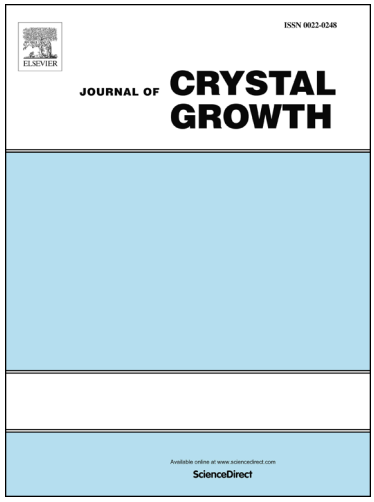

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ABSTRACT:

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