Supplementary material for

Unique "posture" of rose Bengal for fabricating personal protective equipment with enhanced daylight-induced biocidal efficiency

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Supporting information contains:

Supplementary discussion

Supplementary figures S1–S7

Supplementary tables S1–S4

Supplementary references

1. Supplementary discussion

1.1 Fabrication of DBwEE-Cotton by RB at different pH

POP can be positively charged depending on the solution pH, resulting in protonation of the primary and secondary amines in its structure. Thus, the pH of the RB solution may show an impact on the adsorption, driven by the electrostatic interaction between anionic RB and cationic POP. As shown in Fig. S1a, the highest adsorption amount was noticed at pH = 5 (i.e., 12.79 mg/g), whereas the adsorption amount dropped to 7.07 and 5.14 mg/g at pH of 3 and 11, respectively. This phenomenon can be explained by checking the zeta potential of the POP at different pH conditions. In Fig. S1b, the POP showed a cationic character when the solution pH was lower than 10, whereas the zeta potential of the POP dropped to -14.2 mV at pH = 10. According to the pKa values of RB ($p\mathrm{K}_{\mathrm{aOH1}} < 0$, $p\mathrm{K}_{\mathrm{aCOOH}} = 1.89$, $p\mathrm{K}_{\mathrm{aOH2}} = 3.93$),[1] RB performed fewer negative charges when pH = 3, leading to a weaker driving force for RB adsorption. On the other hand, the decrease of RB adsorption at pH = 10 was attributed to the charge repulsion between negatively charged POP and RB.

1.2 Fabrication of DBwEE-Cotton by different initial concentrations of RB

In Fig. S2a, the initial RB concentration was related to the final loading of RB on the fabrics. In the concentration range of 10–250 mg/L, the RB loadings on the DBwEE-Cotton increased as the initial concentration was increased. However, the adsorption amount of RB kept steady by further increasing the concentration to 350 mg/L and 500 mg/L. The over-loading of RB molecules on the fabric can be achieved via hydrophobic interaction between RB molecules with high RB initial concentrations, which can be seen on the CHPTAC@Cotton (Table S1). Nevertheless, because of the size-exclusive guest-host capture of RB on the DBwEE-Cotton, the over-loading of RB was avoided.

The adsorption kinetics of RB onto the SAFE-Cotton (i.e., resulted in DBwEE-Cotton) was studied by controlling the RB initial concentration and the pH as 100 mg/L and 5.5, respectively (Fig. S2b and S2c). The adsorption performed rapidly during the first 4 hours but tending to equilibrium after that. The dye exhaustion at the end of the adsorption (i.e., 24 hours) reached 90.0%, attributed to the high porosity on the SAFE-Cotton. During the first 60 min, the adsorption can be plotted to pseudo-first-order kinetics with a rate constant of -0.0106 min^{-1}.

1.3 Mechanical property of modified fabrics

The tensile strengths and tearing strength of the cotton, SAFE-Cotton, and DBwEE-Cotton were tested with an Instron® 5566 (MA, USA) according to the American Society for Testing and Materials (ASTM) D 5035-06 testing method and an Elmendorf tearing tester (Thwing-Albert Instrument Co., PA, USA) according to ASTM D 1424 testing method with modifications, respectively. Specifically, the sample size of the cotton, SAFE-Cotton, and RB-adsorbed cotton (DBwEE-Cotton$_{100}$) was cut as 2 cm × 7 cm with a testing gauge length of 5 cm for tensile strength tests. The fabric size was set as 2 cm × 7 cm for tearing strength tests. The strength on the filling direction was measured in triplicates. The tensile strength retention (TSR) was calculated based on Equation S1. TS_0 and TS_n refer to the stress at break (MPa) of pristine cotton and treated cotton, respectively.

$$TSR = \frac{TS_n}{TS_0} \times 100\%$$

(S1)

