ЛАБОРАТОРИЯ ИНФОРМАЦИОННЫХ ТЕХНОЛОГИЙ

Wednesday, 13 November 2019, at 15:00

Conference hall

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Development of a method and a set of programs for optimizing the molecular dynamics potential for chemically reactive systems

(based on the PhD thesis)

The work is devoted to the development of a method for optimizing the multi-parameter molecular dynamics potential for chemically reactive systems and to the implementation of this method in the form of a set of programs to search for the ReaxFF potential parameters. The proposed method is a sequence of actions for searching the parameters of the empirical MD potential, including the choice of a potential function, the choice and comparison of search methods, obtaining an optimization set, the analysis of the sensitivity of the potential function to changing parameters and the process of optimizing the potential.

Several optimization methods were implemented in the work, and their comparison was carried out. In particular, the Strongin global search algorithm used by the author was applied to optimize the MD potential for the first time. An own potential function was proposed. The scalability of the created set of programs was investigated. The parameters of the ReaxFF potential for model systems AlH and ZnOH were obtained, and MD simulation of these systems was performed.

The given method can be applied both to the problem of obtaining potential parameters for arbitrary classes of compounds and to the solution of other complex multi-parameter optimization problems.