

Supplementary Information

Enhanced Iodine Capture by Hydrogen Bond Reconstruction Strategy

Ling-Qiong Gou, Yuan-Hao Wang, Shuang-Long Wang, Jia-Ying Liu, Xin Xin, Xinhong Xu, Song Qin, Ling He*, and Guo-Hong Tao*

College of Chemistry, Sichuan University, Chengdu 610064, China

* E-mail: lhe@scu.edu.cn, taogh@scu.edu.cn

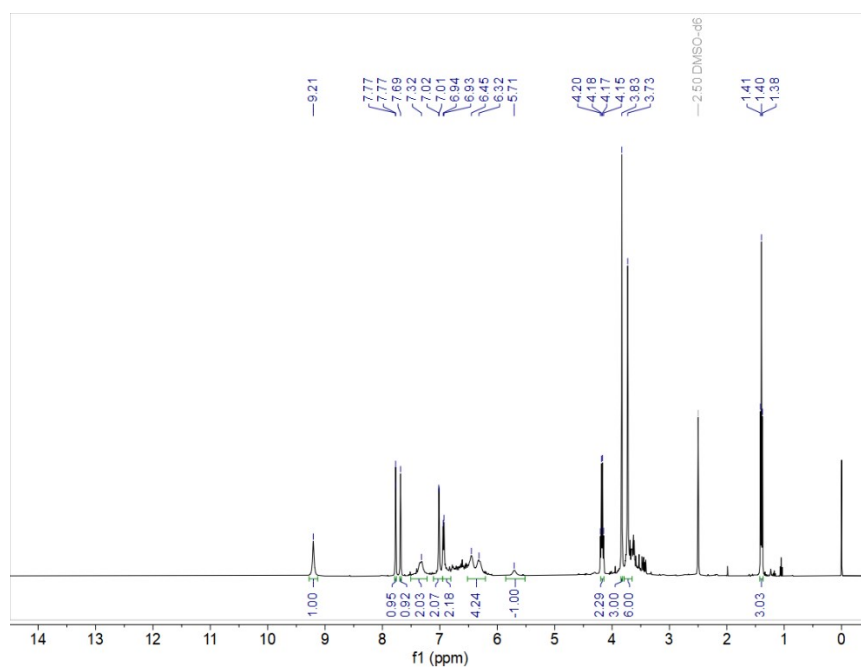


Fig. S1 ^1H NMR spectrum of [Emim][Cur] in $\text{DMSO-}d_6$.

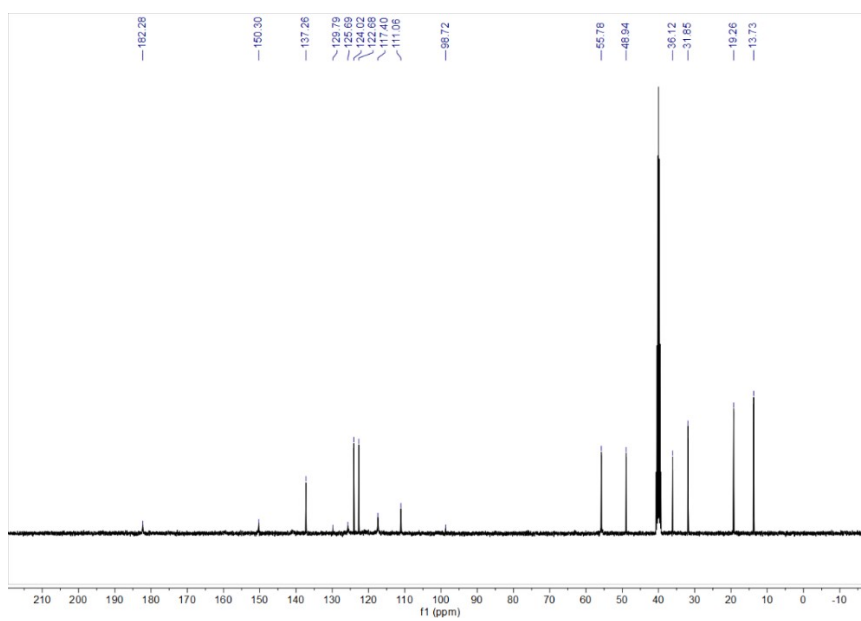


Fig. S2 ^{13}C NMR spectrum of [Emim][Cur] in $\text{DMSO-}d_6$.

