Molecular Modelling on Variation of OH1 Crystal Morphology by Organic Solvents

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As a terahertz generating crystal, OH1(2-(3-hydroxystyryl)-5,5-dimethylcylcohex-2-enylidene) malonontirile) has the potential for various application. In crystallization process, its morphology can have a significant effect on downstream process and this crystal growth habit can be modified by solvents in some cases. In this work, variation of OH1 crystal morphology in organic solvents was studied by molecular modelling approach. Interaction energies between crystal molecules at each surface and solvent molecules were calculated by molecular dynamics simulation and geometry optimization. These energies were applied on attachment energy model for the prediction of morphology. As a result, polar organic solvents resulted in asymmetrical crystal growth habit because it has a strong interaction on (1 1 -1) surface and (1 3 -1) surface by hydrogen bonding. Weakly polar organic solvent had a specific interaction on polar surfaces but influenced almost symmetrically resulting plate-shape morphology. On the other hand, a relatively-high-aspect-ratio morphology was found in nonpolar solvent environment since growth of polar surfaces was almost not influenced. These results were confirmed by experimental work.