Supporting Information

Predicting the crystal habit of Photoinitiator XBPO and elucidating the solvent effect on crystal faces

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Table S1 The crystal habit parameters of XBPO crystals in a vacuum predicted by the AE model[a]

(*h k l*)	Multiplicity	d_{hkl}	E_{att} (Total)	E_{att} (vdW)	E_{att} (Electrostatic)	*Area*(%)
(1 0 0)	2	17.24	-33.59	-30.63	-2.96	46.12
(1 1 0)	4	10.97	-63.39	-60.27	-3.12	28.41
(0 1 1)	4	7.28	-97.32	-89.66	-7.65	12.52
(1 1 -1)	4	7.30	-97.38	-88.92	-8.45	12.95

[a] All energies are in kcal mol^{-1}, distances are in Å.

Table S2 The diffusion coefficient of solvent molecules at the dominant crystal surfaces of XPBO

Solvent	(*h k l*)	$D/\times10^{-9}m^2\ s^{-1}$	ϕ
acetone	(1 0 0)	2.89	1.000
	(1 1 0)	2.91	1.007
	(0 1 1)	2.55	0.882
	(1 1 -1)	4.15	1.436
ethanol	(1 0 0)	1.43	1.000
	(1 1 0)	1.80	1.259
	(0 1 1)	2.43	1.699
	(1 1 -1)	2.80	1.958

Note: the diffusion coefficient (*D*) can be calculated using its mean square displacement (MSD) with respect to time as follows:

$$D = \frac{1}{6}\lim_{t\to\infty}\frac{d}{dt}\sum_{i=1}^{N}\left\langle\left|r_i(t) - r_i(0)\right|^2\right\rangle$$

where N indicates the equivalent particles, $r_i(t)$ is the position of molecule i at time t. The values of D was evaluated using the slope of the MSD versus time (take the 35-135 ps time interval).

Table S3 The calculation details of affinity degree at the dominant crystal surfaces of XPBO[a]

Solvent	(h k l)	ϕ	S	n	E_{ads}	E_{att}	ε
acetone	(1 0 0)	1.000	1.440	18	-10.344	-33.590	0.887
	(1 1 0)	1.007	1.780	18	-11.466	-63.390	0.648
	(0 1 1)	0.882	1.700	18	-12.000	-97.320	0.370
	(1 1 -1)	1.436	1.580	18	-13.694	-97.380	0.638
ethanol	(1 0 0)	1.000	1.440	18	-10.600	-33.590	0.909
	(1 1 0)	1.259	1.780	18	-10.580	-63.390	0.748
	(0 1 1)	1.699	1.700	18	-9.750	-97.320	0.579
	(1 1 -1)	1.958	1.580	18	-13.300	-97.380	0.845

[a] All energies are in kcal mol^{-1}.