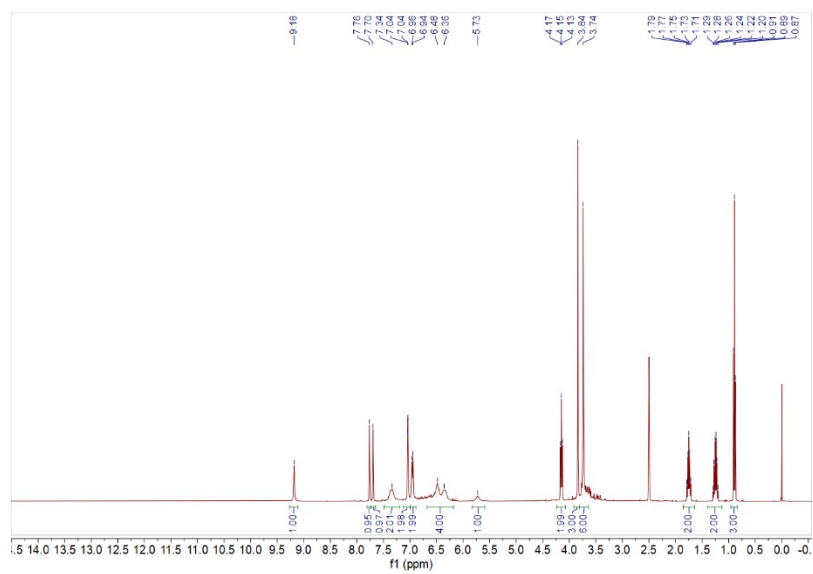


Fig. S3 ^1H NMR spectrum of [Bmim][Cur] in $\text{DMSO-}d_6$.

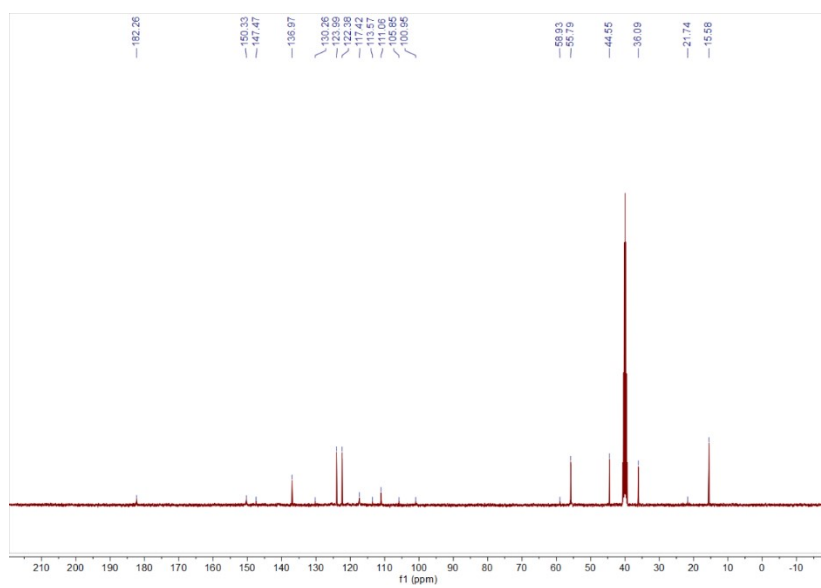


Fig. S4 ^{13}C NMR spectrum of [Bmim][Cur] in $\text{DMSO-}d_6$.

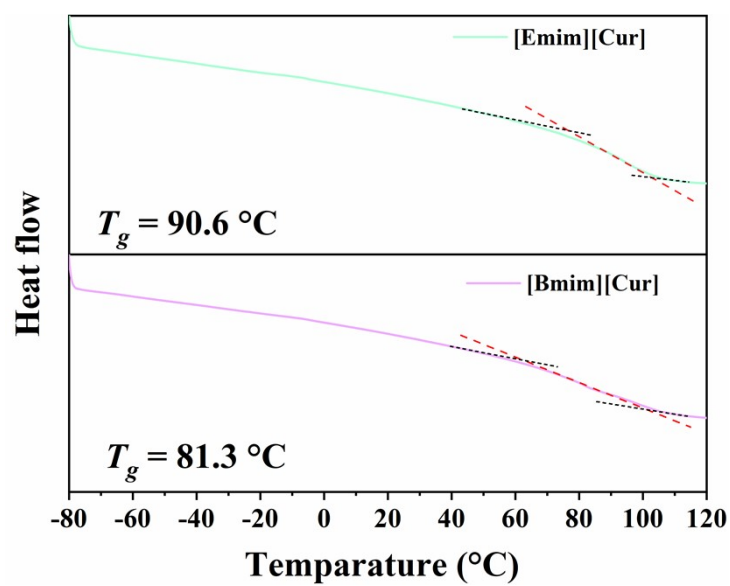


Fig. S5 DSC curves of [Emim][Cur] and [Bmim][Cur].

