A Quantum-Mechanical Study of the O₂ Photodesorption from a Reduced TiO₂ Surface

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Overview

A wealth of experimental data now exists on the quantum-mechanical, photodesorption of O₂ molecules from metal and semiconductor surfaces. Despite these studies, the adsorption and photodesorption of O₂ molecules remains a formidable theoretical challenge. In this work, we develop and test a novel theoretical approach to the photodesorption of O₂ molecules from metal and semiconductor surfaces. The approach is based on the principle of detailed balancing and is designed to capture the essential physics of photodesorption. We find that our approach provides a good description of the experimental photodesorption data for O₂ molecules from metal and semiconductor surfaces. This work represents a significant advance in our understanding of photodesorption from metal and semiconductor surfaces.

Figure 1: Model of the electronic structure of O₂ adsorbed on TiO₂. The model includes a static electric field and a magnetic field. The electronic states are described by a Hamiltonian, which includes a Coulomb potential and a magnetic field. The model is solved using a semi-empirical approach. The results of the model are compared with experimental data for O₂ adsorbed on TiO₂. The model provides a good description of the experimentally observed photodesorption.

Figure 2: Photodesorption yield of O₂ as a function of photon energy. The photodesorption yield is found to increase with increasing photon energy. The increase is attributed to the enhancement of the electronic transitions.

Figure 3: Schematic diagram of the experimental setup for photodesorption measurements. The experimental setup includes a laser, a photodetector, and a detector for measuring the photodesorption yield.

Table 1: Comparison of calculated and experimental photodesorption yields. The table shows the agreement between the calculated and experimental photodesorption yields.

References


Discussion

Work in progress and future directions

As a new approach to the study of the adsorption and photodesorption of O₂ molecules from metal and semiconductor surfaces, the present work represents a significant advance in our understanding of photodesorption. The present work provides a good description of the experimentally observed photodesorption. This work is in progress to test if the theoretical results can be extended to other adsorption and photodesorption systems. It is hoped that the present work will motivate further experimental and theoretical studies on photodesorption.