Electronic Supplementary Information

Wrinkle-Induced High Sorption Makes Few-layered Black Phosphorus a Superior Adsorbent for Ionic Organic Compounds

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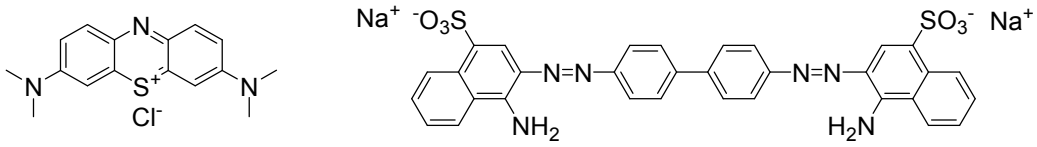

Fig. S1 Chemical structures of methylene blue (left) and Congo red (right).

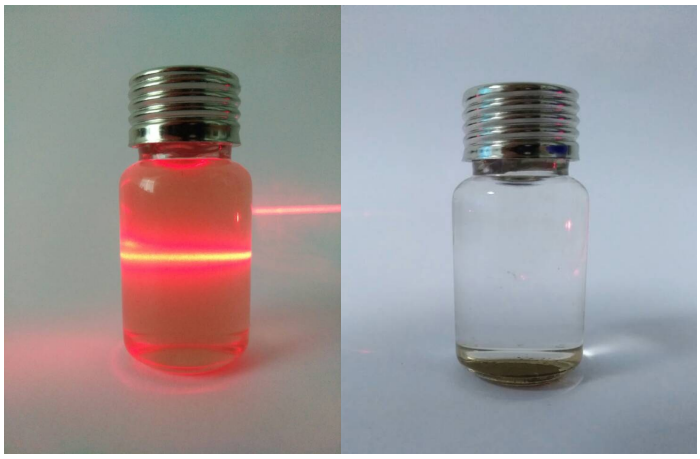

Fig. S2 Tyndal effect observation of the supernatant before and after centrifugation.

