Free Energy-Based Monte Carlo Determination of a Model Microphase Former YUAN ZHUANG, Duke Univ, KAI ZHANG, Yale Univ, PATRICK CHARBONNEAU, Duke Univ — Determining the equilibrium phase behavior of microphase formers from particle-based simulations is particularly challenging because the occupancy of the various microphase features (clusters, layers, cylinders, etc.) fluctuates and varies from one state point to the next. Here, we compute the phase diagram of a schematic microphase former, the square well-linear model, using a novel free energy-based Monte Carlo simulation methodology. Our approach surmounts traditional equilibration difficulties by including modulated reference fields and developing the expanded isothermal-isobaric [N]PT ensemble. Our results for the square-well-linear model goes beyond other descriptions of the equilibrium phase behavior of simple microphase formers by revealing the complex thermodynamic interplay of various microphases with micelle formation and percolation.

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