As shown in Table S4, the TSR of SAFE-Cotton decreased to 46.72%, which is caused by the high temperature, long reaction duration, and the production of hydrochloric acid as the byproduct during the POP in situ synthesis. Nevertheless, the adsorption of RB on the SAFE-Cotton showed no effect to the tensile strength of the material, whose TSR was tested as 45.34%. Similar changing trend can be noticed by evaluating the tearing strength of the fabrics when the testing errors are considered.
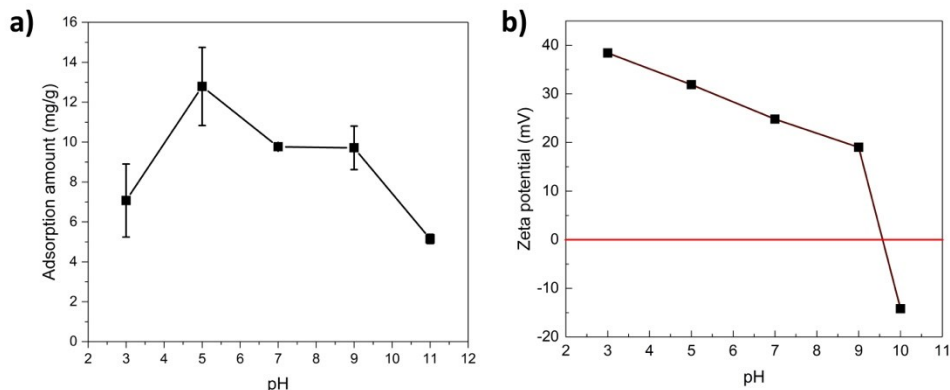
2. Supplementary figures

Fig. S1 a) pH effects on the adsorption behavior of RB on SAFE-Cotton. **b)** Zeta potentials of POP particles in water under specific pH conditions.
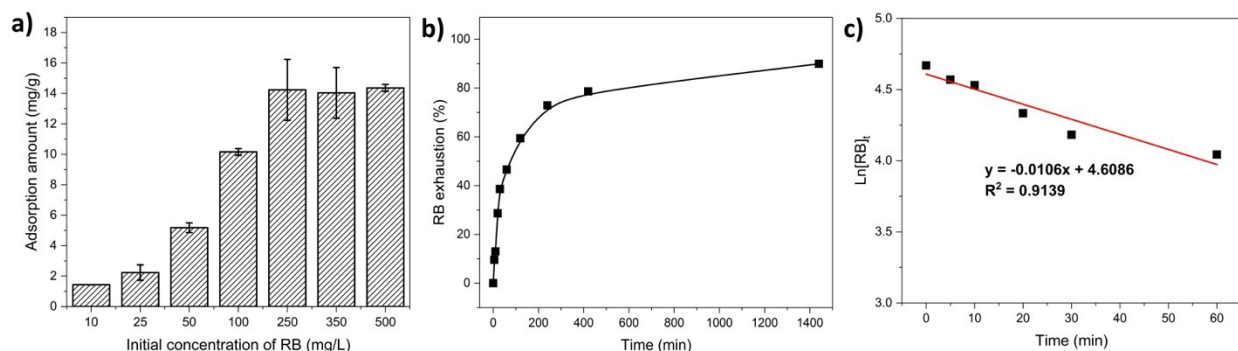

Fig. S2 a) Adsorption amounts of RB on SAFE-Cotton according to different RB initial concentrations. **b)** The exhaustion of 30 mL 100 mg/L RB by SAFE-Cotton (5×5 cm^2) at room temperature according to adsorption time. **c)** Pseudo-first order kinetics of RB adsorption on SAFE-Cotton.
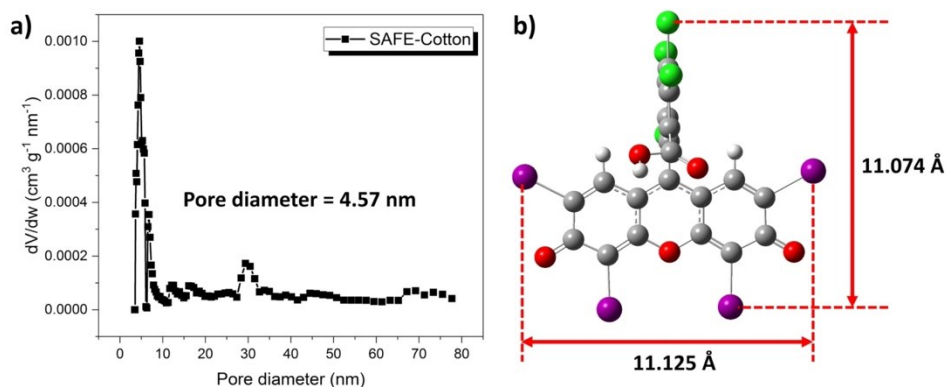

