

Supplementary Information: Thermal Conductivity of ice polymorphs: a computational study

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I. STRUCTURE OF ICE IH, VI, AND VII

In this work, we have carried out molecular dynamics simulations for ice Ih, VI, and VII, which are defined by the structures presented in Fig. S 1:

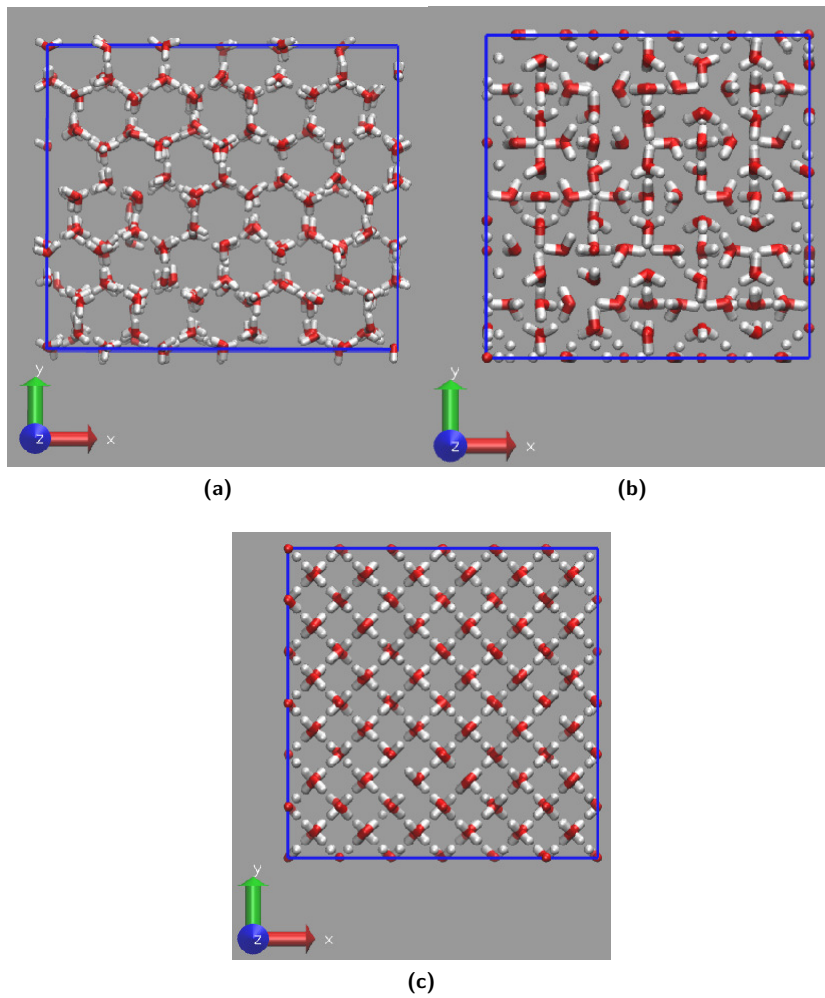


FIG. 1. Crystallographic structures for Ice Ih (a), VI (b), and VII (c). The molecule of water is represented by licorice visualization using VMD software [1]. The red part is the oxygen atoms and the white region corresponds to hydrogen atoms. The simulation box is highlighted using a solid blue line. The 3D projection of the structure in all cases is on the X-Y plane.

II. THERMAL CONDUCTIVITY FOR ICE IH AND VI

We plot in this section of the supplementary information the results of density, pressure and thermal conductivity for Ice Ih and VI. Those values are collected on Table 2 of main text and now plotted in Fig. S 2 and Fig. S 3.

[1] W. Humphrey, A. Dalke and K. Schulten, *Journal of Molecular Graphics*, 1996, **14**, 33–38.