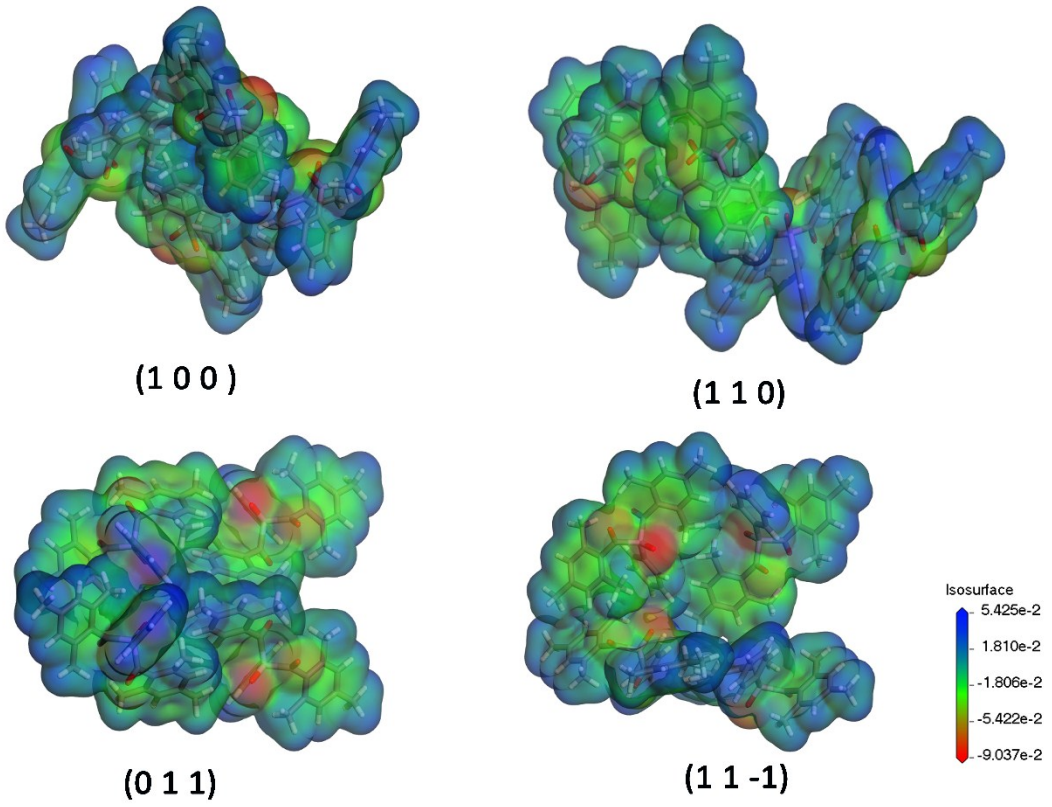


Fig. S1 Electrostatic potential (ESP) maps of important crystal faces.

