2D-confined water. Phases and dielectric response

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Two-dimensionally confined water to 0.8 nm of width was studied by means of molecular dynamics simulations using both empirical force fields (TIP4P 2005), and first-principles forces, following intriguing findings on melting lines of different character (see e.g. Ref [1]). The Structural and dynamical properties will be reviewed for the various phases as well as the response to perpendicular electric fields, for varying lateral pressure and temperature. The anomalously low perpendicular dielectric response observed in Ref. [2] is addressed. It had already been predicted from simulations (see e.g. Refs [3,4]), but not as extremely low as measured. The response is here found to vary relatively little with lateral pressure, with a very slight increase of the effective dielectric constant towards the transition between the liquid and the hexatic phase. The ionic vs electronic response will be discussed.

REFERENCES

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FIGURES

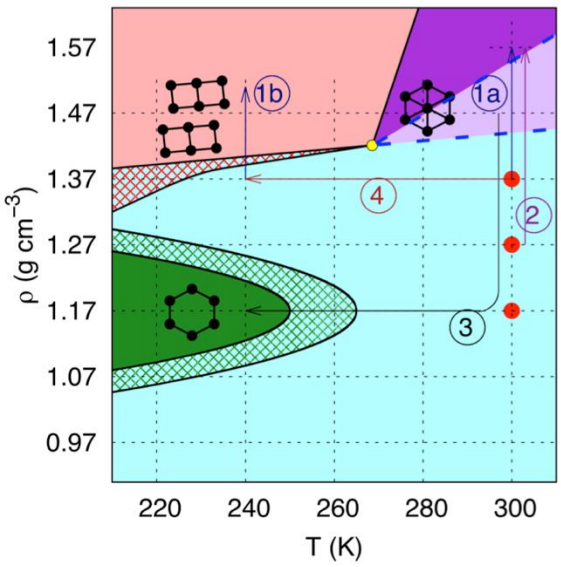

Figure 1: Density-temperature phase diagram for water confined to two dimensions to a thickness of 0.8 nm (bilayer water). Blue indicates the liquid, green and orange indicate solid phases, and light/dark purple indicate a plastic phase in which oxygens order (orientationally or translationally) but hydrogen atoms do not.