

Achieving Post-Hartree-Fock Quality with Force Fields: A Systematic Attempt Through Force Matching

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Room 9341

Molecular simulation is an increasingly powerful tool for elucidating microscopic mechanisms of many physical, chemical and biological processes. The most accurate simulations use electronic structure methods to calculate forces on the atoms to drive the system evolution. Accurate electronic structure methods are very expensive. Even on the fastest super-computer, electronic structure methods are restricted to system sizes of less than 1000 atoms. In order to study systems at a much larger scale, empirical force fields are frequently used to describe the potential energy landscape. However, empirical force fields are usually not very accurate when compared with electronic structure methods. We developed the adaptive force matching (AFM) method that can be used to create force fields that are as accurate as electronic structure methods but without the associated high computational cost. We demonstrated the creation and refinement of accurate force fields for water following the AFM method. We showed that the AFM method can be used to systematically evaluate the importance of force field terms allowing us to use a minimal number of terms to achieve the best accuracy.

Theoretical Chemistry Institute Seminar Series