Multipolar Force Fields in Chemical and Biological Simulations

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Conventional force fields use point charges to represent the electrostatics between interacting sites. Such a procedure is economical but for certain applications the accuracy is not sufficient. In particular for dynamics in spatially constrained environments anisotropic components of the interactions become important. Also, for small molecules with vanishing low-order multipoles, inclusion of higher multipoles becomes mandatory. In my presentation I will discuss applications of multipolar force fields to infrared spectroscopy and vibrational relaxation. Implications for the interpretation of experimental data will also be discussed.