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Entropy and phase diagram of warm dense water MARTIN FRENCH, Universität Rostock, MICHAEL DESJARLAIS, Sandia National Laboratories, RONALD REDMER, Universität Rostock — Under conditions typical for the interiors of Neptune-like planets, water can occur not only as a fluid phase, but also form superionic states or the solid ices VII and X. Here we employ density functional theory (DFT) in combination with molecular dynamics (MD) simulations to construct thermodynamic potentials for the ices VII and X and for the superionic phases with bcc and fcc oxygen lattices. This allows us to determine boundaries between the phases directly from their thermodynamic functions. In doing so, it is necessary to calculate the entropy from the DFT-MD simulations, which is done with the 2PT-MF method [1] generalized to multi-component systems. In the case of ices VII and X, we develop an analytic expression for the free energy using a multi-stage fitting procedure of DFT-MD data [2]. The respective equation of state agrees well with experiments. The calculated phase boundary between the ices and the superionic phase is consistent with that obtained directly from heating and cooling DFT-MD simulations.

[1] M. P. Desjarlais, Phys. Rev. E 88, 062145 (2013)
[2] M. French, R. Redmer, Phys. Rev. B 91, 014308 (2015)

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