Fig. S3 a) Pore size distribution of SAFE-Cotton. **b)** Optimized geometry of rose Bengal from Gaussian calculation. The predicted diameter of rose Bengal is estimated by the distance between the two farthest atoms in the vertical and horizontal directions.
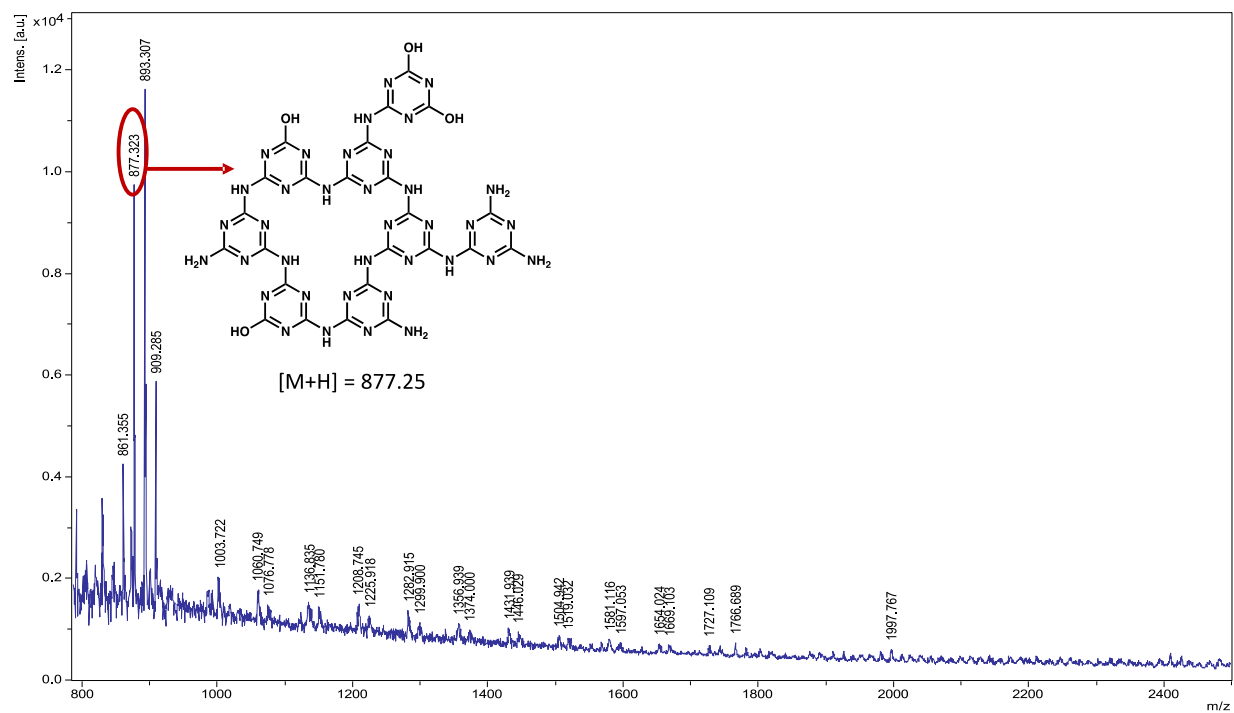
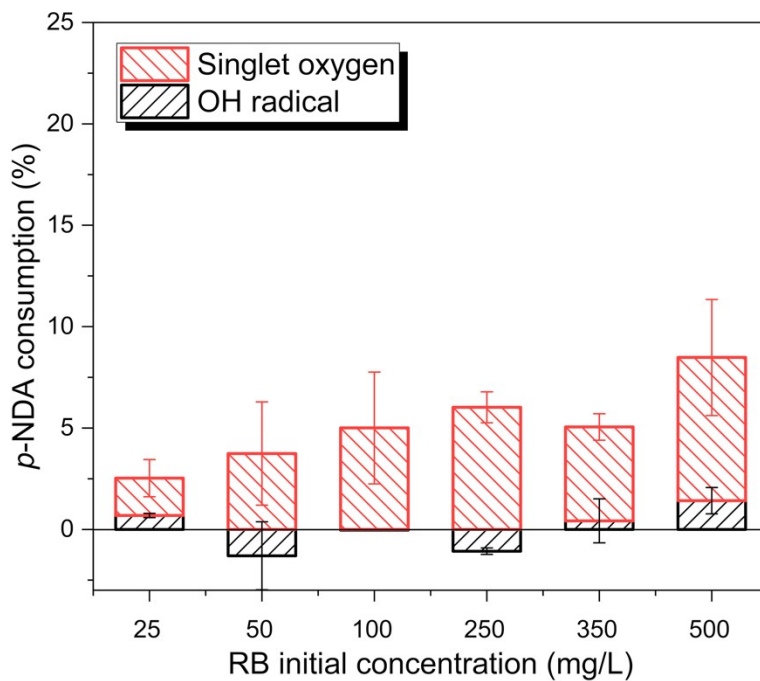**Fig. S4** MALDI-TOF-MS spectrum of POP particles.

