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Real Space Alternatives to the Ewald: Shifted Electrostatics for Multipoles MADAN LAMICHHANE, THOMAS PARSONS, KATHIE NEWMAN, J. DANIEL GEZELTER, Univ of Notre Dame — We have developed three real-space methods for computing electrostatic interactions in Molecular Dynamics (MD): Gradient Shifted Force (GSF), Shifted Potential (SP), and Taylor Shifted Force (TSF) [1]. Electrostatic interaction energies, forces, and torques of the molecules obtained from these methods were tested against an analytical as well as a reference method in a variety of condensed phase environments. Tests show that electrostatic energies, forces, and torques evaluated from our real-space methods show excellent agreement with the computationally expensive Ewald method. Total energy is conserved in molecular systems interacting using GSF and TSF methods. Different structural and dynamical properties of the multipolar fluids have been investigated. Recently, we have developed methods for evaluating dielectric properties for dipolar and quadrupolar fluids. Results for the dielectric constant of dipolar and quadrupolar fluids evaluated using the fluctuation and perturbation method will also be discussed. [1] M. Lamichhane *et al.,* J. Chem. Phys **141**, 134109 (2014); **141**, 134110 (2014).

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