Reproducing high accuracy QM interactions via empirical force fields

Amin Alibakhshi

Department of Theoretical Chemistry, Christian-Albrechts University Kiel
(alibakhshi@pctc.uni-kiel.de)

Reliable and accurate evaluation of inter and intra-atomic interactions is one of the key steps in majority of molecular modeling approaches. Although these interactions can be precisely evaluated via high quality ab initio methods, the computational costs of such approaches specially for large systems has made applying empirical force fields still inevitable.

The empirical force fields typically fractionize the total energy of a molecule into smaller components such as bond stretching, angle and torsional bending and non-bonded interactions and evaluate each one of these energy terms via simple algebraic and empirical expressions. The conventional approaches of parametrizing such empirical force fields typically rely on transferability of force field parameters and determining those parameters such that they reproduce one or few bulk properties of the ensemble as accurate as possible. Nevertheless, remarkable inaccuracies inherent in such parameterization approaches reported in many recent studies has been the motivation of proposing next generation force fields e.g. machine learning based and ab initio derived force fields as well as more rigorous system specific parameterization strategies e.g. via the force matching technique [1].

In the present study we evaluated the performance of several conventional and more rigorous recently proposed empirical force fields in reproducing high accuracy QM interactions. As a benchmark, we carried out QM computations for 1500 configurations of boric acid and borate solvated in a small cluster of 64 water molecules. Each force field was parameterized by force matching technique to reproduce the reference QM forces. The studied configurations were extracted from molecular dynamics snapshots and selected such that they cover a wide combination of various force field variables. According to the results, none of the conventional force fields could reproduce QM forces with average unsigned relative error more accurate than 104%. Nevertheless, through a new empirical force field introduced in the present study which is a slightly modified version of a robust reactive force field recently developed in our group [2], we could achieve 8% accuracy in average unsigned relative error of evaluated forces.

1. Steffen, J. and B. Hartke, *Cheap but accurate calculation of chemical reaction rate constants from ab initio data, via system-specific, black-box force fields.* The Journal of chemical physics, 2017. **147**(16): p. 161701.
2. Hartke, B. and S. Grimme, *Reactive force fields made simple.* Physical Chemistry Chemical Physics, 2015. **17**(26): p. 16715-16718.