Dielectric constant of confined water

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Dielectric constant and charge distribution of confined Tip4p/2005 and OPC water models are calculated. Molecular dynamics was performed in a canonical ensemble (NVT) for systems consisting of 700 to 3000 water molecules. Dielectric constant was calculated by the dispersion of total dipole moment of water system. Calculations were performed using the *Mdtraj* library [1]. Hexagonal boron nitride BN (the BN model is described in [2]) sheets were placed parallel in the $x - y$ plane with periodicity in both directions, and z is the confined direction. Water was confined between these sheets. For each simulation with a different distance between the BN sheets, the dielectric constant of water was calculated. It depends straightly on the confinement size. While the dielectric constant of water under normal conditions for Tip4p/2005 potential is 78, under confinement significantly decreases up to 2. Obtained tenfold decrease in the dielectric constant of confined water corresponds to experimental [3] and computational [4] studies. A utilized method of modelling confined water can be used to predict the dielectric properties of water and other liquids at nanoscales.

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