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The volume isotope effect in ice under high pressure¹ STEFANO DE GIRONCOLI, Scuola Internazionale Superiore di Studi Avanzati (SISSA) and CNR-IOM DEMOCRITOS Simulation Centre, KOICHIRO UMEMOTO, Department of Earth Sciences, University of Minnesota, RENATA WENTZCOVITCH, Department of Chemical Engineering and Materials Science, University of Minnesota — The volume isotope effect (VIE) in ice has recently received considerable attention [1,2]. Ice Ih and XI, prototypical forms of low-pressure ice, have anomalous VIE, i.e., the volume of D₂O (V_{D_2O}) is larger than that of H₂O (V_{H_2O}) [1]. In contrast, the VIE in ice VIII at 0 GPa was reported to be normal, i.e., $V_{D_2O} < V_{H_2O}$ [2]. Here we clarify the origin of this behavior in different forms of ice. Furthermore, we predict a reversal in the VIE in ice VIII under high pressure. [1] B. Pamuk et al., Phys. Rev. Lett. 108, 193003 (2012). [2] E. D. Murray and G. Galli, Phys. Rev. Lett. 108, 105502 (2012).

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