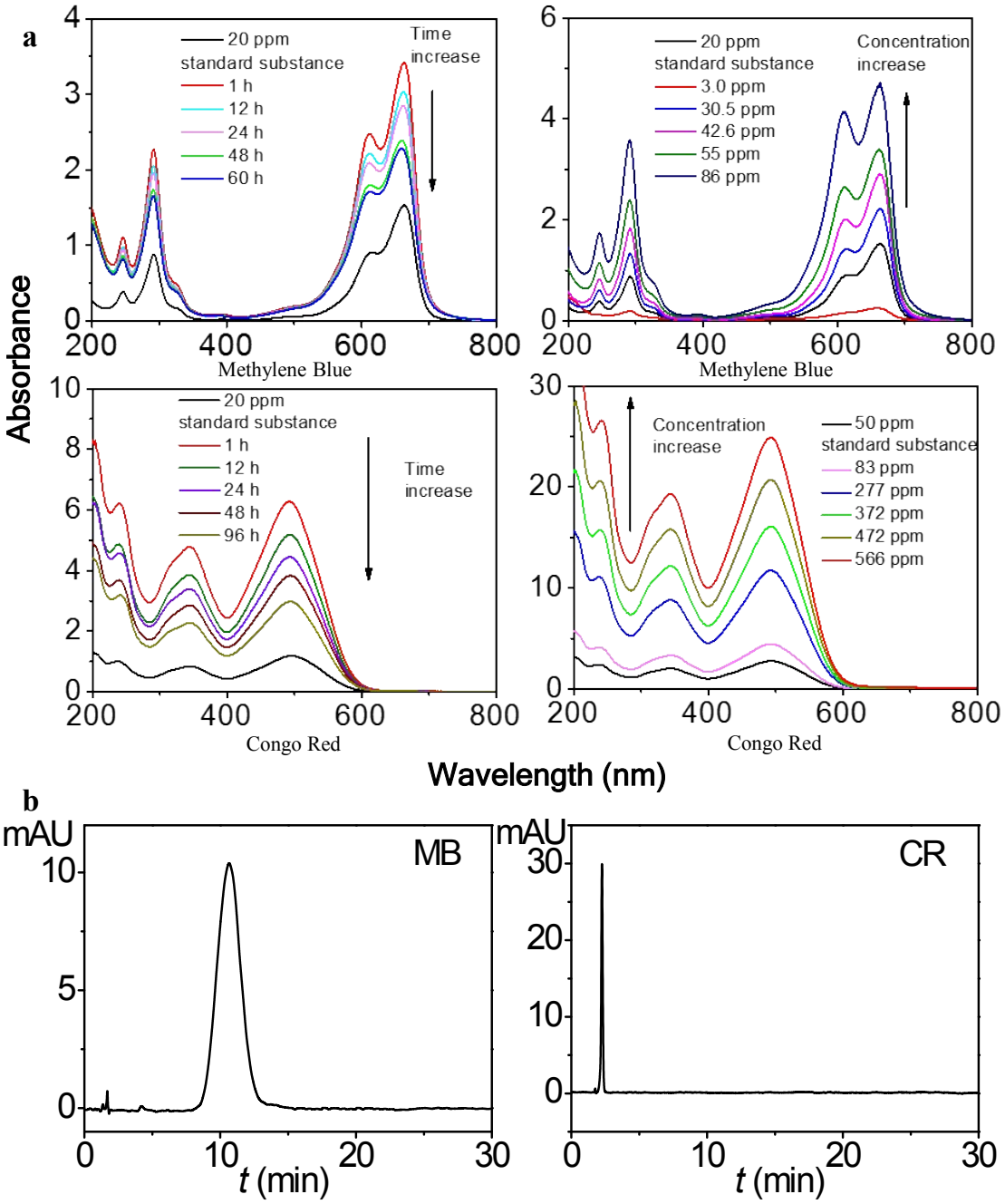

Fig. S3 (a) UV-Vis spectra of MB and CR during sorption varied with time and initial concentration; (b) HPLC spectra of MB and CR after sorption. No new peaks were found in both spectra, suggesting no degradation occurred.

Table S1. Results of LM, FM, and DA models fitted sorption data of two dyes by few-layered BP [a]

LM						
Compounds	Q^0	P of Q^0	b	P of b	RMSEC	r_{adj}^2
MB	856.81±28.61	<0.0001	0.011±0.001	<0.0001	24.912	0.9870
CR	218.59±4.90	<0.0001	0.050±0.005	<0.0001	9.227	0.9800

FM						
Compounds	K_f	P of K_f	n	P of n	RMSEC	r_{adj}^2
MB	38.77±6.67	<0.0001	0.505±0.033	<0.0001	38.81	0.9700
CR	43.82±5.39	<0.0001	0.283±0.024	<0.0001	16.10	0.9394

DA							
Compounds	Q^0	P of Q^0	E	P of E	b	RMSEC	r_{adj}^2
MB	1232±283	<0.0001	20.3±0.9	<0.0001	2.68±0.32	18.268	0.993
CR	230±8.97	<0.0001	26.6±0.1	<0.0001	5.28±0.34	8.535	0.991

[a] All estimated parameter values, their standard error, probability of assuming the null hypothesis (p) and the fitting adjusted square of correlation coefficient (r_{adj}^2) were determined by a commercial software program (Sigmaplot 11.1).

