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Insights into the Molecular Mechanism underlying Polymorph Selection JEROME DELHOMMELLE, CAROLINE DESGRANGES, University of South Carolina — We use molecular simulations to study polymorph selection during the crystallization of charge-stabilized colloidal suspension. By modifying the conditions of crystallization, we invert the stability of two polymorphs and induce the formation of crystallites whose structure is predominantly that of the stable polymorph. However, our simulations reveal that kinetics play a major role not only during the nucleation step but also in the growth mechanism. The growth of post-critical crystallites of the stable polymorph proceeds through a complex mechanism involving the cross-nucleation of a third metastable polymorph followed by the conversion of this third polymorph into the stable structure.

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