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Stability of Polymeric Crystalline Polymorphs¹ DANIEL W. SINKOVITS, SANAT K. KUMAR, Columbia University — In the search for polymeric materials with novel properties, such as high dielectric constant and low loss, an important attribute of a material is its crystal structure. Most polymers can crystallize into multiple polymorphs whose properties vary. Therefore, the question of which polymorphs are thermodynamically preferred under what conditions is of great importance. We generate polymorphs using atomistic molecular dynamics simulations and tackle the question of stability using a combination of molecular dynamics and Monte Carlo techniques.

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