Teorijska hemija / Theoretical Chemistry

TH P 1

Molecular dynamics simulation of ethanol on TiO_2 anatase surface

Olga A. Fedorako[1], Natallia E. Boboriko[1], Yaraslau U. Dzichenka[2]
[1]Belarusian State University, Chemistry Faculty, Minsk, Belarus,
Institute of Bioorganic Chemistry of National Academy of Sciences, Minsk, Belarus,

In the work molecular dynamics simulation of anatase surfaces and ethanol molecules was investigated. Appropriate force field was developed using q= 2.196 e, σ=1.958 Å, ε=0.6070 kcal/mol parameters for Ti atom, and q= -1.098 e, σ=2.875 Å, ε=0.3319 kcal/mol parameters for O atom. Anatase unit cell containing four titanium atoms and eight oxygen atoms was simulated. Using Amber program package (110), (011), and (101) anatase surfaces with 20x20 unit cells size were developed. Each surface was extended with application of boundary conditions. For molecular dynamics calculations NVT ensemble was used, time step was 0.002 fs for each case. Temperature of 300 K was used for each molecular dynamics simulation.

It was established that (110) anatase surface is characterized by the highest preference of interaction with ethanol molecules. This fact was revealed by the analysis of the calculated energies for the simulated systems and relying on the dependencies of ethanol molecules distances from the surface on simulation time.

The force field that was developed in the work can be used for investigation of interactions between anatase surfaces with other molecules including biomolecules and peptides. Investigations of such kind are especially important in the field of chemical sensors and biosensors for directional synthesis of materials with required sensor properties.

This work was partially supported by Belarusian Republican Foundation for Fundamental Research under Contract No. Kh19-046.