Graduate School Seminar

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Statistische Physik

Miscibility gap of hydrogen-helium mixtures

Our focus is the calculation of a demixing phase diagram of hydrogen-helium mixtures for application in planetary and astrophysics.
Hydrogen-helium demixing has been proposed as a possible source of Saturn's excess luminosity: When the planetary isentrope enters the demixing region, helium-rich droplets can form and sink toward the planet's core, thus, acting as an additional source of heat.
Demixing is calculated 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 choice of an exchange-correlation (XC) functional, that captures the relevant physics, is of high importance. It has been shown that standard approximations lack the ability to adequately describe the hydrogen metallization, which is directly connected to the H-He demixing. Functionals, that take non-local correlations into account, e.g., vdW-DF [1], are in better agreement with experiments [2]. Benchmarking studies with many XC functionals against QMC calculations suggest vdW-DF as an appropriate functional also for hydrogen-helium mixtures [3].
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 [4]. Differences and implications for planetary physics are discussed.

[1] Dion et al., PRL 92, 246401 (2004)
[2] Knudson et al., Science 348, 1455 (2015)
[3] Clay et al., PRB 89, 184106 (2014)
[4] Lorenzen et al.,PRL 102, 115701 (2009)

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Slides: English

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