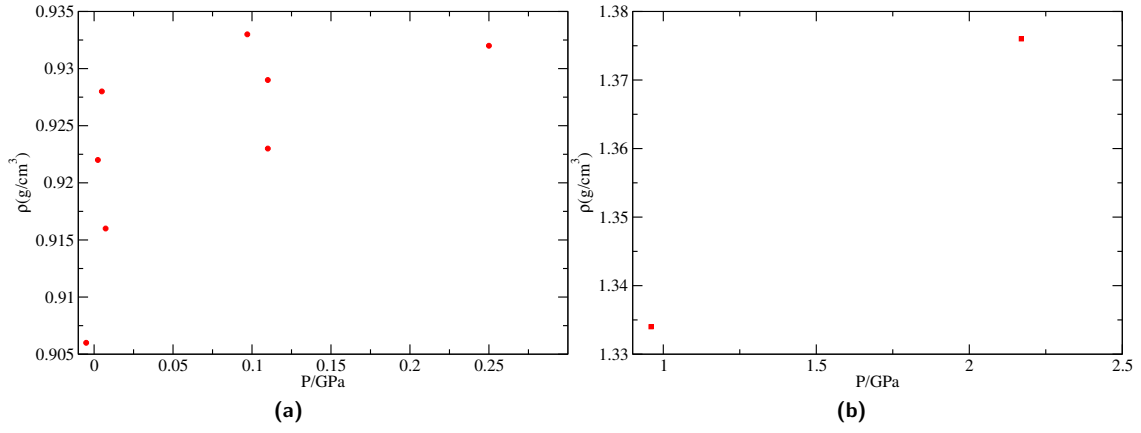


FIG. 2. (a) Density results for Ice Ih plotted with pressure. The solid red dots represents the value of density versus pressure for TIP4P/Ice water model. The thermodynamics state collected in Table 2 of main text are plotted in this figure. (b) Density results for Ice VI plotted with pressure. The solid red squares are the value of density versus pressure for TIP4P/Ice water model. The thermodynamics state collected in Table 2 of main text are plotted in this figure.

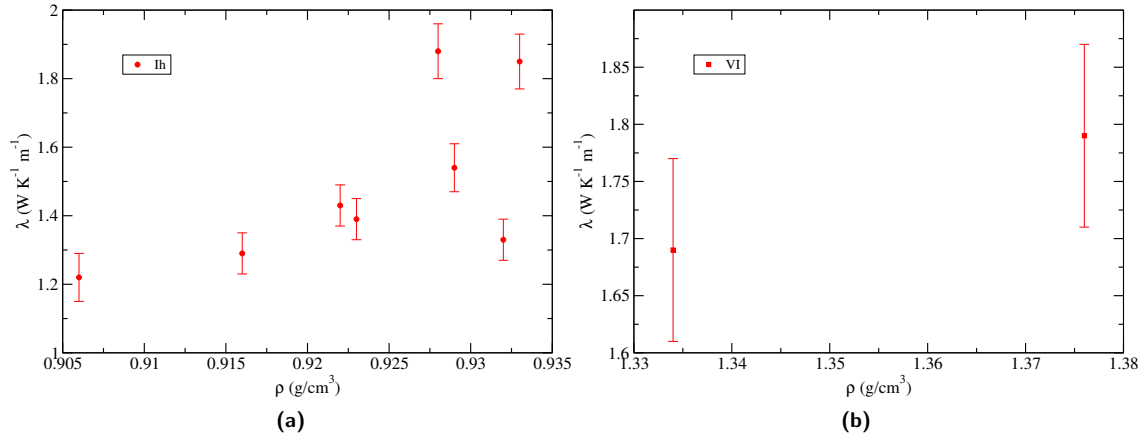


FIG. 3. (a) Thermal conductivity versus density for Ice Ih. The solid red dots represents the value of λ versus ρ for TIP4P/Ice water model. Data from Table 2 of main text. (b) Thermal conductivity with density for Ice VI. The solid red squares are the value of λ versus ρ for TIP4P/Ice water model. Data from Table 2 of main text.