Physico-chemical nanomaterials science

A quantum chemical study on electronic structure and a adsorption potential of nitrogen doped titania thin films

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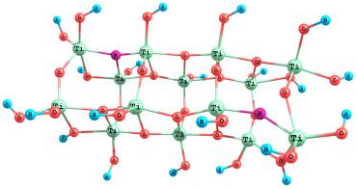
Porous and non-porous nitrogen doped titania thin films were synthesized by sol-gel using ethanolamines as doping agent [1]. It has been shown that the synthesis route influences on the titania particle sizes and, consequently, on the band gap energy values.

Nitrogen incorporation into the lattice structure of 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. Analogous to [2], the total energy values of the optimized geometrical structures of different size



TiO_2 and $TiO_2(N)$ cluster models (including 14 to 21 titanium atoms) were calculated using density functional theory method (DFT) and the hybrid B3LYP potential with basis set 6-31G(d,p) by means of the software package PC GAMESS (version FireFly 8.1.0 by A.Granovsky).

Calculated parameters for the models of TiO_2 surface of different composition have been carried out including those for the titania clusters doped by two and four nitrogen atom. Titanium dioxide structure was represented by clusters with different composition (the values in eV of band gap widths are in parentheses): $Ti_{21}H_8O_{46}$ (3.16), $Ti_{14}H_{22}O_{39}$ (5.23), $Ti_{14}N_2H_{22}O_{37}$ (4.00), $Ti_{14}N_4H_{22}O_{35}$ (3.40). The experimental value is 3.2 eV [1].

The calculation results were as follows: an increase in the number of doping nitrogen atoms leads to the decrease in the width of the band gap.

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. – V. **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 tio$_2$ thin films and on the efficiency of water molecules adsorption onto their *surfaces* // Scientific papers of NAUKMA – 2016. – V. **183**. – P. 67–72.