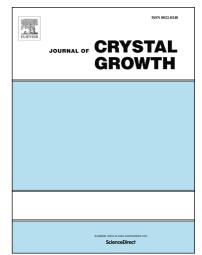
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Crystal Engineering of Ibuprofen Compounds: From Molecule to Crystal Structure to Morphology Prediction by Computational Simulation and Experimental Study

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Crystal Engineering of Ibuprofen Compounds: From Molecule to Crystal Structure to

Morphology Prediction by Computational Simulation and Experimental Study

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ABSTRACT:

We selected the crystal structures of ibuprofen with seven common space groups $(Cc, P2_1/c, P2_12_12_1, P2_1, Pbca, Pna2_1, and Pbcn)$, which was generated from ibuprofen molecule by molecular simulation. The predicted crystal structures of ibuprofen with space group $P2_1/c$ has the lowest total energy and the largest density, which is nearly indistinguishable with experimental result. In addition, the XRD

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