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Metallic Phase of Water Ice Predicted at Megabar Pressures[1]
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We predict water ice to attain two new crystal structures with Pbca and Cmcm symmetry at 7.6 and 15.5 Mbar, respectively [Phys. Rev. Lett. 105 (2010) 195701]. With density functional calculations, we analyze the structural and electronic properties of these phases at zero temperature. The Pbca phase, like the known high-pressure ice phases VII, VIII, X and Pbcm, is insulating and consists of two interpenetrating hydrogen bonded networks, but the Cmcm phase is metallic and consists of corrugated sheets of H and O atoms. The H atoms are squeezed into octahedral positions between next-nearest O atoms while they occupy tetrahedral positions between nearest O atoms in lower-pressure phases. Our predictions may be testable with ramp compression experiments that can reach megabar pressures at lower temperatures than conventional shock wave experiments. The predicted insulator-to-metal transition would lead to an increase in reflectivity that can be measured with spectroscopic techniques.

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