【Grant-in-Aid for Transformative Research Areas（B）】

Section II

Title of Project： Surface Hydrogen Engineering: Utilization of Spillover Hydrogen and Verification of Quantum Tunneling Effect

MORI Kohsuke
(Osaka University, Graduate School of Engineering, Associate Professor)

Number of Research Area：21B206　Researcher Number：90423087

【Purpose of the Research Project】

The principle of the "hydrogen spillover" phenomenon, in which hydrogen atoms diffuse rapidly on the solid surface, is still a black box (Fig. 1). The first purpose of this area is to understand the control factors for the active hydrogen species generated by spillover, and to propose protocol to utilize it.

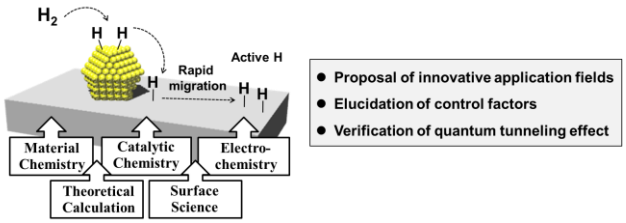

Fig. 1. Elucidation and utilization of hydrogen spillover phenomenon

The "quantum tunneling effect of hydrogen" has been attracting attention as a new reaction paradigm that has the potential to control chemical reactions. In classical mechanics, the reaction is accelerated with increasing temperature according to the Arrhenius equation. On the other hand, regardless of thermodynamics, the chemical reaction may proceed through the potential barrier due to the quantum tunneling effect. In this area, we aim to verify the involvement of the quantum tunneling effect in the hydrogen spillover phenomenon, and finally construct a theory (surface hydrogen engineering) as a new reaction control paradigm that overturns the conventional kinetic and thermodynamic concepts. In order to achieve the goal, the next generation, whose major topics are material chemistry, catalytic chemistry, electrochemistry, surface science, and theoretical calculation, will collaborate with the target of new material design, discover of novel function and principle.

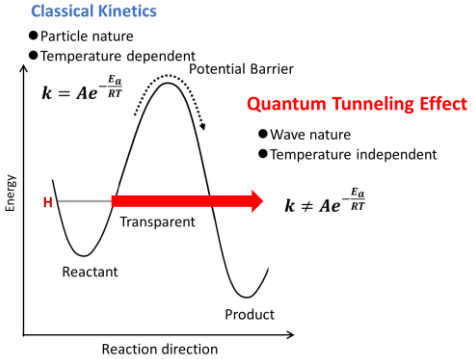

Fig. 2. Conceptual diagram of quantum tunneling

【Content of the Research Project】

The major achievements in this area are "proposal of innovative application fields", "elucidation of control factors/theory construction", and "verification of contribution of quantum tunneling effect". The Mori group (A01), Motokura group (A02), and Aoki group (A03) are working on the synthesis of innovative materials, new catalytic processes, and the development of electrochemical cells, respectively, and finally propose new strategy to use hydrogen spillovers. The Miwa group (A04) aims to acquire basic information of the spilled hydrogen atoms, such as charge, position, diffusion rate, etc. by directly observing the dynamic behavior of spillover hydrogen using muons as a probe. The Hinuma group (A05) independently promotes the theoretical and systematic understanding of the spillover mechanism, and further provides theoretical support to the experimental group.

【Expected Research Achievements and Scientific Significance】

"Hydrogen utilization technology" is regarded as an important issue for the energy strategy and plays a crucial role in the growth strategy that will support Japan's economic growth in the future. The theme of this research, "Construction of Guiding Principles for Freely Manipulating Highly Active Spillover Hydrogen that Moves on Solid Surfaces at High Speed," can be a key technology for the hydrogen production, storage, transportation, and utilization technologies aiming at next-generation hydrogen society.

【Key Words】

Hydrogen spillover: A phenomenon that involves the surface migration of dissociated H atoms at a metal adsorbed on the oxide surface driven by a concentration gradient.
Quantum tunneling effect: A phenomenon in which a chemical reaction proceeds through a potential barrier regardless of thermodynamics because the wave nature is remarkable for electrons and H atoms.

【Term of Project】 FY2021-2023

【Budget Allocation】 104,600 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.mat.eng.osaka-u.ac.jp/surface-hydrogen-engineering
mori@mat.eng.osaka-u.ac.jp