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Supporting Information

Formation Mechanism of Liquid Inclusions in Dicumyl Peroxide Crystals

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According to Table S1, it was found that the COMPASS force field was suitable for the molecular dynamics (MD) simulation of the DCP crystal as the relative errors were less than 5% compared with the experimental results.

Table S1 Comparison of the experimental and optimized lattice parameters of DCP

Lattice parameter	*a* (Å)	*b* (Å)	*c* (Å)	*α* (°)	*β* (°)	*γ* (°)
Exp	10.040	7.477	21.016	90.00	90.00	90.00
COMPASS	9.591	7.412	21.801	90.00	90.00	90.00
Relative error (%)	-4.472	-0.869	3.735	0	0	0

Dicumyl peroxide PXRD analysis was performed on the DCP crystals were obtained by recrystallization from all experimental organic solvents. As shown in Figure S1, PXRD analysis confirmed that the crystal forms of DCP crystals with different habits were consistent.

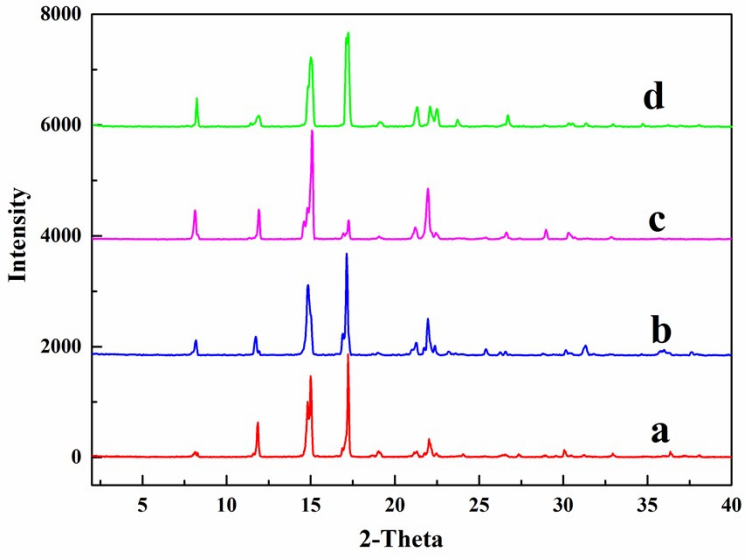

Fig S1. Powder x-ray diffraction patterns of DCP crystals: (a) original material, (b) habit I crystals, (c) habit II crystals, (d) habit III crystals.

Dicumyl peroxide PXRD analysis was performed on the crystals suspended in a saturated solution during the all experimental solvents. The experimental solvent included seven pure organic solvents and different ratios of ethanol-water binary solvents and DMF-water binary solvents. Figure S1 show the patterns of the Dicumyl peroxide PXRD analysis, where (i) ethanol-water mixed solvent represents the analysis results of the crystals in all mixed solvents, where (j) DMF-water mixed solvent represents the analysis results of the crystals in all mixed solvents.

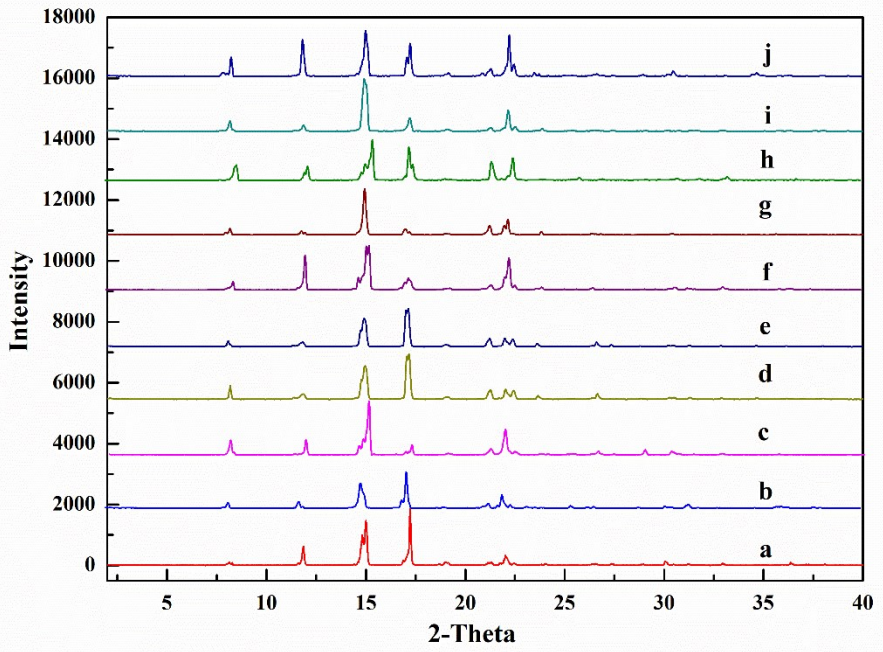

Figure S2. Powder x-ray diffraction patterns of undissolved dicumyl peroxide in different solvents. (a) original material; (b) methanol; (c) ethanol; (d) 1-propanol; (e) 2-propanol; (f) 1-butanol; (g) 2-butanol; (h) DMF; (i) ethanol-water mixed solvent; (j) DMF-water mixed solvent.