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The Phase Diagram of Superionic Ice¹ JIMING SUN, Phys Dept, Princeton Univ, BRYAN CLARK, Phys Dept, University of Illinois at Urbana-Champaign, ROBERTO CAR, Phys Dept and Chem Dept, Princeton Univ — Using the variable cell Car-Parrinello molecular dynamics method, we study the phase diagram of superionic ice from 200GPa to 2.5TPa. We present evidence that at very high pressure the FCC structure of the oxygen sublattice [1] may become unstable allowing for a new superionic ice phase, in which the oxygen sublattice takes the P21 structure found in zero-temperature total energy calculations [2]. We also report on how the melting temperature of the hydrogen sublattice is affected by this new crystalline structure of the oxygen sublattice.

[1] Hugh F. Wilson, Michael L. Wong, and Burkhard Militzer. Superionic to superionic phase change in water: Consequences for the interiors of uranus and neptune. *Phys. Rev. Lett.*,110:151102, Apr 2013.

[2] Andreas Hermann, N. W. Ashcroft, and Roald Hoffmann. High pressure ices. *Proceedings of the National Academy of Sciences*, 109(3):745-750, 2012.

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