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# New insights into the behavior of water ices VII and VIII under extreme pressure and temperature

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We examine the origin of longstanding anomalies in the dense solid phases of $H_2O$ ices VII, VIII, and X using a combination of first-principles methods. We propose the existence of a ferroelectric phase, which is competitive with the established antiferroelectric ice VIII form under pressure. The existence of domains of the ferroelectric form explains previously observed splittings in diffraction data and the appearance of new bands in vibrational spectra starting above 10 GPa. The ferroelectric form is stabilized by density and is accompanied by the onset of spontaneous polarization. The presence of local electric fields triggers the preferential parallel orientation of the water molecules in the structure, which could be stabilized in bulk using new high-pressure techniques.

We analyze the behavior of ice VII at high temperature over a wide pressure range from large-scale molecular-dynamics calculations. We compute its equation of state along two isotherms. We look at the energetic cost of the spontaneous hydrogen hopping in the structure, and provide insights about the formation of the superionic form of water at high temperatures.