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Form 3

# Abstract of Thesis

| Name （LI, Fengxuan） | |
|---|---|
| Title | Study of surface structures of the rutile $TiO_2$(110)-(1 x 2) surface and its water adsorption reaction<br>（ルチル型 $TiO_2$(110)-(1×2) 表面構造および水吸着反応に関する研究） |


Abstract of Thesis

This study aims to investigate the adsorption behavior and mechanism of water molecules on the $TiO_2$(110)-(1x2) reconstructed surface. It provides a theoretical basis for understanding the adsorption process of surface water molecules.

The study established a reliable $TiO_2$(110)-(1x2) surface structure model, combined with scanning tunneling microscopy (STM) and density functional theory (DFT) , to verify the surface configuration and the relationships among different parts, thereby conducting theoretical verification of the experimental results and explaining the mechanism of water adsorption. Through the mutual confirmation of experiments and theory, this research proposed the basic mechanism of water molecule adsorption and reaction on the $TiO_2$(110)-(1x2) surface at the atomic scale.

Firstly, the study verified the single link structure based on the asymmetric (1x2) model. This model was confirmed to be reasonable through the comparison of simulated images with experimental STM images and the comparison of DFT total energies. Further, three different types of double link structures were constructed and analyzed. It was found that the formation mechanism of the double link structure was mainly influenced by the relative orientation of the single link, local atomic positions, and vacancies. The types of double link structures could be controlled by the single link structure. The simulated STM images of these models were highly consistent with the experimental results, verifying their reliability.

And then, the behavior of water molecule adsorption on the $TiO_2$(110)-(1x2) surface was studied. The results showed that water molecules mainly existed in the form of molecular adsorption at room temperature and preferentially adsorbed in the (1x2) region without influencing from other parts on the surface. After low-temperature annealing, a double-cross-linked structure was formed on the surface, and this structure gradually disappeared as the temperature was further increased, and the surface returned to its original configuration, indicating that this structure is reversible. The surface structure changes caused by water molecule adsorption were mainly related to the partial dissociation behavior of water molecules under thermal excitation conditions. The participation of oxygen promoted the rearrangement of surface atoms, thereby inducing the formation of new link structure.

Overall, this study systematically revealed the atomic-level characteristics of the $TiO_2$(110)-(1×2) surface single link and double link structures, and deeply explored the adsorption behavior of water molecules on this surface and the regulatory mechanism of its influence on the surface structure.

様式７

# 論文審査の結果の要旨及び担当者

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## 論文審査の結果の要旨

本論文は、$TiO_2$(110)-(1×2)再構成表面における水分子の吸着挙動とその機構を原子レベルで解明することを目的とし、走査トンネル顕微鏡（STM）と密度汎関数理論（DFT）計算を組み合わせた実験・理論融合型の手法により体系的に検討したものである。まず、非対称(1×2)モデルに基づくシングルリンク構造を提案し、シミュレーションSTM像と実験像の比較および全エネルギー評価により、その妥当性を検証した。さらに、三種類のダブルリンク構造を構築して形成要因を解析し、シングルリンクの相対配置、局所原子位置、空孔の存在が構造形成を支配することを明らかにした。これらのモデルは実験結果と高い一致を示し、構造理解の信頼性を裏付けている。続いて、水分子の吸着挙動を詳細に調べた結果、室温では主として分子状で吸着し、他領域の影響を受けることなく(1×2)領域に優先的に吸着することを示した。低温アニール後には二重架橋構造が形成されるが、さらなる加熱により消失して元の表面構造に戻ることから、この構造変化が可逆的であることを明らかにした。これらの変化は熱励起下での水分子の部分解離と酸素の関与による表面原子の再配列に起因し、新たなリンク構造の形成を誘起することが示唆された。以上より、本論文は$TiO_2$(110)-(1×2)表面におけるリンク構造の原子レベルの特徴と水分子吸着による表面構造制御機構を体系的に解明し、酸化物表面反応の理解に重要な知見を提供するものである。よって、本論文は博士（工学）の学位論文として価値のあるものと認める。