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Polarization as a field variable from molecular dynamics simulations KRANTHI K. MANDADAPU, JEREMY TEMPLETON, JONATHAN LEE, Sandia National Laboratories — In this talk, we show that polarization density, an important quantity in electromagnetism, can be obtained from molecular dynamics simulations. We show that the Irving and Kirkwood procedure used for obtaining stresses and heat fluxes in terms of the microscopic quantities can be extended to the case of electrostatics where the macroscopic electrostatic equation can be derived starting with the microscopic electrostatic equation, microscopic density of charges and using a phase-space distribution function and a suitable localization function. As a result, we obtain an expression for polarization density as a field variable in terms of the microscopic dipole moments and quadrupole moments and higher order terms depending upon the degree of the polynomial used for the localization function. Finally, we apply this method to obtain the dielectric constant of bulk water and to study the polarization effects in electric double layer calculations. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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