Molecular Modeling Study for Solvent Effect on Morphology of Succinic Acid Crystal

최인영, 김우식[1], 강정원†
고려대학교; [1]경희대학교
(jwkanag@korea.ac.kr†)

Crystal morphology is significant for the process design since it has a great impact on efficiency of downstream process in industrial crystallization process. The morphology of crystals grown from solution is mainly affected by the intrinsic properties of crystal or external effects such as solvent and addtives. In these days, molecular modeling methods has been applied for the prediction of crystal morphology and the investigation of solvent effects on the shape of a growing crystal. In this work, the influence of solvents on succinic acid crystal morphology was investigated by a systematic molecular modeling approach. The attachment energy method was applied with molecular dynamics simulation and energy minimization of solvent molecules on crystal faces. The attachment energies and interaction energies between solvents-solutes were calculated by Material Studio with COMPASS force-field, based on molecular mechanics theory. The succinic acid crystal morphology generated by molecular modeling methods exhibited the similar results of experimental observation. Furthermore, the major faces of a crystal shape was predicted and the effects of functional groups of solvents was identified in a systematic manner.