One-step synthesis of triazine-based covalent organic frameworks at room temperature for efficient photo-degradation of bisphenol A under visible light irradiation

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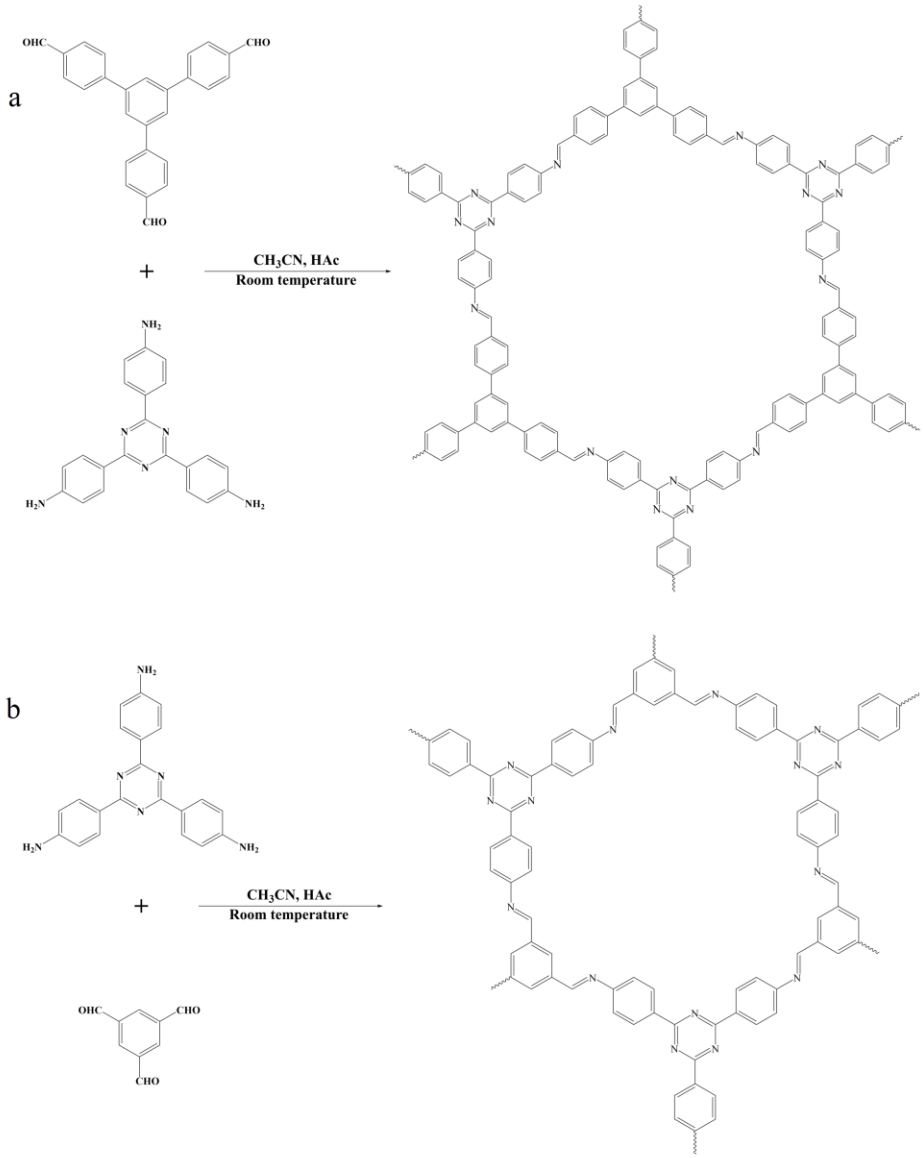
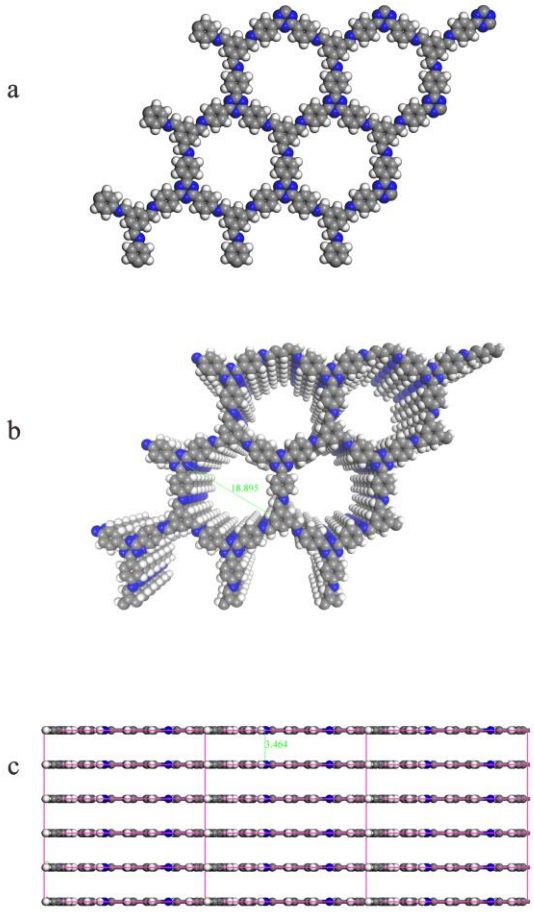
Supplementary materials



