Thematic Section: Quantum-Chemical Research. **Full Paper**
Subsection: Inorganic Chemistry. *Reference Object Identifier* – ROI: jbc-02/17-49-4-105
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Submitted on April 26, 2017.

Comparison of methods for the study of water sorption on the titanium oxide

© **Andrey A. Degtyarev**,[1]* **Alexander G. Tarakanov**[2+]
[1] *Department of Chemistry and Chemical Technologies. Tambov State Technical University. Soviet St., 106. Tambov, 392000. Russia. Phone: +7 (4752) 63-44-44. E-mail: ad.dycost@gmail.com*
[2] *Department of Chemistry and Chemical Technologies. Tambov State Technical University. Soviet St., 106. Tambov, 392000. Russia. Phone: +7 (4752) 63-44-44. E-mail: uazqaaz@gmail.com*

*Supervising author; [+]Corresponding author

Keywords*:* DFT, pseudopotentials, BSSE, titanium(IV) oxide, rutile, water, sorption.

Abstract

The work investigated the influence of the cluster size of the titanium oxide(IV) and the method of molecular modeling, computational costs and the accuracy of the calculation of geometrical and energy characteristics of adsorption of water molecules on the surface (110) of rutile.

The calculations by methods of molecular dynamics, semi-empirical quantum chemistry and *ab initio* methods in the bases with pseudopotentials (LANL2DZ and SBKJC) and full-electronic basis (3-21G(d,p), 6-31G(d,p), 6-31++G(d,p)). Used *ab initio* methods – Hartree-Fock and the density functional theory with hybrid functional B3LYP5. Of the studied methods method was chosen, which is optimal on the basis of computational cost and accuracy of the calculation.

Computational cost was evaluated on the basis of time of one optimization step for fixed software and hardware. The calculation accuracy was estimated on the basis of two factors: the energy of adsorption of one water molecule in the center of the cluster and the distance between the water oxygen and the nearest atom of the (100) surface cluster. Comparison of the used methods was carried out with experimental data and quantum-chemical calculations in full-electronic basis (from published data and own calculations) adopted as a benchmark.

In addition to the methods demonstrated acceptable results for precision values, the influence of BSSE on the value of the energy of sorption.

Optimal was adopted the calculation method of the density functional theory with hybrid functional B3LYP5, full-electronic basis 6-31G(d,p) for atoms H, O and the basis of a pseudopotential LANL2DZ for Ti atoms with the subsequent calculation of BSSE.

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