

The Dielectric Constant of Ice

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The dielectric properties of materials can be exploited to great advantage in many electronic devices. Furthermore, the dielectric constant of solvents is a crucial property determining the solubility of electrolytes. However, calculation of the dielectric susceptibility by means of computer simulations has been a great challenge for many years. On the one hand, the electromagnetic boundary conditions considered may affect the output considerably and need to be carefully implemented. On the other hand, dielectric relaxation is usually a very slow process which required extremely long simulation times. This sampling problem is essentially unsurmountable when one considers condensed phases with very stiff directional forces, such as ice. The random hydrogen bond network in such cases has relaxation times which are extremely slow, to the point that the ordered phase of pure ice at ambient pressure has never been observed. In this work we exploit a recently developed algorithm for the sampling of hydrogen bond networks in order to study the dielectric susceptibility of ice. We will report results for several ice models and study the anisotropy of the dielectric constant, which is found to be very large at certain conditions.