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Molecular Surface Science: Uncovering Reaction Mechanisms in Electronics and Catalysis

Surface and interface science serves as the foundation for numerous applications, ranging from microelectronics to bio-sensing to heterogeneous catalysis. Surface chemistry thus informs important technologies of today that drive multibillion dollar industries, and understanding the fundamental chemistry at a molecular level is key to future advances. This talk will examine my group's studies of molecular surface science in two key areas: electronics and catalysis.

On the topic of electronic materials, I will describe our work on the adsorption of organic molecules at semiconductor surfaces, aimed at the ultimate goal of controlling the chemical and electrical properties of these hybrid systems. The presentation will examine model systems of molecular adsorption on the Ge(100)-2×1 surface using a combination of experimental and theoretical methods. The reactivity of different functional groups will be described, with particular focus on reactions of bi- and trifunctional molecules. The results help elucidate the way in which the molecular structure as well as the identity of the reactive moieties affects the product distribution of the molecules upon adsorption.

On the topic of heterogeneous catalysis, I will describe recent studies on supported metal catalysts for the conversion of synthesis gas ($\text{CO} + \text{H}_2$) to synthetic liquid fuels and high-value chemicals. The interactions between the metal, the support and promoters, and adsorbed reaction intermediates are of particular interest. Experimental and theoretical studies provide strong evidence of structure sensitivity in syngas conversion on Rh catalysts. Further, atomic layer deposition is applied as a method to achieve atomic scale catalyst design, allowing study of the important effects of promoters and supports, which strongly influence the performance of Rh catalysts. Our results show that the activity and selectivity is highly sensitive to the identity as well as the placement of the promoters, and *in situ* spectroscopy combined with theoretical calculation helps provide a mechanistic understanding of the relationship between surface reaction intermediates and the desired products.

【講師紹介】 Bent 教授は、現在、スタンフォード大学化学工学科学科長、TomKat Center on Sustainable Energy のセンター長を務められるなど、米国を代表する表面科学者の一人です。本講演では、半導体表面での分子吸着や触媒反応について、解りやすく解説いただきます。

談話会委員 長谷川 幸雄、加藤 岳生