Fig. S5 ROS production of RB-CHPTAC@Cotton dyed with different RB initial concentrations.
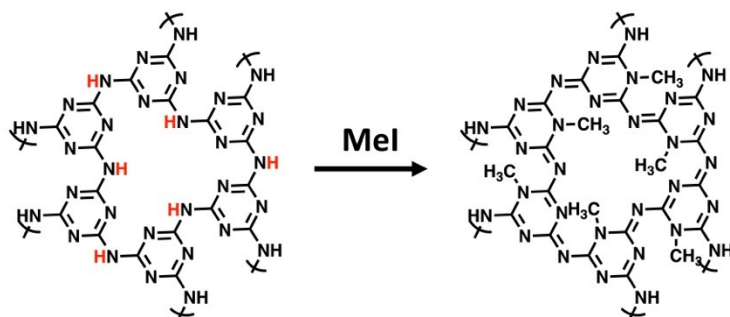
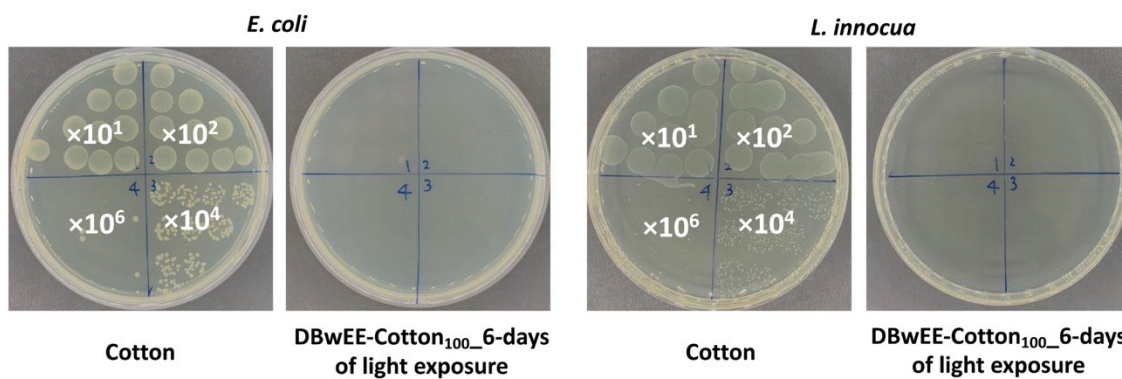**Fig. S6** Chemical structural changes of POP before and after MeI alkylation.

Fig. S7 Antibacterial results (30 min of daylight irradiation) of DBwEE-Cotton$_{100}$ after 6-days of daylight exposure.

