1-nc	1, 3, 5-triformylphloroglucinol+ p-phenylenediamine
COF-V (synthesized by Li et al.)	V inyl-incorporated COF (2,5-Divinylterephthalaldehyde (DVA) + 1,3,5-tris(4"-aminobiphenyl)benzene (TABPB))
COF-V (synthesized by Sun et al.)	Vinyl-functionalized COF (2,5-divinylterephthalaldehyde (Dva) + 1,3,5-tris(4-aminophenyl)-benzene (Tab))
COM	COF membrane
COOH@COF	Carboxyl functionalized COF
CR	Congo red
CTX	cefotaxime
CuP-DMNDA-COF	Imine-linked functionalized COFs
CuTAPP	5,10,15,20-tetra(p-aminophenyl) porphyrinatocopper(II)
CV	crystal violet
DBA	4,4’-diamino-[1,1’-biphenyl]-3,3’-dicarboxylic acid
DBd	4,4’-diamino-[1,1’-biphenyl]-2,2’-dicarboxylic acid
DCC	Dynamic covalent chemistry
DFS-4BS	direct fast scarlet 4BS
DFT	Density functional theory
DHBD	3,3′-dihydroxybenzidine
DMBD	2,2′-dimethyl-[1,1′-biphenyl]-4,4′-diamine-COF
DMNDA	2,6-dimethoxynaphthalene-1,5-dicarbaldehyde
DMTA	2,5-dimethoxyterephthalaldehyde
DMTP	dimethoxyterephthaldehyde
DT	4,4″-diamino-pterphenyl
EB-COF:Br	1,3,5-trifomylphloroglucinol (TFP) + ethidium bromide (EB)
EDC	endocrine-disrupting chemicals
EIS	electrochemical impedancespectroscopy
EPA	Environmental Protection Agency
EXAFS	Extended X-ray absorption fine structure spectroscopy
Fe0/TAPB-PDA COFs composites	1,3,5-tris(4-aminophenyl)benzene (TAPB) + terephthalaldehyde (PDA) + zero-valent iron (Fe0) nanoparticles
Fe_3O_4@TpPa-1	1,4-diaminobenzene (Pa-1) + 1, 3, 5-triformylphloroglucinol (Tp) + amino-functionalized magnetic Fe3O4 (Fe3O4-NH2)
FT-IR	Fourier transform infrared spectroscopy
g-C_3N_4	Graphitic carbon nitride
GenX	ammonium perfluoro-2-propoxypropionate
GO	Graphene oxides
IARC	International Agency for Research on Cancer
IAST	A method established for evaluation of metal ion uptakes by variety of adsorbents

Kd	Constant of distribution, L/g
Ksp	The solubility product constant, Ksp, is the equilibrium constant for a solid substance dissolving in an aqueous solution. It represents the level at which a solute dissolves in solution. The more soluble a substance is, the higher the Ksp value it has
LDHs	Layered double hydroxides
LMS	Layered metal sulfides
M18	monolith with 16% COF powder
M28	monolith with 28% COF powder
MB	Methylene blue
M-COF	Melamine-based COF
M-COF-SH	Thiol-functionalized COF composite
MO	Methyl orange
MOFs	Metal organic frameworks
MSPE	magnetic solid-phase extraction
MW	molecular weight
NACs	nitroaromatic compounds
NCCT	$NiFe_2O_4$/COF/CS/TPA nanocomposites film
ND	1,5-naphalenediamine
NZVI	Nanoscale zero-valent iron
OA	okadaic acid
OMC	Ordered mesoporous carbon
Pa-2	p-phenylenediamine (2,5-dimethyl-pphenylenediamine)
PAHs	Polycyclic aromatic hydrocarbon
PA-POFs	COFs with tetra-coordinated phosphate functional groups
PDA	p-phenylenediamine
PFAS	Per-/polyfluorinated alkyl substances
PFOA	perfluorooctanoic acid
pHzpc	The pH at zero-point charge
POFct-1	3D porous organic framework (crystal-type)
POFct-2	3D porous organic framework (amorphous)
POPs	Persistent organic pollutants
PPCPs	pharmaceutical and personal care products
PTSA	ptoluene sulfonic acid
P-WCA-POFs	COFs with hexa-coordinated phosphorus moieties
PXRD	powder X-ray diffraction pattern
QG-scaffolded COFs	Q-graphene (QG) + melanine (MA) + paraformaldehyde (PA) + phenol (Phen)
RhB	Rhodamine B
SA	succinic anhydride
SAXS	Small-angle X-ray scattering
SMT	Sulfamerazine
SNW-1	Schiff-based networks

TAPB	1,3,5-tris(4-aminophenyl) benzene
TAPB-BMTTPA-COF	1,3,5-tris(4-aminophenyl)benzene (TAPB) + 2,5-bis(methylthio)terephthalaldehyde (BMTTPA)
TC	Tetracycline
TCC	Triclocarban
TCOF/ T-COF	Triazine-based COF
TCS	Triclosan
TFBODH	Oxalyldihydrazide (ODH) + 1,3,5-triformylbenzene (TFB)
TFP	1,3,5-Triformylphloroglucinol
TFPM	tetra(4-formylphenyl)methane
TFPOT	1,3,5-triazine and 2,4,6-tris(4-formylphenoxy)-1,3,5-triazine
TFPPy-CHYD	1,3,6,8-tetrakis(4-formylphenyl)pyrene (TFPPy) + carbohydrazide (CHYD)
TFPT–COF	1,3,5-tris-(4-formyl-phenyl)triazine(TFPT)+ 2,5-diethoxy-terephthalohydrazide
TGA	Thermogravimetric analysis
Tp	2,4,6-triformylphloroglucinol
TPA	terephthalaldehyde
TPB	1,3,5-tri-(4-aminophenyl)benzene
TpBD	1,3,5-triformylphloroglucinol and benzidine
TPB-DMTP-COF-SH	triazole and thiol groups-functionalized COF (2,5-dimethoxyterephtaldehyde (DMTA) + 2,5-bis(prop-2-in-1-yloxy)terephtaldehyde (BPTA) + 1,3,5-Tris-(4-aminophenyl)benzene (TAPB))
TPhP	Triphenyl phosphate
TpND	a COF synthesized with Tp and ND
TpODH	Oxalyldihydrazide (ODH) + 1,3,5-triformylphloroglucinol (Tp)
TpPa-NH2@EDTA	EDTA-functionalized COF (triformylphloroglucinol (Tp) + 2-nitrobenzene-1,4-diamine (Pa-NO2) + ethylenediaminetetraacetic dianhydride (EDTA dianhydride))
TPT-CHO	2,4,6-tris(p-formylphenoxy)-1,3,5-triazine
TS-COF-1	Triazine-polyimide-COF
TS-COF-2	Task-specific Triazine-Schiff base-COF
TTB-COF	Thioether-functionalized COF (2,5-bis(2-(ethylthio)ethoxy) terephthalohydrazide (BETH) + 1,3,5-triformylbenzene (TFB))
Tz	1,3,5-tris(4-formyl-phenyl) triazine
TzDBd	1,3,5-tris(4-formyl-phenyl) triazine + 4,4'-diamino-[1,1'-biphenyl]-2,2'-dicarboxylic acid
U.S. EPA	The United States Environmental Protection Agency
VSM	vibrating sample magnetometer
WHO	World Health Organization
XAFS	X-ray absorption fine structure
XANES	X-ray absorption near-edge structure spectroscopy

XPS	X-ray photoelectron spectroscopy
λex	Wave length of external UV

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