世纪物理情·系列讲座

A deep variational free energy approach to dense hydrogen

【报告人】

王磊

中科院物理所

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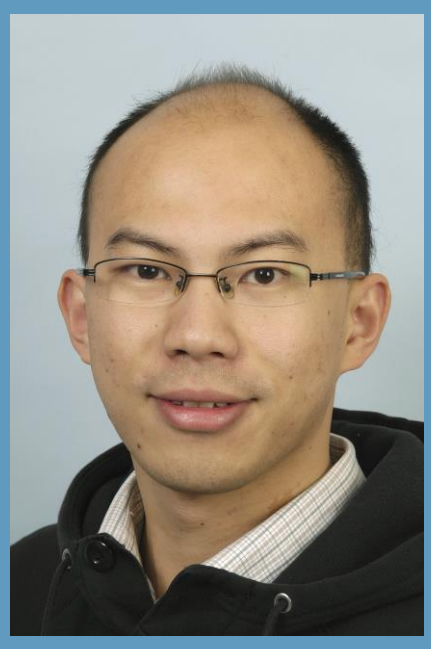
清华大学高等研究院

科学馆104报告厅

【摘要】

Dense hydrogen, the most abundant matter in the visible universe, exhibits a range of fascinating physical phenomena such as metallization and high-temperature superconductivity, with significant implications for planetary physics and nuclear fusion research. Accurate prediction of the equations of state and phase diagram of dense hydrogen has long been a challenge for computational methods. In this talk, we present a deep generative model-based variational free energy approach to tackle the problem of dense hydrogen, overcoming the limitations of traditional computational methods. Our approach employs a normalizing flow network to model the proton Boltzmann distribution and a fermionic neural network to model the electron wavefunction at given proton positions. The joint optimization of these two neural networks leads to a comparable variational free energy to previous coupled electron-ion Monte Carlo calculations. Our results suggest that hydrogen in planetary conditions is even denser than previously estimated using Monte Carlo and ab initio molecular dynamics methods. Having reliable computation of the equation of state for dense hydrogen, and in particular, direct access to its entropy and free energy, opens new opportunities in planetary modeling and high-pressure physics research.

【报告人简介】



王磊2006 年本科毕业于南京大学，2011 年在中国科学院物理研究所获得博士学位， 此后在苏黎世联邦理工学院从事计算量子物理的博士后研究，2016 年加入中科院物理所工作。王磊的主要研究兴趣是深度学习与量子多体计算。

主办单位:清华大学高等研究院