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Polar nanoregions in water - a study of the dielectric properties of TIP4P/2005, TIP4P2005f and TTM3F[1] DANIEL ELTON, MARIVI FERNANDEZ-SERRA, State Univ of NY- Stony Brook — Using molecular dynamics simulation we present a critical comparison of the dielectric properties of three models of water - TIP4P/2005, TIP4P/2005f and TTM3F. Dipole spatial correlation is measured using the distance dependent Kirkwood function along with one dimensional and two dimensional dipole correlation functions. We find that the introduction of flexibility alone does not significantly affect dipole correlation and only affects $\varepsilon(\omega)$ at high frequencies. By contrast the introduction of polarizability increases dipole correlation and yields a more accurate $\varepsilon(\omega)$. Additionally the introduction of polarizability creates temperature dependence in the dipole moment even at fixed density, yielding a more accurate value for $d\varepsilon/dT$ compared to non-polarizable models. To understand the physical origin of the dielectric properties of water we make analogies to the physics of polar nanoregions (PNRs) in relaxor ferroelectric materials. We show that $\varepsilon(\omega, T)$ and $\tau_D(T)$ for water have striking similarities with relaxor ferroelectrics, a class of materials characterized by large frequency dispersion in $\varepsilon(\omega, T)$, VFT behaviour in $\tau_D(T)$, and the existence of PNRs.

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