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Phase transitions and critical phenomena of ice under high pressure

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Water distributes ubiquitously among the solar system and outer space in a wide variety of solid forms, i.e. more than ten kinds of crystalline ice, two types of amorphous ice, and clathrate hydrates. These polymorphs often play crucial roles in the planetary geology. Diversity of the stable ices and hydrates also suggests the existence of the various kinds of stable and metastable phases yet to be discovered [1]. Computer simulations and the theoretical treatments are useful to explore them. In this talk, we introduce the phase transitions of ice VII, which is one of the highest-pressure ice phases. The melting curve of ice VII to high-pressure liquid water has not been settled by experiments. We have proposed the intervention of a plastic phase of ice (plastic ice) between ice VII and liquid water, based on molecular dynamics (MD) simulations and the free energy calculations [2], which enables to account for large gaps among the various experimental curves of ice VII. In plastic ice, the water molecules are fixed at the lattice points, while they rotate freely. Interestingly, our additional survey by large-scale MD simulations elucidates that the phase transition between ice VII and plastic ice is first-order at low pressure as it was already predicted, while it is found to be second-order at higher pressures, where a tricritical point joins these phase boundaries together [3]. The critical fluctuations may give a clue for determining the phase boundary experimentally. We also argue about the phase transition dynamics of liquid water to ice VII at their direct phase boundary where metastable plastic ice phase plays an important role.

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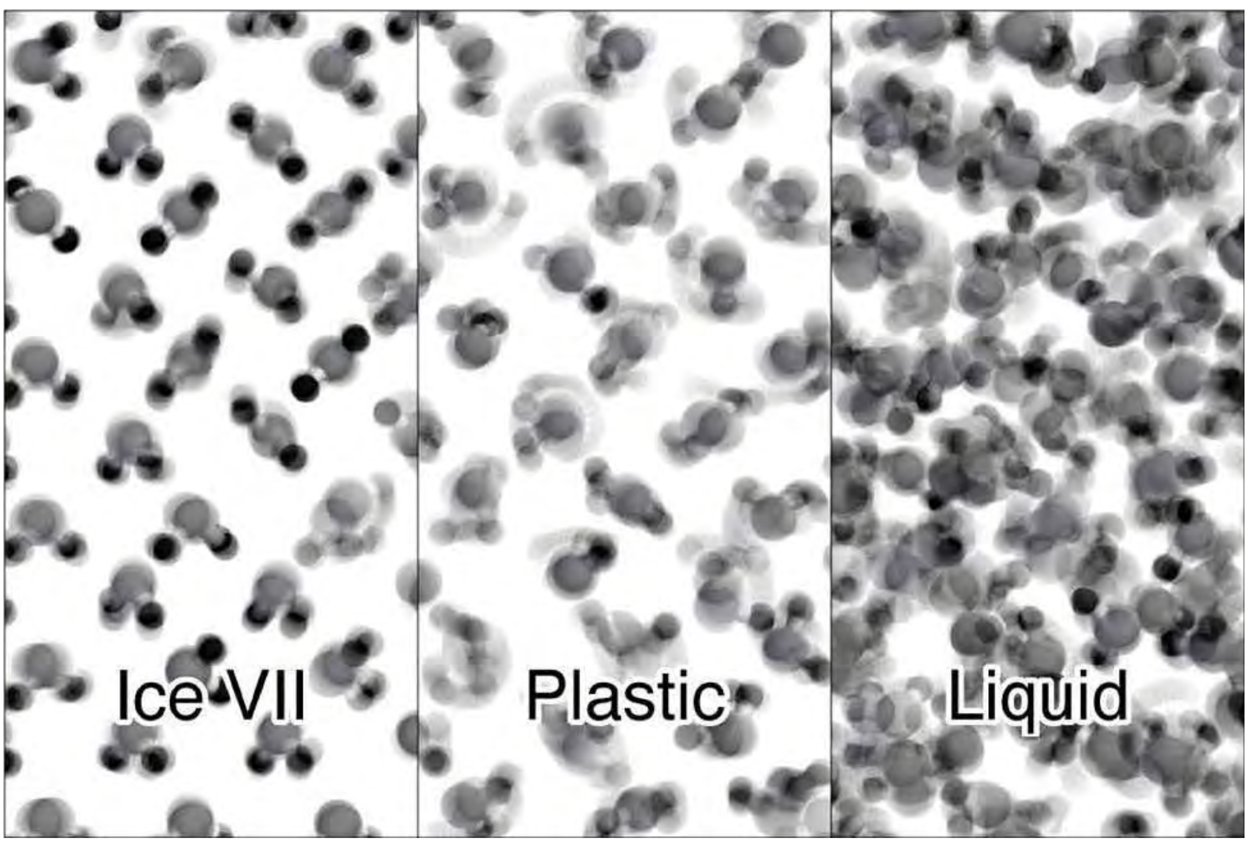

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