THE MINISTRY OF EDUCATION AND SCIENCE OF THE RUSSIAN FEDERATION
NATIONAL RESEARCH TOMSK STATE UNIVERSITY

# CATALYSIS: FROM SCIENCE TO INDUSTRY

*Proceedings of*
*VII International scientific school-conference for young scientists*

October 11-15, 2022

Tomsk 2022

# Electronic and optical properties of Ti-doped bismuth metasilicate

D.A. Perminova, E.A. Kovaleva, O.V. Vodyankina

*Tomsk State University, Tomsk, Russia*

darya.work.perminova@mail.ru

Renewable energy sources have gained research interest for decades. Solar energy catalysis is considered to be one of safe and sustainable alternatives to fossil fuel. There are a few Bi-based materials with promising photocatalytic properties. Though being promising photocatalysts, bismuth silicates are less investigated comparing to other bismuth compounds. Bismuth metasilicate $Bi_2SiO_5$ is of a particular research interest due to its perovskite-like structure and higher photocatalytic activity. Recently, Ti-doped structures of $Bi_2SiO_5$ were synthesized with titanium content up to 0.5. In present work, their electronic and optical properties were studied by means of density functional theory.

Calculations were performed using OpenMX quantum chemical package. PBE exchange-correlation functional and standard recommended PAO and VPS settings were used. The Monkhorst-Pack scheme was implemented for k-point Brilloin zone sampling. 1×6×6 *k*-point mesh was used for geometry optimization according to bismuth metasilicate unit cell size while the number of *k*-points was doubled in each direction for DOS calculations.

First, $Bi_2SiO_5$ unit cell was optimized. Lattice parameters were found to be in good agreement with experimental data [1]. Then, $Bi_2Si_{0.75}Ti_{0.25}O_5$ and $Bi_2Si_{0.5}Ti_{0.5}O_5$ structures were modeled by replacing one or two silicon atoms with titanium. Less than 1.5% lattice expansion is observed for $Bi_2Si_{0.75}Ti_{0.25}O_5$ with respect to original structure, and 1.6–2.7% expansion depending on the direction is observed for $Bi_2Si_{0.5}Ti_{0.5}O_5$.

Band structure of the doped bismuth metasilicates preserves nature of their counterpart, being direct semiconductor. Band gap slightly decreases when Ti is introduced in structure. However, it doesn't change much as its concentration increases. PDOS analysis shows that titanium states mostly contribute to the bottom of the conduction band. Optical absorption edge shifts from 511 nm for pristine $Bi_2SiO_5$ to 557 nm for both doped compounds.

*This work was supported by Russian Science Foundation, grant no. 19-73-30026.*

**References**

1. Ketterer, J.; Kramer, V. *Neues Jahrb. fur Mineral.* **1986**, *1*, 13–18.