Scheme S1 A schematic illustration for the room-temperature synthesis of TrCOFs.

The synthesis reaction of TrCOF materials is Schiff-base reaction. Acetonitrile and acetic acid are used as solvent and catalyst, respectively. Ultrasound provides enough energy for the reaction to overcome the energy barrier required for the reaction.



Scheme S2 (a) Illustration of the Forcite GeomOpt of TrCOF2. **(b)** Top and **(c)** side views of the offset AA stacked structure of TrCOF2.

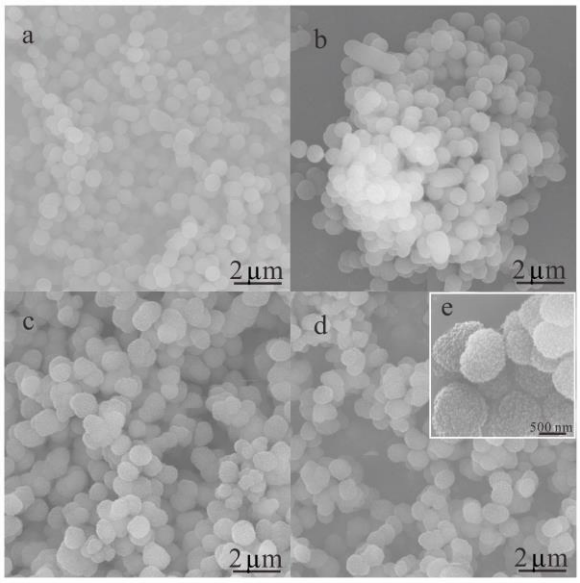


Fig. S1 SEM images of **(a)** TrCOF1-12, **(b)** TrCOF1-72, **(c)** TrCOF2-12, and **(d)(e)** TrCOF2-72.

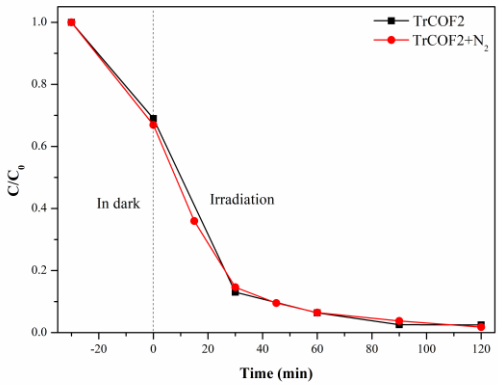


Fig. S2 Photocatalytic activities over TrCOF2-72 with/without bubbling N_2.

The Kubelka–Munk function is:

$$(\alpha h\nu)^n = B(h\nu - E_g)$$

where h, ν, B, α, and E_g represent the Planck's constant, the frequency of light, the proportional constant, the absorbance, and the bandgap energy, respectively; n is 1/2 for the indirect bandgap semiconductor and 2 for the direct bandgap semiconductor.

Table S1 Fractional atomic coordinates for the unit cell of TrCOF2 ($a = b = 26.2510$ Å, $c = 3.5$ Å, $\alpha = \beta = 90.00°$ and $\gamma = 120.00°$)

