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Melting Points via Pseudo-supercritical Path Monte Carlo Simulations: Carbon Dioxide and Benzene

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Abstract

The melting points of carbon dioxide and a newly developed benzene model are calculated via thermodynamic integration along a pseudo-supercritical path connecting the liquid and solid phases and subsequent multiple histogram reweighting using Monte Carlo simulations. For carbon dioxide, the melting point obtained here for the TraPPE model at a pressure of 10 atm agrees well with a previous estimate of the triple point temperature via Gibbs ensemble simulations with an explicit interface as well as the experimental data. For the TraPPE all-atom benzene model, slightly different values of the magnitude of the partial charges were explored to find a model that matches the experimental normal melting point.

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