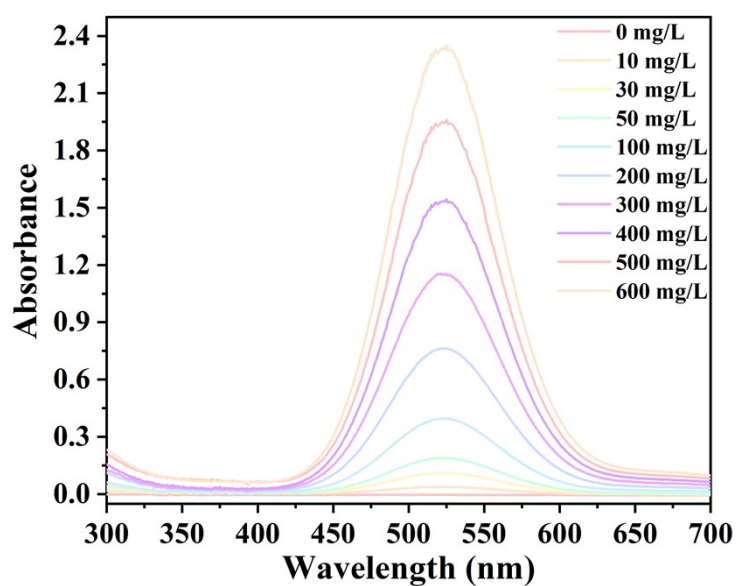


Fig. S6 Concentration-dependent UV-vis absorption spectra of iodine/cyclohexane solution.

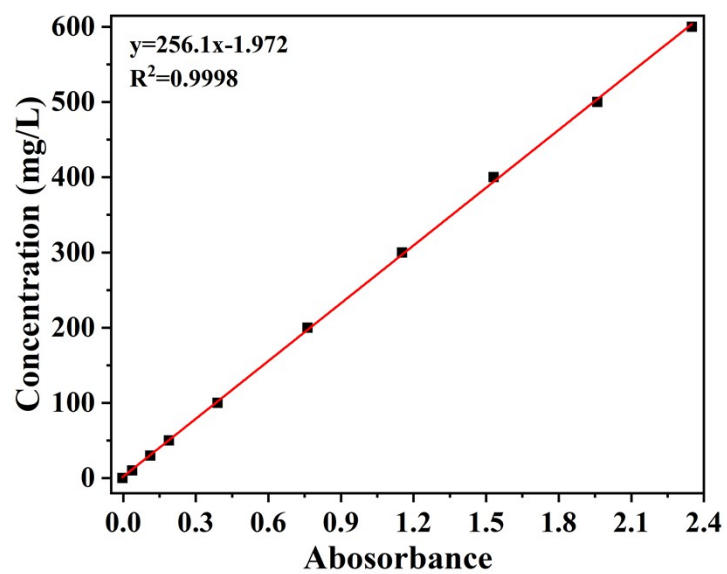


Fig. S7 Standard curve equation of iodine concentration in cyclohexane.

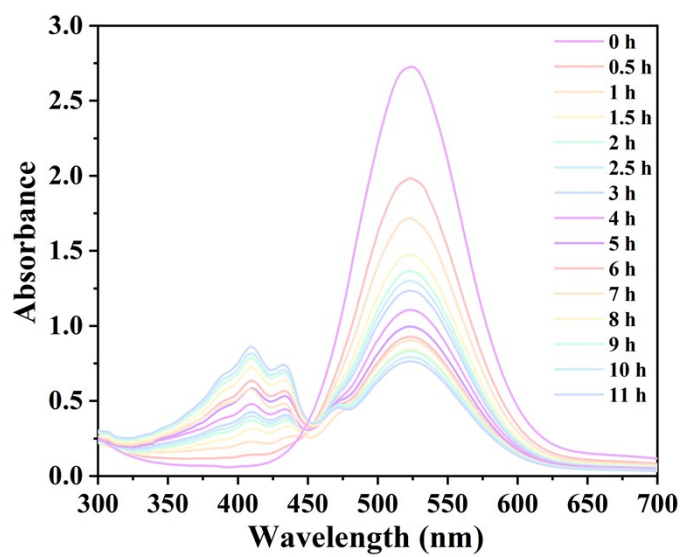


Fig. S8 Time-dependent UV-vis absorption spectra of iodine/cyclohexane solution.

