

Abstract Submitted
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New ultrahigh pressure phases of H₂O ice predicted using an adaptive genetic algorithm¹ MIN JI, CAI-ZHUANG WANG, Iowa State University, KOICHIRO UMEMOTO, University of Minnesota, KAI-MING HO, Iowa State University, RENATA WENTZCOVITCH, University of Minnesota — We propose three new phases of H₂O under ultrahigh pressure. Our structural search was performed using an adaptive genetic algorithm which allows an extensive exploration of crystal structure at density functional theory(DFT) accuracy. The new sequence of pressure-induced transitions beyond ice X at 0 K should be ice X → Pbcm → Pbca → Pmc2₁ → P2₁ → P2₁/c phases. Across the Pmc2₁-P2₁ transition, the coordination number of oxygen increases from 4 to 5 with a significant increase of density. All stable crystalline phases have nonmetallic band structures up to 7 TPa.

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