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Ab initio calculations of the equations of state for hydrogen, helium, and water and the relevance to the giant planets

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Since the interior structure of giant planets inside or outside our solar system cannot be probed directly by experiments, planetary models have been developed to gain further insight. Such models require accurate equations of state (EOS) for the major components (H, He, and heavier compounds like water) up to extreme thermodynamic conditions (pressures of several ten megabars and temperatures of more than ten thousand degrees Kelvin) [1]. Ab initio methods that combine finite temperature density functional theory (FT-DFT) for the electrons with classical molecular dynamics (MD) for the ions have proven to be a powerful tool to calculate such accurate EOS data. In addition, the FT-DFT-MD also generates structural information, transport and optical properties and, most important, information on phase diagrams and demixing regions. Based on our recently calculated ab initio data for H, He, and water, we derive interior models of Saturn and Jupiter and discuss the role of H-He demixing [2] and of the plasma phase transition in hydrogen on the planetary interiors. We also present new models for Uranus and Neptune which offer conditions to allow the formation of the exotic superionic phase of water [3]. The ab initio data can also be applied in planetary evolution scenarios and dynamo simulations of solar and extrasolar planets.

[1] J. J. Fortney, N. Nettelmann, Space Sci. Rev. 152, 423 (2010)
[2] W. Lorenzen, B. Holst, R. Redmer, Phys. Rev. Lett. 102, 115701 (2009)
[3] M. French, T. R. Mattsson, N. Nettelmann, R. Redmer, Phys. Rev. B 79, 054107 (2009)