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Exploring complex chemical composition spaces of planetary ices

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The interiors of icy planets are thought to comprise H/He-rich atmospheres followed by vast 'hot ice'mantle regions and, possibly, small rocky cores. The 'hot ice'layers, the largest water reservoirs in planetary systems, are chemically very complex and while individual constituents (water, methane, ammonia) have been studied in great detail both computationally and experimentally, their mixtures are much less explored. However, molecular mixtures allow for chemical changes that can drastically alter their properties at specific conditions, with consequences for internal stratification, depth-density profiles, thermal conduction, convection, magnetism, etc.

In this talk I will discuss some of the recent computational progress in studies of complex molecular mixtures at extreme conditions, including 'hot ice'mixtures (such as ammonia-water), ad-mixtures of atmospheric materials (such as methane-hydrogen), and the structure of the full H-C-N-O quaternary chemical space near Neptune's core pressure conditions, as explored via unbiased crystal structure searching. I will show that planetary ice mixtures can exhibit properties not found in their constituting compounds, and argue that the full complexity of these mixtures needs to be considered to fully capture their behaviour.

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