Physico-Chemical nanomaterials science

QUANTUM CHEMICAL STUDY ON WATER MOLECULES ADSORPTION ON N-DOPED ANATASE FACE (001)

O.V. Smirnova, A.G. Grebenyuk, V.V. Lobanov

Chuiko Institute of Surface Chemistry of National Academy of Sciences of Ukraine,17 General Naumov str., Kyiv 03164, Ukraine.
E-mail: osmirnova@isc.gov.ua

Titanium dioxide is an important material used in photochemical applications and technology. Nitrogen incorporation into the titania films was proved by XPS measurements. Quantum chemical calculations were performed to find out the difference between the pure titania and nitrogen doped titania films.

We present hybrid DFT calculations for large TiO_2 cluster models in the gas phase: pure, N-doped and with an oxygen vacancy. All the clusters investigated are derived from the anatase bulk structure.

The surfaces are passivated with hydroxyl ligands. The geometrically optimized bonding patterns, structures, and electronic properties are similar in all clusters.

An analysis of the results of calculations suggests that modeling of XPS spectra for all of the above mentioned structures gives an opportunity to clarify the experimental data [1,2]. Based on the results of the calculation, it can be concluded that insertion of nitrogen atoms into oxygen positions in anatase crystalline structure leads to a shift of O $2p_{1/2}$ peak to low energies (from 521 to 520 eV).

1. *Linnik O.P., Shestopal N.O. , Smirnova N.P. [et al.]* Sol-gel synthesis, optical properties, morphology and photocatalytic activity of titania films modified with ethanolamines as nitrogen source // Surface. – 2012. – **4**(19). – P.105–110.

2. *Smirnova O.V., Grebenyuk A.G., Linnik O.P., Chorna N.O., Lobanov V.V.* Effect of nitrogen doping on the spatial and electronic structure of TiO2 thin films and on the efficiency of water molecules adsorption onto their surfaces // Scientific papers of NAUKMA. – 2016. – **183**. – P. 67–72.