3. Supplementary tables

Table S1. CIELab color parameters, ASTM whiteness index, and yellowness index of different fabrics

	L^*	a^*	b^*	Color difference	Whiteness index	Yellowness index
Cotton	87.9	-0.49	0.49	0.00	69.53	0.60
	87.54	-0.47	0.53	0.36	68.61	0.70
	87.94	-0.29	0.58	0.22	69.51	0.81
	87.71	-0.47	0.44	0.20	69.37	0.52
Average	87.77±0.18	-0.43±0.09	0.51±0.06	0.20±0.15	69.16±0.48	0.66±0.13
SAFE-Cotton	82.4	1.9	14.9	15.61	2.21	31.39
	82.4	1.91	14.9	15.61	2.22	31.40
	82.76	1.78	14.75	15.33	2.96	30.91
	82.61	1.84	13.26	14.02	2.69	28.27
Average	82.54±0.18	1.86±0.06	14.45±0.80	15.14±0.76	2.52±0.37	30.49±1.50
DBwEE-Cotton$_{10}$	65.08	42.81	-8.19	49.60	--	--
	63.98	45.63	-7.94	52.53	--	--
	66.51	41.83	-7.14	47.92	--	--
	67.70	40.29	-6.21	45.89	--	--
Average	65.82±1.62	42.64±2.25	-7.37±0.89	48.98±2.80	--	--
DBwEE-Cotton$_{50}$	50.25	56.58	-2.56	68.32	--	--
	45.08	59.68	-1.89	73.77	--	--
	46.33	59.15	-2.49	72.64	--	--
	50.16	56.96	-3.25	68.72	--	--
Average	47.96±2.64	58.09±1.55	-2.55±0.56	70.86±2.75	--	--
DBwEE-Cotton$_{100}$	42.48	60.23	-19.79	78.49	--	--
	42.12	59.62	-19.56	78.17	--	--
	40.51	60.2	-16.05	78.76	--	--
	42.11	59.45	-17.44	77.53	--	--
Average	41.81±0.88	59.88±0.40	-18.21±1.79	78.24±0.53	--	--
DBwEE-Cotton$_{250}$	41.69	65.71	-22.43	83.81	--	--
	41.00	65.62	-22.61	84.17	--	--
	43.55	67.94	-21.68	84.39	--	--
	40.64	65.29	-21.62	83.85	--	--
Average	41.27±1.29	66.14±1.21	-22.09±0.51	84.05±0.28	--	--
DBwEE-Cotton$_{500}$	38.81	63.09	-22.43	83.42	--	--
	37.91	61.80	-20.96	82.58	--	--
	35.37	58.89	-21.55	82.17	--	--
	40.40	64.91	-22.87	84.02	--	--
Average	38.12±2.10	62.17±2.53	-21.95±0.86	83.05±0.83	--	--

Table S2. Adsorption amount of RB on CHPTAC@Cotton.

Initial concentration (mg/L)	Adsorption amount (mg/g)
10	1.417
25	3.346

50	8.257
100	10.625
250	12.625
350	14.875
500	18.710

Table S3. Antibacterial functions of organic PS-incorporated fabrics

Materials	light source	time	Bacterial reduction (gram-negative/gram-positive)	Reference
Wool/acrylic blend	visible light	60 min	1–2 log/~4 log	[2]
RB-modified cotton	green light	4 hours	6 log/6 log	[3]
Porphyrinic MOFs/cotton	visible light	45 min	6 log/6 log	[4]
RB/Polyurethane coated on leather	Fluorescent light	1.5 hours	6 log/N/A	[5]
RB-DEAE@Cotton	cold white	60 min	6 log/6 log	[6]
DBwEE-Cotton	cold white	5 min	1.87 log/1.67 log	**This work**
		10 min	4.78 log/2.76 log	
		20 min	>6 log/>6 log	

Table S4. Tensile strength, tensile strength retention, and tearing strength of treated fabrics.

Sample	Stress at break (MPa)	TSR (%)	Tearing strength (º)
Cotton	88.46±1.37	100.00	46.12±9.46
SAFE-Cotton	41.33±5.51	46.72	26.63±9.52
BDwEE-Cotton$_{100}$	40.11±1.22	45.34	19.88±8.61

4. Supplementary references

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