Computation of the Gibbs free energy difference between polymorphs[1] DANIEL W. SINKOVITS, SANAT K. KUMAR, Columbia University — Semi-crystalline polymers commonly crystallize into several different polymorphs; for example, the alpha and beta phases of isotactic polypropylene. While it is possible to favor particular polymorphs by kinetic means, such as with varying degrees of supercooling or through the use of different solvents in solution casting, we focus on the question of thermodynamic stability; that is, which polymorph possesses the lowest Gibbs free energy for a given temperature and pressure. We implement a version of the Bennett Acceptance Ratio method and find phase diagrams for several polymers. We also demonstrate agreement with phonon analysis in the quasi-harmonic approximation. The advantages and drawbacks of these methods will be discussed.

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