# Water-ammonia mixtures at high pressures

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The interior of the Giant Planets Uranus and Neptune contains large amounts of water, ammonia and methane (referred to as ”planetary ices”). Many observable properties of these planets, such as luminosity, gravitational moments and magnetic fields, are thought to be determined by the physical and chemical properties of matter within this ice layer. Hence, the phase diagrams, equations of state and structural properties of these materials and their respective mixtures are of great interest.
We present equation of state data for water-ammonia mixtures at pressures up to several Mbar and in the temperature range from 500 K to 10000 K obtained by ab initio simulations based on density functional theory using the VASP code [1]. Furthermore, we investigate the impact of the complex chemistry on the fluid properties as well as exotic phases forming at these high pressures. In particular we discuss superionic phases, which have been predicted for the pure compounds water [2,3] and ammonia [2,4]. These superionic phases are characterized by highly mobile hydrogen ions in a lattice of oxygen and nitrogen ions, respectively, and might be present in the mixture as well.

[1] G. Kresse and J. Hafner, Phys. Rev. B, 47, 558 (1993).
[2] C. Cavazzoni et al., Science , 283, 44 (1999).
[3] M. French et al., Phys. Rev. B 79, 54107 (2009).
[4] M. Bethkenhagen et al., J. Chem. Phys. 138, 234504 (2013).