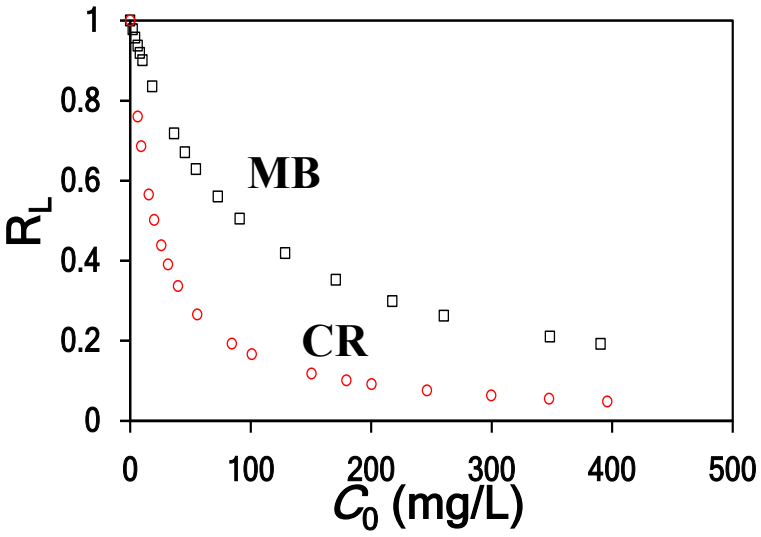

Fig. S4 Variation of separation factor R_L with dyes' initial concentration C_o.

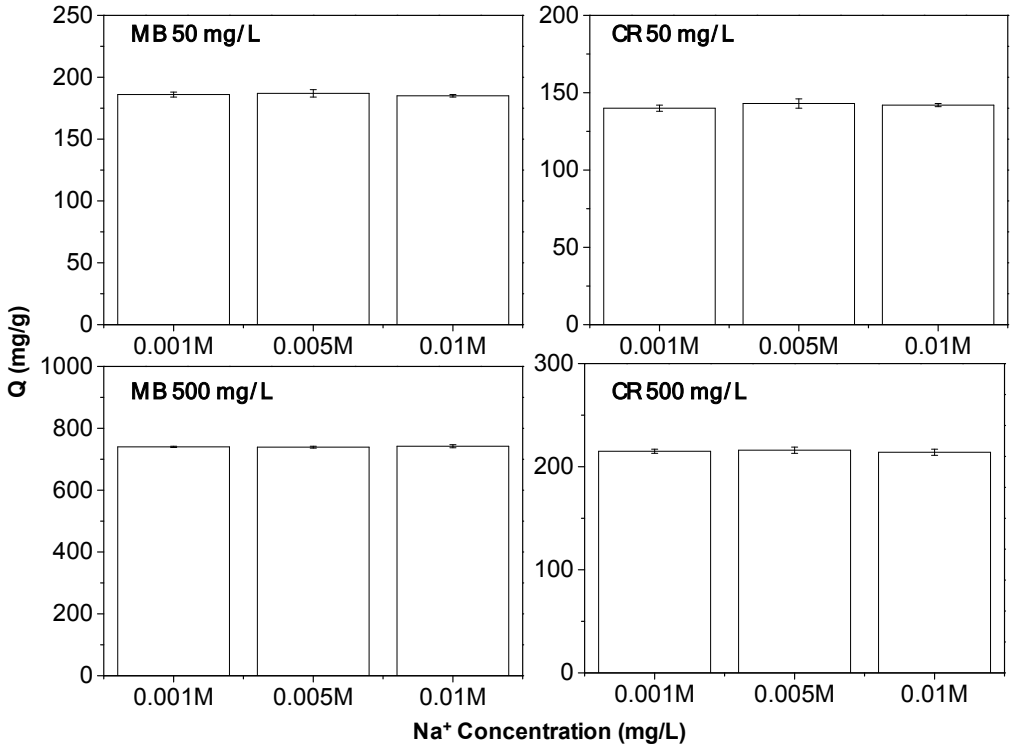

Fig. S5 Comparison of amount sorption of two dyes at different Na^+ concentration levels at initial concentration of 50 and 500 mg/L respectively.

