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## Molecular mixtures at high pressures

The interiors of the giant planets Uranus and Neptune are dominated by a mixture of the molecular compounds water, ammonia and methane. 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. [1]

In particular, the superionic phases of water and ammonia, characterized by highly mobile hydrogen ions diffusing through a lattice of oxygen and nitrogen ions, respectively, have gained much attention. For water, the influence of such a phase on the properties of the giant planets as well as on exoplanets has been discussed widely [2,3], while it is an open question how the properties of such a water layer change when other compounds are introduced.

To address this question we performed ab initio simulations based on density functional theory using the VASP code [4] for a variety of molecular mixtures starting with a 1:1 water-ammonia mixture. Heating up structures which we had found from evolutionary crystal prediction calculations with XtalOpt [5] we find superionic water-ammonia structures present up to several Mbar. Adding methane to the water-ammonia mixtures we observe amorphous structures of nitrogen and oxygen while carbon forms short chains. Evaluating the equation of state and structural properties such as diffusion coefficients and bond autocorrelation functions for varying mixing ratio we discuss general trends with respect to the N:O:C concentration. The obtained results are essential to construct new interior models for Uranus and Neptune as well as Neptunelike exoplanets. [6]

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