**Title:** Simulations of water and aqueous solutions under extreme conditions: the important role of molecular dynamics simulations

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**Abstract:**

Water is a complex system where computer science plays a crucial role. Computer molecular dynamics simulations in particular are pivotal to study the behavior of water and aqueous solutions under extreme conditions. Especially in the supercooled region that is to-date only partially accessed by experiments. I will show water systems where computer simulations show results in line with experiments and produce further results in regions of the phase diagram not explored so far by experiments. I will show results on thermodynamics, slow dynamics and structure upon cooling of bulk water, and water in solutions with inorganic and organic solutes. The results that I will discuss are of interest also for outer planets science, and in particular for the research about water on Mars, and for cryoprotection techniques.

**Keywords**: Supercooled water (1); Computer simulations (2); aqueous solutions (3).

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