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Gibbs-ensemble Monte Carlo simulations for binary mixtures

Armin Bergermann, Martin French, and Ronald Redmer

Institut für Physik, Universität Rostock, D-18057 Rostock, Germany

We explore the performance of the Gibbs-ensemble Monte Carlo simulation method by calculating the miscibility gap of H₂-He mixtures with analytical exponential-six potentials [1]. We calculate demixing curves for pressures up to 500 kbar and temperatures up to 1800 K. Our results are in good agreement with *ab initio* simulations in the non-dissociated region of the phase diagram. Next, we determine new parameters for the Stockmayer potential [2] to model the interactions in the H₂O-H₂O system for temperatures of 1000 K < *T* < 2000 K. The corresponding miscibility gap of H₂-H₂O mixtures was determined and we calculated demixing curves for pressures up to 150 kbar and temperatures up to 2000 K. Our results show reasonable agreement with previous experimental data of Bali *et al.* [3]. These results are important for interior and evolution models for ice giant planets [4].

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