Understanding Ice

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Frozen water has abnormally low compressibility and applying pressure decreases rather than increases the critical temperature for phase transitions.

Chang Sun, Nanyang Technological University, Singapore, and colleagues show that the anomalities of ice under pressure are due to Coulomb repulsion between bonding and non-bonding electron pairs. They have developed a method to simulate these properties accurately.

The key to their model is in considering O···H–O as the basic structural unit of ice. The repulsion between the lone pair and bonding pair causes the O···H hydrogen bond to shorten and the O–H real bond to lengthen. At sufficiently high pressure, the hydrogen bond and real bond become equivalent in length. The change in binding energy of the real bond dominates, causing the observed effects on physical quantities as it lengthens and weakens.

This model works better for the system than commonly used rigid non-polarizable models, as they have a fixed molecular geometry and cannot intrinsically account for changes in the molecular geometry.

The hidden force opposing ice compression,
C. Q. Sun, X. Zhang, W. Zheng,
Chem. Sci. **2012**.
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