

MAR08-2007-000294

Abstract for an Invited Paper
for the MAR08 Meeting of
the American Physical Society

Development of a polarizable force field based on the classical Drude oscillator¹

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Empirical force field development requires a systematic approach allowing for the development of a practical potential energy function and optimization of physically realistic parameters that reproduce a range of target data. Ongoing efforts in our laboratory include the development of a polarizable force field based on the classical Drude oscillator for a range of molecules representative of biological systems. A central theme in these efforts is the accurate treatment of both atomic interactions as well as condensed phase properties. To achieve this goal extensions of the energy function have been implemented and parameter optimization has been performed targeting a variety of quantum mechanical results and experimental condensed phase properties. An overview of these studies will be presented.

¹Financial support from the NIH (GM051501 and GM072558) is acknowledged.