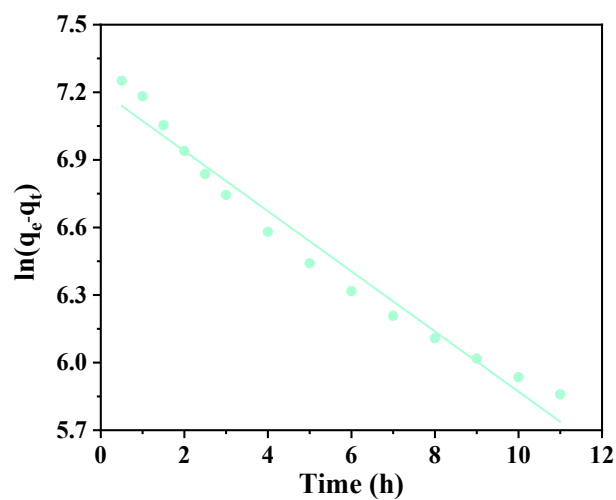


Fig. S9 Pseudo-first-kinetics model of [Emim][Cur], the concentration of iodine/cyclohexane solution is 700 mg L⁻¹.

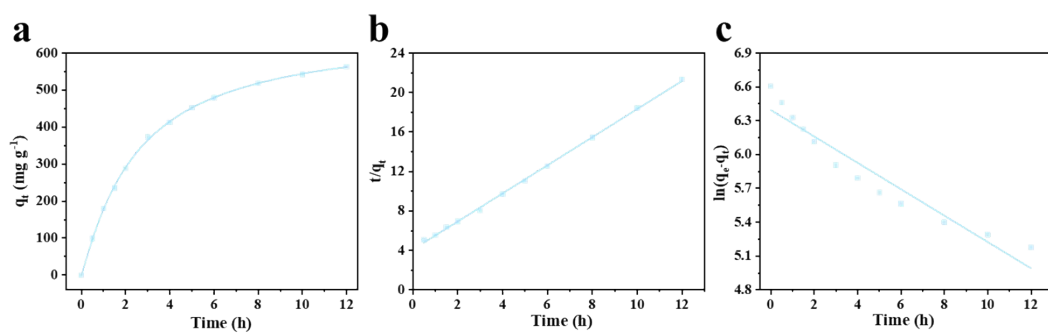


Fig. S10 Kinetic curves of iodine adsorption, pseudo-first-kinetics model, and pseudo-first-kinetics model of [Emim][Cur], the concentration of iodine/cyclohexane solution is 200 mg L⁻¹.

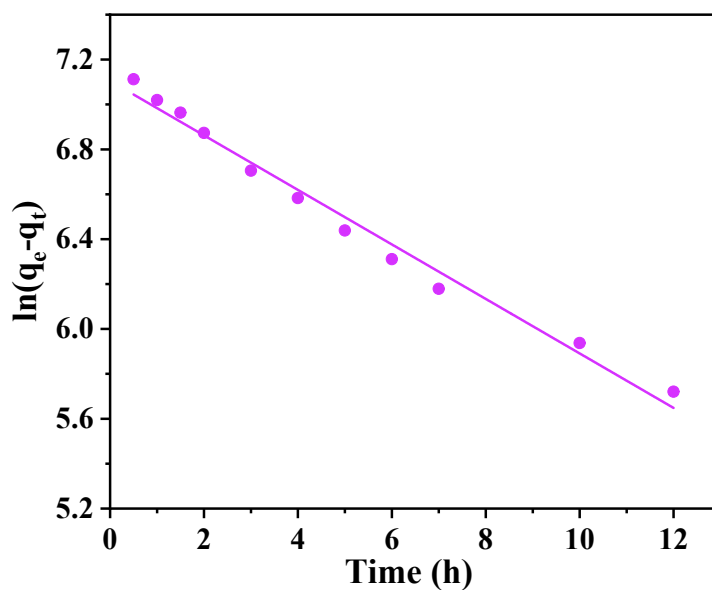


Fig. S11 Pseudo-first-kinetics model of [Bmim][Cur], the concentration of iodine/cyclohexane solution is 700 mg L⁻¹.

