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An integral method to compute Helmholtz free energies of crystalline solids[1] ZHIYUE LU, CHRISTOPHER JARZYNSKI, University of Maryland at College Park — We describe a method to compute the Helmholtz free energy of a crystalline solid by direct evaluation of the partition function. In the many-dimensional conformation space of all possible arrangements of N particles inside a periodic box, the energy landscape consists of localized islands corresponding to different solid phases. Calculating the partition function for a specific phase involves integrating over the corresponding island. Introducing a natural order parameter that quantifies the net displacement of particles from lattices sites, we write the partition function in terms of a one-dimensional integral along the order parameter, and evaluate this integral using umbrella sampling. We validate the method by computing free energies of both face-centered cubic (FCC) and hexagonal close-packed (HCP) hard sphere crystals with a precision of $10^{-5}k_BT$ per particle.

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Zhiyue Lu
University of Maryland at College Park

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