

Water Polarization under Thermal Gradients

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We investigate the response of bulk liquid water to a temperature gradient using nonequilibrium molecular dynamics simulations. It is shown that the thermal gradient polarizes water in the direction of the gradient, leading to a non-negligible electrostatic field whose origin lies in the water reorientation under nonequilibrium conditions. The dependence of the magnitude of the electrostatic field with the temperature gradient is in agreement with nonequilibrium thermodynamics theory. We conclude that temperature gradients of the order of 10^8 K/m could result in fairly large polarizations $\sim 10^6$ V/m.