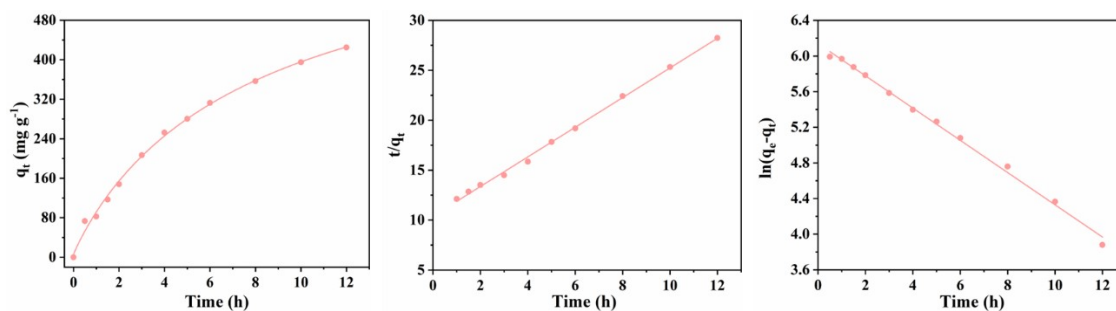


Fig. S12 Kinetic curves of iodine adsorption, pseudo-first-kinetics model, and pseudo-first-kinetics model of [Bmim][Cur], the concentration of iodine/cyclohexane solution is 200 mg L⁻¹.

Table S1

Kinetic parameters for I₂ removal by [Emim][Cur] and [Bmim][Cur] in 200 mg L⁻¹ I₂/cyclohexane solution.

Adsorbent	q _e (exp) (mg g ⁻¹)	Pseudo-first order			Pseudo-second order		
		q _e (cal) (mg g ⁻¹)	k ₁ (h ⁻¹)	R ²	q _e (cal) (mg g ⁻¹)	k ₂ (g g ⁻¹ h ⁻¹)	R ²
[Emim][Cur]	740.2	598.2	0.1169	0.9183	702.1	0.4966	0.9991
[Bmim][Cur]	658.3	464.3	0.1811	0.9659	673.5	0.2122	0.9980

Table S2

Kinetic parameters for I₂ removal by [Emim][Cur] and [Bmim][Cur] in 700 mg L⁻¹ I₂/cyclohexane solution.

Adsorbent	q _e (exp) (mg g ⁻¹)	Pseudo-first order			Pseudo-second order		
		q _e (cal) (mg g ⁻¹)	k ₁ (h ⁻¹)	R ²	q _e (cal) (mg g ⁻¹)	k ₂ (g g ⁻¹ h ⁻¹)	R ²
[Emim][Cur]	1813	1348	0.1336	0.9699	1770	0.3245	0.9962
[Bmim][Cur]	1695	1218	0.1214	0.9834	1585	0.3061	0.9875

Table S3

Langmuir and Freundlich isotherm parameters for I₂ removal using [Emim][Cur] and [Bmim][Cur].

Adsorbent	Adsorbate	Langmuir constants			Freundlich constants		
		q _m (cal) (g g ⁻¹)	k _L (L mg ⁻¹)	R ²	k _f (L g ⁻¹)	n _f (L mg ⁻¹)	R ²
[Emim][Cur]	I ₂	3.867	794.9	0.9956	0.1851	0.3483	0.9458
[Bmim][Cur]	I ₂	3.843	963.9	0.9888	0.0936	0.4261	0.9269