Element	Atom number	Fractional coordinates of atoms		
		u	v	w
H	1	1.013028	0.864960	0.500000
H	2	0.956965	0.756670	0.500000
H	3	0.795127	0.760835	0.500000
H	4	0.850069	0.867736	0.500000
H	5	0.600474	0.373752	0.500000
H	6	0.538058	0.169633	0.500000
H	7	0.434173	0.106416	0.500000
H	8	0.407990	0.255222	0.500000
H	9	0.511542	0.320900	0.500000
H	10	0.333442	0.088698	0.500000
H	11	−0.864960	0.148068	0.500000
H	12	−0.756670	0.200296	0.500000
H	13	−0.760835	0.034291	0.500000
H	14	−0.867736	−0.017668	0.500000
H	15	−0.373752	0.226722	0.500000
H	16	−0.169633	0.368425	0.500000
H	17	−0.106416	0.327757	0.500000
H	18	−0.255222	0.152768	0.500000
H	19	−0.320900	0.190642	0.500000
H	20	−0.088698	0.244744	0.500000
H	21	−0.148068	−1.013028	0.500000
H	22	−0.200296	−0.956965	0.500000

H	23	−0.034291	−0.795127	0.500000
H	24	0.017668	−0.850069	0.500000
H	25	−0.226722	−0.600474	0.500000
H	26	−0.368425	−0.538058	0.500000
H	27	−0.327757	−0.434173	0.500000
H	28	−0.152768	−0.407990	0.500000
H	29	−0.190642	−0.511542	0.500000
H	30	−0.244744	−0.333442	0.500000
C	1	0.935882	0.874836	0.500000
C	2	0.965432	0.842545	0.500000
C	3	0.933772	0.781043	0.500000
C	4	0.872307	0.750426	0.500000
C	5	0.842448	0.782487	0.500000
C	6	0.874001	0.844039	0.500000
C	7	0.969349	0.940169	0.500000
C	8	0.629087	0.356284	0.500000
C	9	0.690313	0.395699	0.500000
C	10	0.537759	0.253306	0.500000
C	11	0.512435	0.191171	0.500000
C	12	0.451518	0.153507	0.500000
C	13	0.413280	0.175976	0.500000
C	14	0.436928	0.236929	0.500000
C	15	0.497788	0.274904	0.500000
C	16	0.349078	0.135327	0.500000
C	17	−0.874836	0.061046	0.500000
C	18	−0.842545	0.122886	0.500000
C	19	−0.781043	0.152729	0.500000
C	20	−0.750426	0.121881	0.500000
C	21	−0.782487	0.059960	0.500000
C	22	−0.844039	0.029962	0.500000
C	23	−0.940169	0.029180	0.500000
C	24	−0.356284	0.272803	0.500000
C	25	−0.395699	0.294614	0.500000
C	26	−0.253306	0.284454	0.500000
C	27	−0.191171	0.321265	0.500000
C	28	−0.153507	0.298012	0.500000
C	29	−0.175976	0.237303	0.500000
C	30	−0.236929	0.199998	0.500000
C	31	−0.274904	0.222883	0.500000
C	32	−0.135327	0.213751	0.500000
C	33	−0.061046	−0.935882	0.500000
C	34	−0.122886	−0.965432	0.500000
C	35	−0.152729	−0.933772	0.500000
C	36	−0.121881	−0.872307	0.500000
C	37	−0.059960	−0.842448	0.500000
C	38	−0.029962	−0.874001	0.500000

C	39	−0.029180	−0.969349	0.500000
C	40	−0.272803	−0.629087	0.500000
C	41	−0.294614	−0.690313	0.500000
C	42	−0.284454	−0.537759	0.500000
C	43	−0.321265	−0.512435	0.500000
C	44	−0.298012	−0.451518	0.500000
C	45	−0.237303	−0.413280	0.500000
C	46	−0.199998	−0.436928	0.500000
C	47	−0.222883	−0.497788	0.500000
C	48	−0.213751	−0.349078	0.500000
N	1	0.940607	0.971033	0.500000
N	2	0.312774	0.155465	0.500000
N	3	−0.971033	−0.030426	0.500000
N	4	−0.155465	0.157309	0.500000
N	5	0.030426	−0.940607	0.500000
N	6	−0.157309	−0.312774	0.500000

Table S2 Comparison of BPA degradation efficiency by different materials

Photocatalyst	Irradiation time/min	Catalyst concentration/($g \cdot L^{-1}$)	Pollutant concentration/($mg \cdot L^{-1}$)	Degradation efficiency/%	Ref.
Co-BiOCl	120 (visible)	0.67	10	95	[1]
CxCN	90 (visible)	0.2	10	100	[2]
CdS/COF	180 (UV)	0.3	–	85.68	[3]
CSCF	180 (visible)	0.67	3	94.0	[4]
TrCOF2	60 (vislbe)	0.2	2	98	this work

References

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