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# Miscibility gap of hydrogen-helium mixtures

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## Abstract

We calculate the high-pressure demixing phase diagram of hydrogen-helium mixtures [1], which is important for applications in planetary physics, in particular, for calculating the interior and evolution of gas giants. The separation of hydrogen and helium has long been proposed as a possible source of Saturn's excess luminosity: The initially hot planet cools down with increasing age and when the planetary isentrope intersects with the demixing region [2], helium-rich droplets can form and sink toward the planetary core, thus, acting as an additional source of heat; see, e.g., [3].

The region of demixing is observed from thermodynamic relations by computing the free enthalpy G(x,P,T) at constant pressure P and temperature T for different helium fractions x. We use finite-temperature density functional theory molecular dynamic simulations to obtain the equation of state for given volumes and temperatures. The non-ideal entropy of mixing is calculated using a combination of coupling-constant integration and thermodynamic integration of the equation of state.

The choice of an appropriate exchange-correlation (XC) functional is of paramount importance. It has been shown that standard approximations such as PBE lack the ability to adequately describe the metallization transition in hydrogen [4], which is directly connected to the H-He demixing. Functionals that take into account non-local correlations such as vdW-DF [5] are in better agreement with recent experiments [4]. Benchmarking studies with many XC functionals against QMC calculations suggest vdW-DF as an appropriate functional also for hydrogen-helium mixtures [6].

Here, we present a demixing phase diagram of H-He mixtures calculated with vdW-DF and compare with previous calculations derived with the PBE functional [7, 8]. Differences and implications for planetary physics are discussed, in particular, for the gas giants Jupiter and Saturn.

## References

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