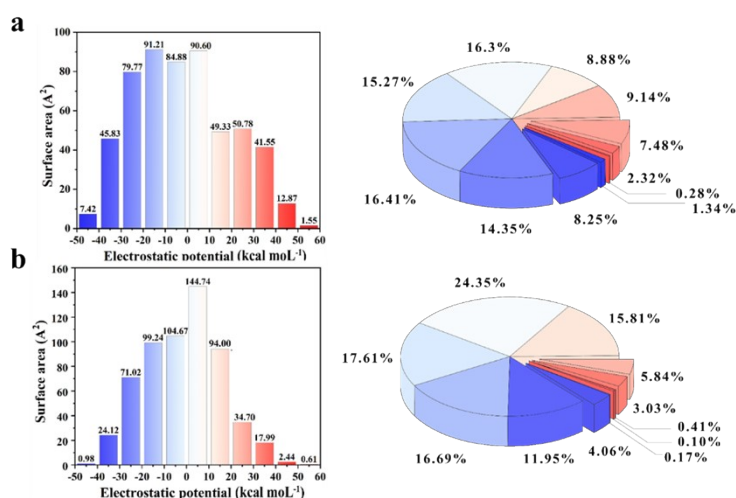


Fig. S13 Surface area and area percent of each ESP range on the vdW surface for (a) [Emim][Cur] and (b) [Bmim][Cur].

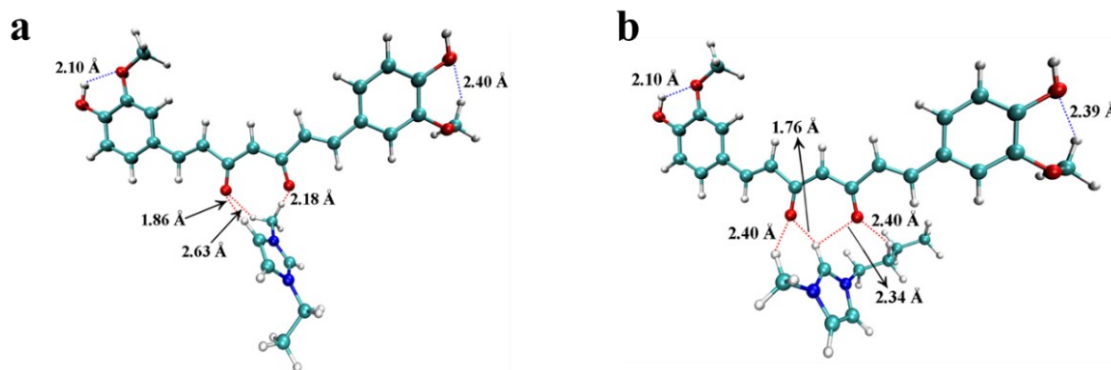


Fig. S14 QTAIM analysis for simplified structure of [Emim][Cur] and [Bmim][Cur].

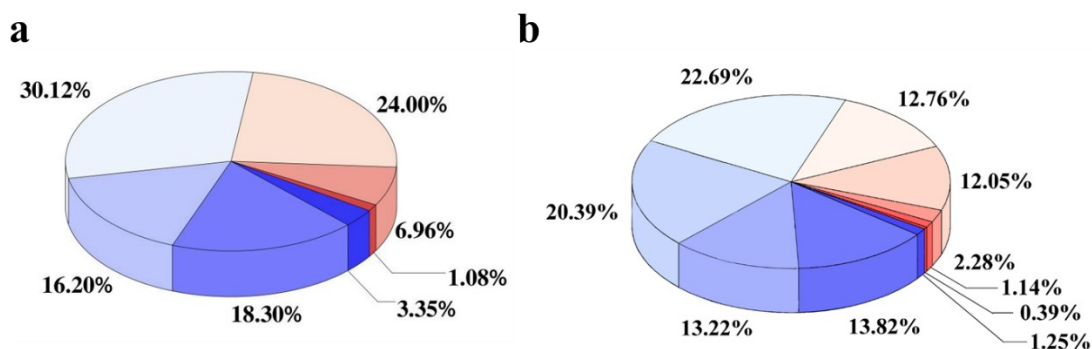


Fig. S15 Area percent of each ESP range on the vdW surface for (a) neutral Cur-I₂ and [Cur]⁻-I₂.