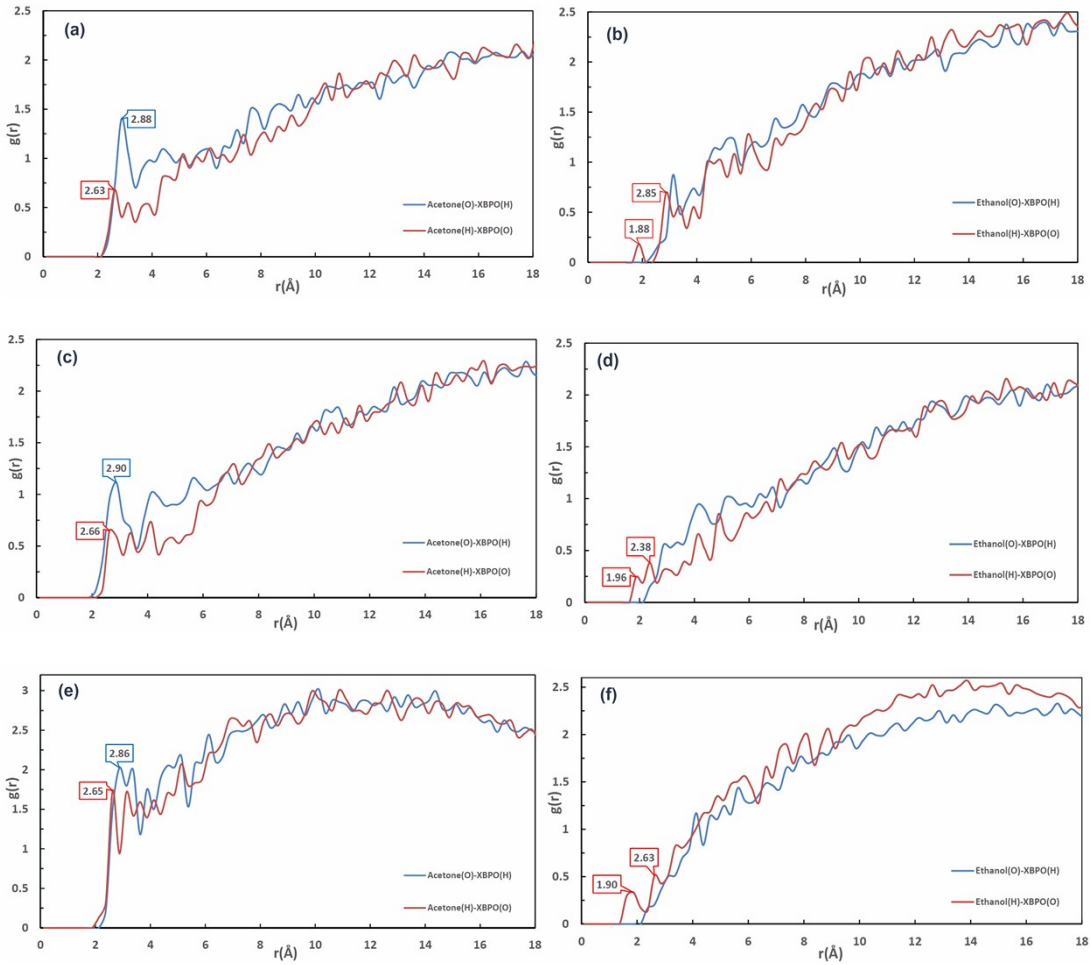
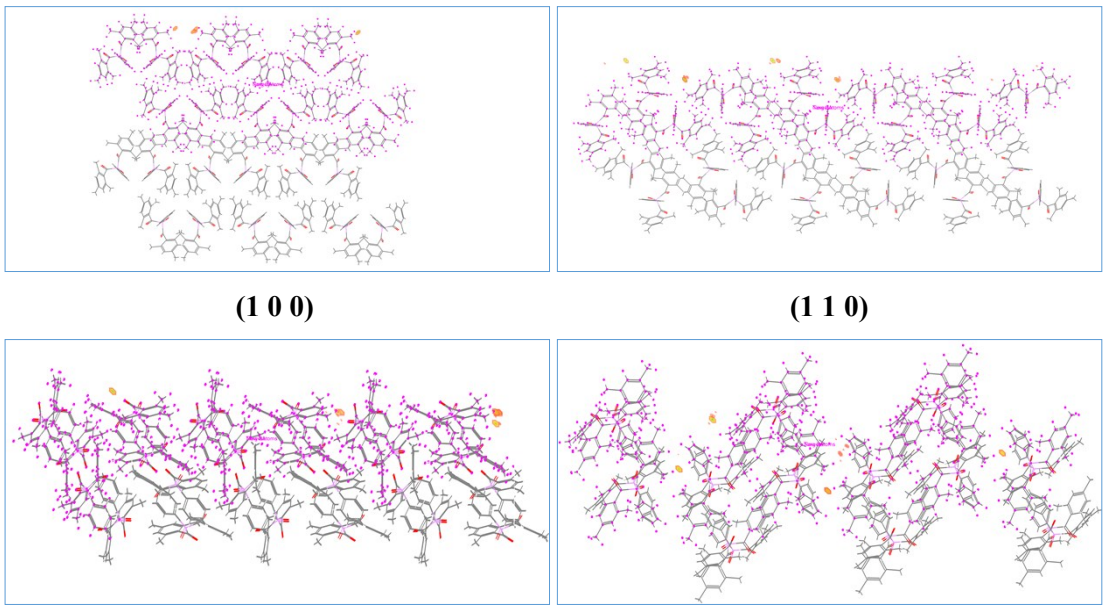