Table S2. Results of PFOM, PSOM, and IPDM fitted with sorption kinetic data of two dyes by few-layered BP [a]

PFOM						
Compounds	q_e	P of q_e	k_1	P of k_1	RMSEC	r_{adj}^2
MB	174.32±16.81	<0.0001	-1.2725±0.6457	<0.0001	36.923	0.5976
CR	171.18±18.47	<0.0001	-0.0234±0.0057	<0.0001	15.386	0.9048
PSOM						
Compounds	q_e	P of q_e	k_2	RMSEC	r_{adj}^2	
MB	251.52±14.99	<0.0001	0.00088	32.277	0.9622	
CR	174.89±16.61	<0.0001	0.00032	17.205	0.8867	
IPDM						
Compounds	k_i	P of k_i	θ	P of θ	RMSEC	r_{adj}^2
MB	27.24±1.85	<0.0001	47.10±7.41	<0.0001	13.403	0.947
CR	14.55±0.47	<0.0001	6.42±2.48	<0.0001	4.973	0.984

[a] All estimated parameter values, their standard error, probability of assuming the null hypothesis (p) and the fitting adjusted square of correlation coefficient (r_{adj}^2) were determined by a commercial software program (Sigmaplot 11.1).

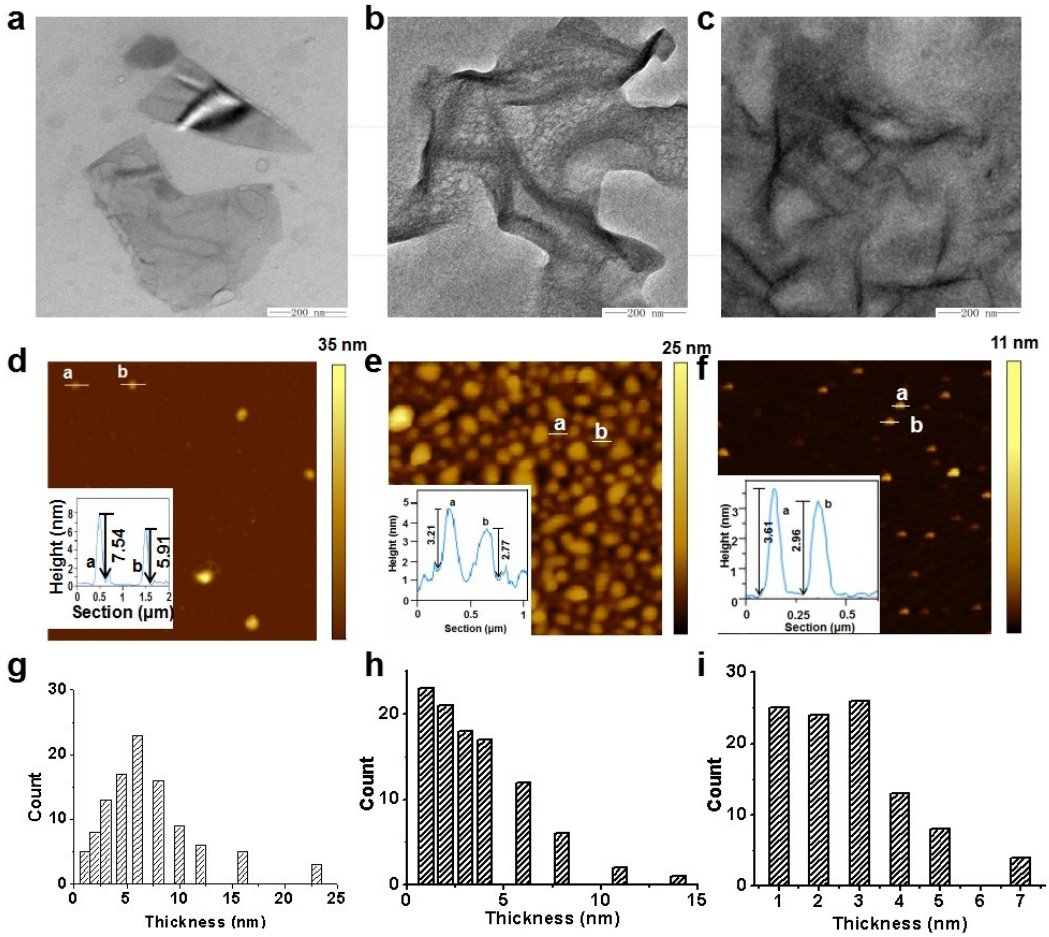

Fig. S6 TEM images (a-c), AFM images (d-f), and statistical analysis of the thickness (g-i) of few-layered BP before (a, d, and g) and after sorption at the initial CR concentration of 50 mg/L (b, e, and h) and 500 mg/L (c, f, and i).

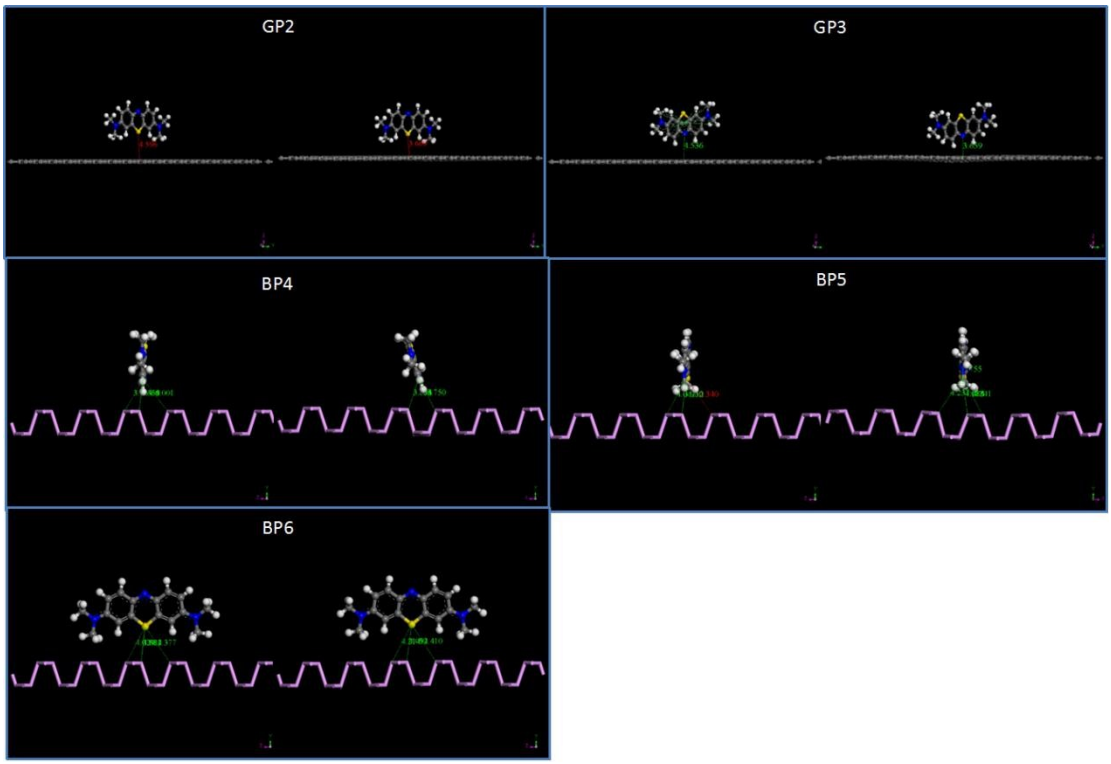

Fig. S7 Intial (left panel) and energy minimized (right panel) configurations of adsorption complex, the relatively unfavorable cases: MB adsored on graphene (GP2-3) and phosphorene (BP4-6) (Dark gray balls: C atoms; Light gray balls: H atoms; blue balls: N atoms; yellow balls: S atoms; Pink balls: P atoms; Unit for distance is Å).