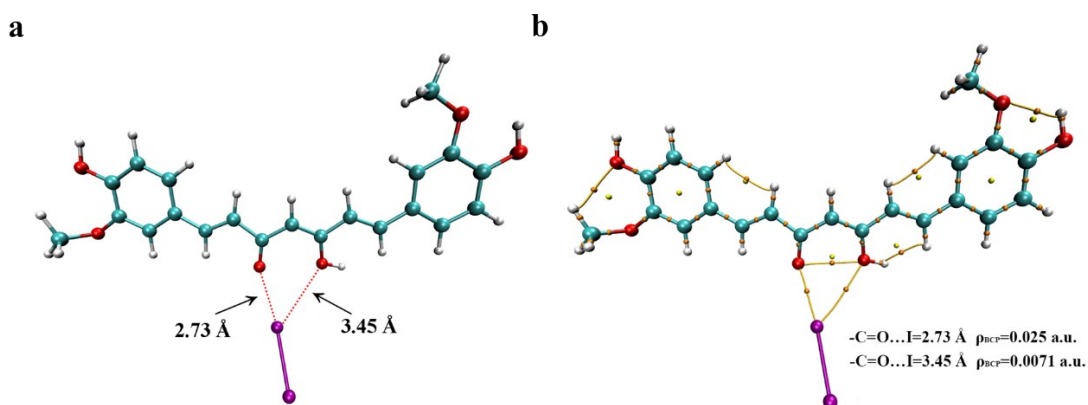


Fig. S16 QTAIM analysis for simplified structure of neutral Cur-I₂.

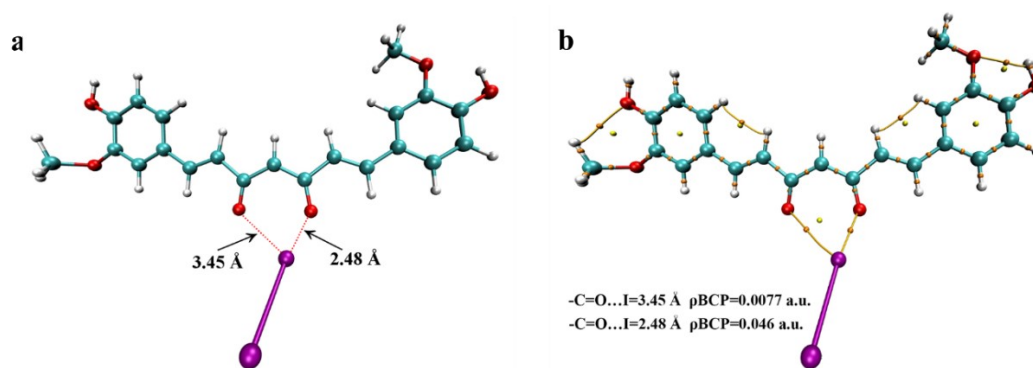


Fig. S17 QTAIM analysis for simplified structure of [Cur]⁻-I₂.

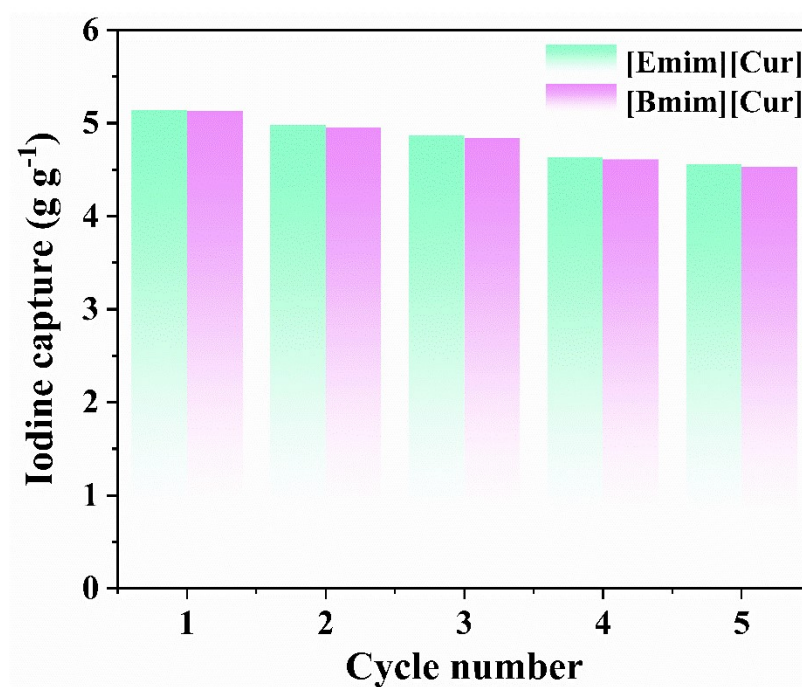


Fig. S18 Reusability of [Emim][Cur] and [Bmim][Cur].