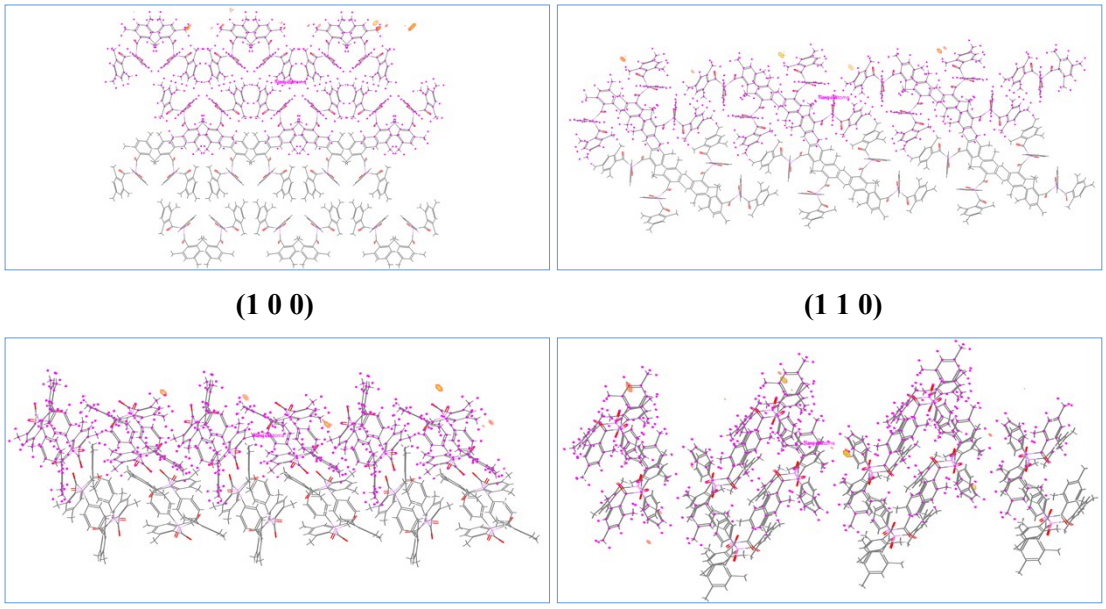
Fig. S2 The RDF analysis between the solvent molecules and the surface of XBPO crystal in acetone/ethanol solvents. (a)(b) Correspond to the surface (1 0 0); (c)(d) Correspond to the surface (1 1 0); (e)(f) Correspond to the surface (0 1 1).



(1 0 0) **(1 1 0)**

(0 1 1) **(1 1 -1)**

Fig. S3 The field of adsorption sites on different crystal faces (acetone molecule).



(1 0 0) **(1 1 0)**

(0 1 1) **(1 1 -1)**

Fig. S4 The field of adsorption sites on different crystal faces (ethanol molecule).

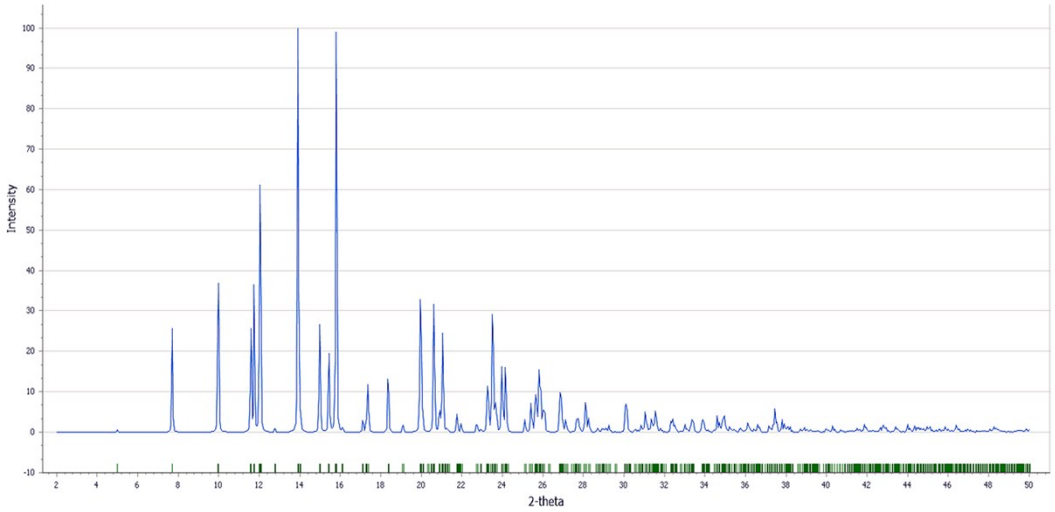


Fig. S5 The simulated pattern of the XBPO crystal.