Supporting Information

Solvent effects on catechol crystal habits and aspect ratios: a combination of experiments and molecular dynamics simulation study

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**Table S1.** The cleaved depth and size of catechol crystal faces to form a simulation supercell.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Crystal Faces (h k l)** | ***dhkl*** | ***m*** | ***n*** | ***a\** (Å)** | ***b\**(Å)** | ***c\**(Å)** |
| (1 0 -1) | 2 | 6 | 3 | 33.328 | 32.907 | 20.529 |
| (1 0 1) | 3 | 2 | 6 | 32.804 | 33.328 | 25.027 |
| (0 1 1) | 4 | 4 | 3 | 38.349 | 34.677 | 29.126 |
| (1 1 0) | 4 | 4 | 3 | 40.548 | 33.241 | 27.117 |
| (0 0 2) | 3 | 4 | 6 | 38.349 | 33.328 | 21.717 |
| (1 1 -1) | 4 | 3 | 3 | 32.907 | 33.241 | 25.958 |

1 *a\**, *b\** and *c\** represents the parameter of the catechol supercell.

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**Figure S1.** The simulated XRD pattern of catechol crystal.

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**Figure S2.** The RDF analysis between catechol and methyl acetate on the (1 1 0) face.