【Grant-in-Aid for Scientific Research (S)】

Dynamics of spin, proton and charge at solid surfaces

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Project Information	Project Number : 24H00040 Project Period (FY) : 2024-2028 Keywords : hydrogen, surface spin structure, spin relaxation, adsorption/reaction

Purpose and Background of the Research

● Outline of the Research

To utilize hydrogen as an energy source, it is necessary to generate, store, and convert hydrogen into energy, where the dynamics of hydrogen on solid surfaces play a crucial role. Being the lightest element with spin degrees of freedom, hydrogen exhibits quantum nature such as quantum tunneling and rotation in its dynamics. The present study aims to deepen the understanding of hydrogen dynamics at solid surfaces from the perspectives of spin, proton, and charge while exploring the possibility to control surface reactions utilizing magnetism and magnetic fields.

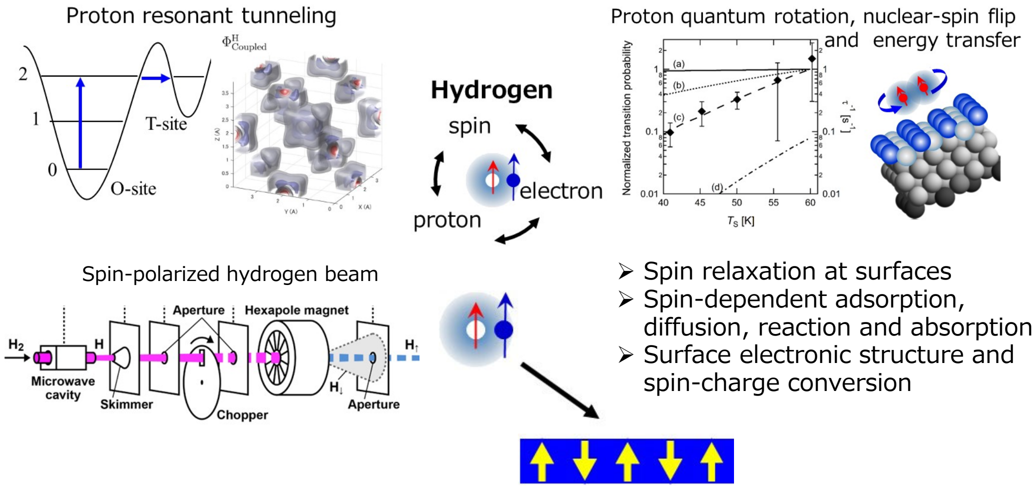

Figure 1. Outline of the research

● Background and purpose

Protons and electrons, the constituent elements of hydrogen, possess spin degrees of freedom. Recently, it has acquired much attention to control molecular adsorption and reactions by utilizing surface magnetism and molecular spins. However, the role of spin in hydrogen surface dynamics remains unclear. Our group has recently developed a spin-polarized hydrogen beam, where a spin polarization of >98% is achieved as demonstrated by a Stern-Gerlach spectrometer in Figure 2.

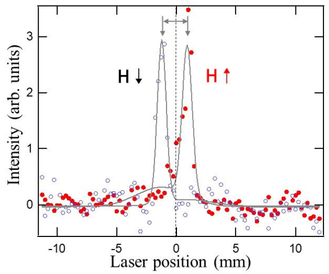

Figure 2. Results of spin-polarization measurements.

On the other hand, solid surfaces exhibit various spin structures. Ferromagnetic materials reveal either perpendicular or inclined magnetization. Furthermore, materials without macroscopic magnetism often possess electronic structures with electron spin and momentum coupled due to spin-orbit interaction, as demonstrated by the Rashba and topological effects. On such surfaces, hydrogen-surface interaction possibly depends on the spin direction of hydrogen thereby inducing spin-dependent adsorption and reactions.

The present study aims to investigate hydrogen dynamics on surfaces with various spin structures. The questions to be answered are how fast the spin relaxation is, how the hydrogen spin state influences the proton motion, and how the spin state is correlated with the surface electronic states. By answering these questions, we aim to elucidate the detailed hydrogen dynamics on surfaces and explore the possibility to control the reactions by magnetism and external magnetic fields.

Expected Research Achievements

● Research strategy

A key strategy of this study is to investigate the spin relaxation and spin dependence in adsorption, diffusion, and reactions on surfaces with various spin structures using the spin-polarized hydrogen beam. With the aid of the theoretical analysis, the spin-proton correlation and spin-charge correlation in hydrogen dynamics at surfaces will be clarified. Specific surfaces to be studied include ferromagnetic Ni thin films, Rashba-split Ag(111)-Bi_xPb_{1-x}, Bi_2Se_3 topological insulator, and Pt among others.

● Spin relaxation

By measuring the spin polarization of the scattered hydrogen on the aforementioned surfaces using a Stern-Gerlach spectrometer and laser resonance ionization (Figure 3), the surface spin relaxation rate will be analyzed. The correlation between the surface spin structure and spin relaxation rate will be elucidated.

● Spin-proton correlation

The spin dependence of the hydrogen adsorption and reactions such as abstraction of adsorbed hydrogen (molecular hydrogen generation), reduction of adsorbed oxygen (water molecule generation), and hydrogenation of hydrocarbons will be examined. Combined with quantum-dynamics analysis, the spin dependence of the hydrogen-surface interaction potential will be clarified (Figure 4). Additionally, the effects of tunneling and non-adiabatic transitions will be revealed.

● Spin-electron correlation

The spin-polarized hydrogen is expected to selectively interact with the spin-polarized states (Figure 5), where spin-induced currents are anticipated. Combining with photoemission spectroscopy, the detailed spin-dependent electronic interaction during hydrogen adsorption, diffusion, and reactions will be elucidated.

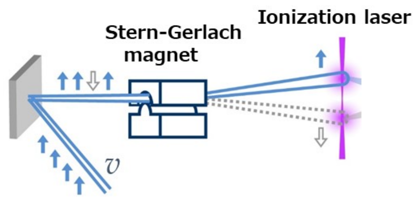

Figure 3. Schematic of spin-relaxation measurements

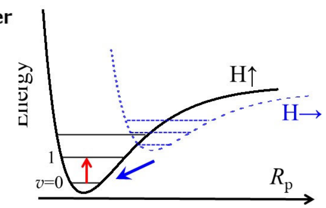

Figure 4. Schematic of spin-dependent H-surface potential.

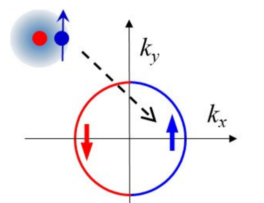

Figure 5. Interaction of spin-polarized H with topological surface state.

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