ЛАБОРАТОРИЯ ИНФОРМАЦИОННЫХ ТЕХНОЛОГИЙ

Tuesday, July 3, 2018 at 15.00

Room 310

K.S. Shefov (St. Petersburg State University)

Development of a technique and a program complex for optimization of molecular dynamics potential for chemically reactive systems

The work is devoted to the development of methods for optimization of multiparameter molecular dynamic potential for chemically reactive systems and the implementation of this technique in the form of a software complex to find parameters of the ReaxFF potential. The proposed method is a sequence of actions to find the parameters of the empirical MD-potential including the choice of an objective function, selection and comparison of search methods, obtaining an optimizing set, analysis of the sensitivity of the objective function to changes in the parameters and the actual process of optimizing the potential.

A. V. Gagin (St. Petersburg State University)

Bayesian methods in the problem of determining the crystal structure of a substance

The seminar deals with the Bayesian approach to the problem of accounting for systematic errors (SE) in diffraction experiments on an example of the Rietveld method as well as the problem of the full neutron scattering. Proposed is a methodology that extends the standard Bayesian approach and allows one to take into account nonparametrized SE. In the framework of this approach, probabilistic models for SE of different types will be constructed which allow one to supplement the experimental model with information about the possible presence of SE.