

20th May 2021, 15:00 s.t. – 16:00

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AG Statistical Physics

Gibbs-ensemble Monte Carlo simulations for binary mixtures

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 500kbar and temperatures up to 1800K. Our results are in good agreement with *ab initio* simulations in the non-dissociated region of the phase diagram [3]. Next, we determine new parameters for the Stockmayer potential [3] to model the interactions in the H₂-H₂O system for temperatures of 1000K < T < 2000K. The corresponding miscibility gap of H₂-H₂O mixtures was determined and we calculated demixing curves for pressures up to 150kbar and temperatures up to 2000K. Our results show reasonable agreement with previous experimental data of Bali *et al* [4]. These results are important for interior and evolution models for ice giant planets because H₂-H₂O demixing would induce compositional gradients which could inhibit convection and, therefore, the cooling of those planets [5, 6].

References

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3. W. Stockmayer, J. Chem. Phys. **9**, S. 398-402 (1941)
4. E. Bali, A. Audétat and H. Keppler, Nature, **495**, 7440 (2013)
5. R. Helled, N. Nettelmann and T. Guillot, Space Sci. Rev., **216** (2020)
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