138h A New Method to Calculate the Melting Temperature of a Binary Mixture
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We present a new thermodynamic integration method that directly connects the liquid and the solid phases of a binary mixture by a reversible pathway. The method allows us to calculate the chemical potential difference between the two phases at a given state point. This information is then used to locate the solid-liquid coexistence points. We show that the melting temperatures predicted by our method agree well with those predicted by Gibbs-Duhem integration for a truncated and shifted Lennard-Jones system with a cutoff radius of 2.5σ. The method is simple, robust, and provides a very accurate estimate of the coexistence points.