Researchers predict properties of surface structure of known catalyst

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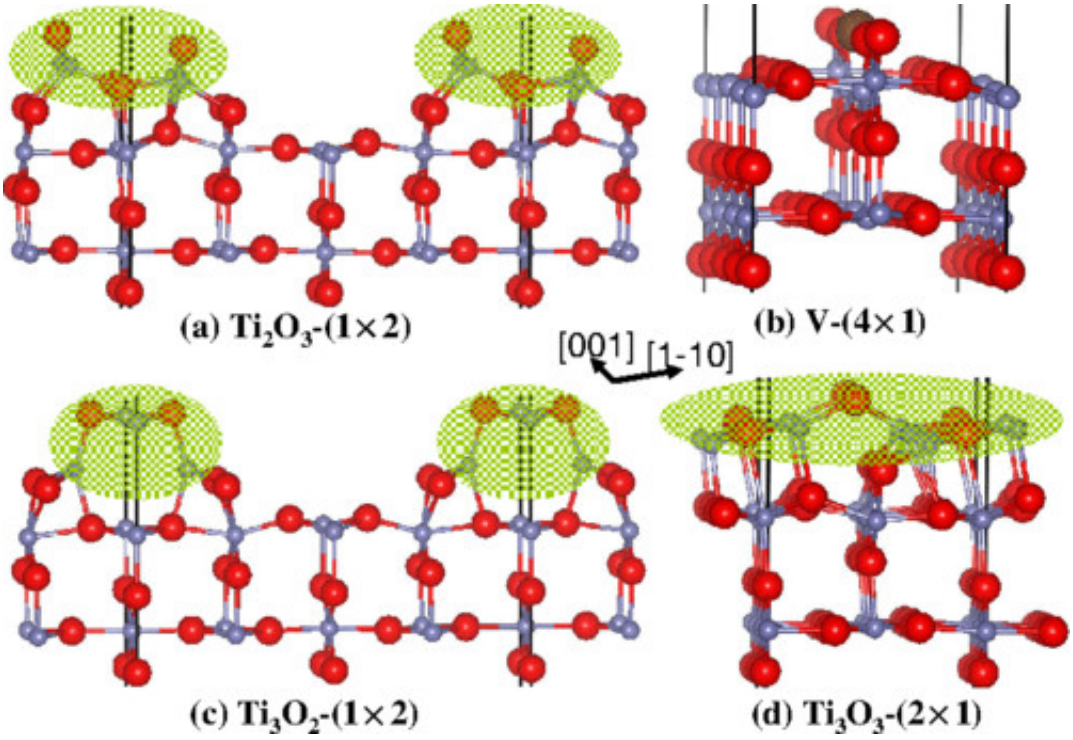

Side views of stable structures of rutile TiO2(110): (a) Ti2O3-(1×2), previously proposed in Refs. [7,9], (b) V-(4×1), (d) Ti3O3-(2×1), as well as (c) metastable Ti3O2-(1×2). Ti and O atoms are represented by small gray and big red balls, respectively. An O vacancy in V-(4×1) is represented by the dark gray ball. Structural features are highlighted by yellow shades Credit: Qinggao Wang

An article in *Physical Review Letters*, which was written by a group of researchers led by Qinggao Wang from MIPT's Laboratory of Computer

Design of New Materials, investigates the surface of titanium dioxide crystals.

"We chose this substance because rutile, a mineral composed primarily of titanium dioxide (TiO2),is one of the most commonly used catalysts in chemistry, "Qinggao Wang said about choosing the subject of research.

In their work, the researchers used the USPEX method, developed by the head of the laboratory, Artem Oganov, who co-authored the article. Professor Oganov explains in detail:

"One of the most promising and challenging areas of materials design is predicting and describing the properties of the surface of a substance, where special surface phases are formed, whose chemical composition and structure may differ significantly from the internal structure. It's very difficult to describe and predict these surface phases, proceeding from basic elementary data.

"Theoretical methods of calculating the properties of surfaces are complicated by some major hindrances, but we've developed a very powerful and effective way to predict the structure and properties of crystal surfaces, based on our USPEX algorithm. We used it for one of the most studied types of surfaces, rutile, a catalyst consisting of titanium dioxide.

"There's a great number of articles about its surface, which purport to understand rutile's catalytic properties. However, if you look at these articles, you'll see that they contradict each other.

"Our method helped us predict how the structure and chemistry of the surface of rutile crystals will change, resolving existing discrepancies between empirical and theoretical data and paving the way to

understanding how chemical reactions occur on the surface of this catalyst. This shows the potential of our theory for predicting surface phases, and we expect to obtain a large amount of data in this field."

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