

Development of a charge-implicit ReaxFF potential for describing interactions in organic systems

Computer simulations allow for mimicking and explaining phenomena which cannot be examined by any experimental approach. For example, some processes are so fast that it is not possible to detect them experimentally. Molecular dynamics is one of the best tools which can be used for analysis of such phenomena. However, in order to recreate reality by computer simulations a description of interactions among atoms is required. The better the description (called a force field or a potential) is, the better is the simulation in reflecting reality.

One of the most important topics of modern chemistry is modelling of chemical reactions. One of the best potentials for this goal is ReaxFF. This potential has many advantages, but it is not free from some drawbacks. Its largest disadvantage is a low speed of computations, which drastically restricts sizes of systems, which can be simulated in a reasonable time. Our goal is to create a new version of this potential, which will be significantly faster. On the way we will try to solve its other problems too. For example, in the present ReaxFF potential atoms can move through each other if their kinetic energy is high enough. Such a phenomenon does not occur in nature and it restricts a utilization of the ReaxFF to describe low-energy collisions. However, in our world an enormous number of phenomena occurs with high energies. Such processes cannot be described by the present ReaxFF potential.

In order to increase speed of computation we will change a way of calculating electrostatic interactions. Instead of a tedious procedure of charge equilibration on each atom in a system, and explicit calculation of electrostatic interactions, we will incorporate electrostatic interaction implicitly into other terms calculating energies and forces. It will lead to a significant acceleration of computations, because algorithms connected with charges are the most time-consuming part of calculations. In order to remove the phenomenon of atoms penetrating each other during high-energy collisions we will add a barrier to the potential which will properly describe interactions at small interatomic distances.

We would like to create a potential which will accurately describe interactions among six elements, namely carbon (C), hydrogen (H), oxygen (O), nitrogen (N), sulphur (S), and phosphorus (P), which will allow for modelling structures and chemical reactions occurring in systems made of biomolecules. In order to do that, we will combine results of interatomic interactions obtained from quantum-mechanical (QM) calculations with a semi-empirical descriptions, where analytic formulae, fitted to results of QM computations, will be used to a fast prediction of forces and energies which occur in polyatomic systems.

The new potential will allow for, for example, investigating interactions between high-energy projectiles and organic or biological samples. Such phenomenon, called sputtering, is a basis of an analytic technique, called secondary ion mass spectroscopy (SIMS). This method allows for a 3D chemical imaging of samples. For example, it can detect where a drug is absorbed inside a cell, which may be used for developing new medicine faster. However, because of a lack of a proper force field, which would allow for description of interactions in such systems, it is still not understood how the SIMS works, especially when it is employed for studying organic and biologic samples. Our research will allow for modelling processes occurring in such systems. It may lead to develop more efficient analytical instruments with a better resolution, which will allow for imaging smaller systems with a higher precision.