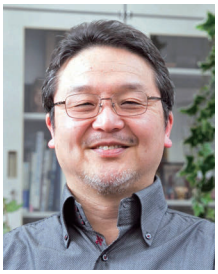
【Grant-in-Aid for Scientific Research (S)】

Broad Section E



Title of Project : Exploring Interface Science by Concerted Use of Advanced Spectroscopy and Theory

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Research Project Number : 18H05265 Researcher Number : 60217164
Keyword : Interface, Nonlinear Spectroscopy, Ultrafast, MD Simulation, Molecular Science

【Purpose and Background of the Research】

Although interfaces play crucial roles in many areas of science and technology, our understanding of interfacial phenomena is insufficient. In this research, researchers who have been developing new experimental and theoretical methodologies collaborate and promote research on liquid interfaces. We clarify static and dynamic processes at the interfaces and elucidate their mechanisms at the molecular level.

【Research Methods】

By using phase-controlled interface selective nonlinear spectroscopy and molecular dynamics simulation, we investigate liquid interfaces by focusing on the following three issues.

(1) Ultrafast interfacial vibrational dynamics

Elucidation of the ultrafast phenomena is the frontier of science. In particular, elucidation of ultrafast dynamics of the hydrogen bonding is essentially important. Ultrafast hydrogen-bond dynamics of bulk water has been intensively studied, but the dynamics at the interface is not elucidated. We investigate it by femtosecond time-resolved phase-controlled sum-frequency generation spectroscopy and its extension to two-dimensional spectroscopy.

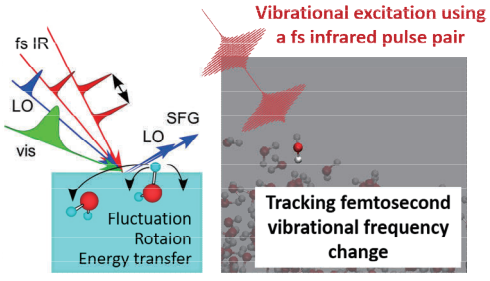

Figure 1 Ultrafast dynamics at liquid interfaces

(2) Structure of liquid interfaces and reactions

Reactions at the liquid interface are thought to be different from those in the solution, but it has not been clarified. We elucidate the structure of liquid interfaces and clarify their effects on the reactivity of interfacial molecules. Furthermore, we observe the interfacial reaction process by the time-resolved measurement directly.

(3) Buried interfaces and complex real interfaces

"Buried interfaces" such as solid/liquid interfaces are an unexplored area. We elucidate the properties of the buried interfaces at the molecular level, from oxide/water interfaces to complex interfaces that are widely utilized in the real world such as the electrode interface.

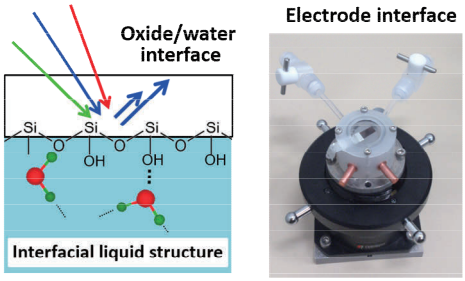

Figure 2 Buried interface and real complex interface

【Expected Research Achievements and Scientific Significance】

The outcomes of this research not only greatly advance interfacial science, but also provide solid basis to a wide range of science and technology including environmental chemistry and electrochemistry where interfacial phenomena play major roles.

【Publications Relevant to the Project】

・Nihonyanagi, S.; Yamaguchi, S.; Tahara, T. Ultrafast dynamics at water interfaces studied by vibrational sum-frequency generation. *Chem. Rev.* **2017**, *117*, 10665-10693.
・Ishiyama, T.; Imamura, T.; Morita, A. Theoretical studies of structures and vibrational sum frequency generation spectra at aqueous interfaces. *Chem. Rev.* **2014**, *114*, 8447-8470.

【Term of Project】 FY2018-2022

【Budget Allocation】 148,400 Thousand Yen

【Homepage Address and Other Contact Information】

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