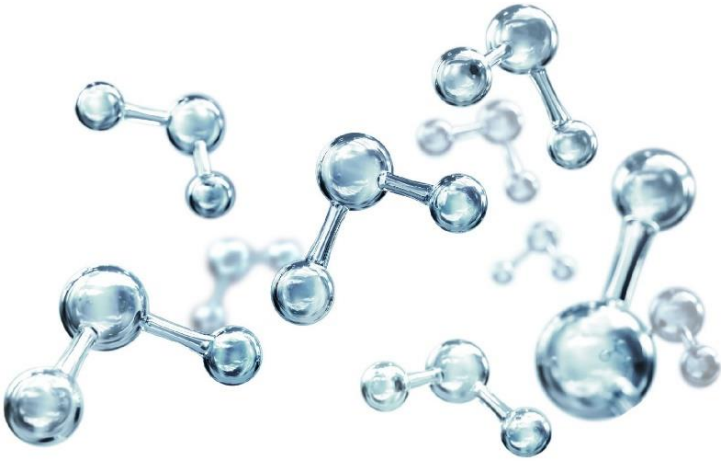
Seminar

CMWS Centre for Molecular Water Science

10th of February 2022
17:00 h

Zoom Virtual Meeting:

https://desy.zoom.us/j/84703564086
Meeting-ID: 847 0356 4086
Password: 570173



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The phase behavior of supercooled water: Recent computational results

Water plays a central role in the physical and chemical processes that sustain life as we know it. Its ubiquity and importance notwithstanding, there remain major open questions concerning the microscopic origin and thermodynamic consequences of water's physical properties, which are anomalous by comparison to those of most other liquids. Water's oddities become more pronounced at low temperatures, especially in the supercooled regime, where the liquid is metastable with respect to crystallization. The existence of a first-order phase transition between two liquid forms of water, terminating at a critical point under deeply supercooled conditions, has been proposed as a thermodynamically consistent way of interpreting experimental observations (Mishima and Stanley, Nature, 396, 329, 1998). I will present recent computational results on metastable criticality in realistic models of water (Debenedetti et al., Science, 369, 289, 2020), supercooled water thermodynamics probed with an ab-initio deep neural network model (Gartner et al., PNAS, 117, 26040, 2020), and the relationship between the long-range structure of water glasses and criticality (Gartner et al., Nature Communications, 12, 3398, 2021). These studies are consistent with the existence of a second, metastable critical point in water.