



## Solubility of sodium chloride in superionic water ice

Jean-Alexis Hernandez and Razvan Caracas

École Normale Supérieure de Lyon, Lyon, France (jeanalexis.hernandez@ens-lyon.fr)

In icy planets, complex interactions are expected to occur at the interface between the rocky core and the icy mantle composed of mixtures based on water, methane, and ammonia [1, 2]. The hydration of the silicate layer produces salts (MgSO<sub>4</sub>, NaCl, KCl) that could mix with the ice, and change considerably its properties [3]. Here, we used first-principles molecular dynamics to investigate the stability and the properties of the binary system NaCl-H<sub>2</sub>O at the relevant thermodynamic conditions for planetary interiors up to ice giants. In these conditions, pure water ice undergoes several transitions that affect considerably its ionic conductivity and its elastic properties [4]. We calculated the Gibbs free energy of mixing along the NaCl-H<sub>2</sub>O binary by applying Boltzmann statistics to account for energy differences between configurations. We evaluated vibrational entropy from the vibrational spectra of the nuclei motion using the recently developed two phases thermodynamic memory function (2PT-MF) model for multicomponent systems [5, 6]. We show that the solubility of NaCl in water ice at 1600 K is less than 0.78 mol%. We find that salty ices present an extended superionic domain toward high pressures in comparison to pure water ice. Finally, we predict that the complete symmetrization of the hydrogen bonds (i.e. transition to ice X) occurs at higher pressure than in pure water ice, as observed in LiCl doped water ice at ambient temperature [7].

### References:

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