SUMMARY

The work contains 119 p., 16 fig. 8 Table. 3 ext. 44 source.

Actuality – studying the interaction of molecules of oxygen, which is in the gas phase mainly electronic state has multiplicity 3 (that is a triplet state) with a solid surface, spin state which singlet is essential, given the possibility of triplet-singlet transition in adsorption complex. Drhuhoryadne but not least is to ascertain the influence of oxygen vacancies on the surface of titanium dioxide adsorption on molecules in the gas phase gap, which determines the efficiency of utilization of solar radiation crystalline oxide of titanium (IV).

Purpose – using quantum chemical calculations to establish the sequence of elementary acts of interaction between oxygen molecules, the basic electronic triplet state which, with mold surface clusters TiO_2, which are in the singlet state, to determine the conditions of their interaction.

Object of study - computer-integrated technologies for the study of perfect crystalline anatase verge, brink anatase with oxygen vacancy, potential energy surface, singlet-triplet transition.

Purpose of the study – the spatial structure and electronic structure of cluster models, the energy complex formation of adsorption properties of triplet-singlet transition.

Research methods – quantum-chemical method of density functional theory of exchange-correlation functional basis in V3LYP 6-31 G **.

Scientific novelty of the results is as follows:

1) The formation of oxygen vacancies on the edge (001) anatase leads to a reduction in the band gap TiO2.

2) adsorption of molecular oxygen on the verge of defect-free (001) Titanium dioxide occurs.

3) H_2O adsorption on the verge oxygen vacancies (001) anatase preceding triplet-singlet transition in the system [001 Cluster + H_2O].

4) The formation of oxygen vacancies, followed by adsorption of H_2O molecules in it leads to further reduce the band gap, opening the way for on the basis of anatase efficient converters of solar radiation.

Publications. Based on work published 4 abstracts at international and Ukrainian conferences.

TITANIUM DIOXIDE, QUANTUM-CHEMICAL CALCULATION CRYSTAL FACES, OXYGEN VACANCIES, O_2 MOLECULES, H_2O MOLECULES, ADSORPTION COMPLEX, TRIPLET-SINGLET TRANSITION.