校長講話

水素社会を実現する21世紀の播磨灘物語

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液体水素運搬船の進水式が12月11日、川崎重工業、神戸工場で行われました。水素は-253℃で液体になり、体積が800分の１になります。オーストラリア、ヴィクトリアに埋蔵する褐炭から水素を取り出し、液化し、液体水素を運搬船に積んで、日本へ輸送する計画だそうです。水素サプライチェーンの一つであり、この完成により、水素社会の実現が期待されます。東京オリンピック、パラリンピック開催時に、デモンストレーションが行われるとの事。楽しみですね。

液体水素を入れる“魔法瓶”は播磨工場でつくられています。液体状態を安定的に持続するには、水素の核スピンを制御する必要があり、これに関する研究開発を共同で進めた経緯から、その当時の研究メンバー、川崎重工業の山下さん矢嶋さんに案内をお願いし、進水式に参加することができました。SUISO Frontier（すいそ　ふろんてぃあ）が船名です。感激しました。

水素と固体表面との相互作用、水素の表面近傍での挙動に関する著書を執筆中です。その中で液体水素運搬船のことも少し触れる予定にしています。以下に前書きの一部を記載します。

John Bockris, in his 1970 talk at the General Motors (GM) Technical Center, coined the term “hydrogen economy” to describe a hypothetical future system of delivering energy through the use of hydrogen. That future is now. After about 50 years, the fulfillment of Bockris’ vision of a hydrogen-powered future is gradually taking shape in our time. In many countries around the world, active efforts to decarbonize energy systems have turned hydrogen into the centerpiece of grand master plans for clean and sustainable replacement to fossil fuels.

While the decarbonization of energy landscape has propelled the contemporary research interest in the conversion, storage, and delivery of hydrogen, its interaction with surfaces has laid the foundation of cornerstone concepts in surface science. Because of its simple electronic structure, studies on hydrogen-metal systems have allowed the derivation of the fundamental principles of surface reactivity and mechanism of bond-forming and bond-breaking processes, which are of great technological and scientific importance. Furthermore, the quantum effects in surface dynamics due to the light mass of hydrogen have made it a profoundly interesting benchmark system from a fundamental point-of-view.

Albeit the study of hydrogen has been a long tradition in surface science, significant advancements in theoretical and computational methods over the past years, in addition to the recent development of high-performance supercomputers, have paved the way to more sophisticated treatment and understanding of hydrogen-surface interactions. In particular, density functional theory-based first principles calculations have matured enough to address the long-standing problem of surface reactivity, such as the solutions to the failure of widely used functionals to predict the experimentally observed structures and stabilities of molecules on surfaces. Also, recent studies on hydrogen and hydrogen-containing molecules have taken major leaps in the understanding of adsorbate-induced segregation in bimetallic catalysts, novel hydrogen storage materials, and other contemporary topics of interest in the general surface science community. Among other things, these recent research accomplishments and the earlier mentioned key role of hydrogen in addressing our energy need, have inspired the concept of this book, which was meticulously written to elucidate both the fundamental concepts of hydrogen-surface interactions and its role in hydrogen economy.

CO_2 を排出しない新たなエネルギーとして注目されている水素。経済産業省・資源エネルギー庁のホームページにも、省エネルギー・新エネルギーとして、大きく取り上げられています。水素社会の実現は目前です。

Towards Hydrogen-based Society

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The ability to unravel and alter the physical properties of materials at the atomic level is one of the themes of our years of work. We work with quantum dynamical calculations to develop materials for “intelligent design”. Intelligent design creates relevant and novel materials aimed at a specific purpose. The mechanism is drawn by so-called computational materials design (CMD). In CMD, mathematical models are used to simulate the system of interest and the obtained data are analyzed to draw physical mechanisms, knowing how a system works through understanding these physical mechanisms is useful for materials design, as it can be used to alter certain conditions and parameters to generate a novel or modified system. Verification can then involve collaboration with experimental groups. Through this process, several groundbreaking results have been developed e.g., in the field of renewable energy and environmental applications.

In this CMD36, we introduce Hydrogen-based technology, one of the many areas we explore in the field of intelligent design research. This topic encompasses R&D toward realizing an innovative energy-saving hydrogen society, centering on quantum dynamics. Utilization of hydrogen as an energy source is being disseminated, e.g. for the fuel cell vehicles. Prompt realization of a hydrogen society it is essential to optimize the energy mix and energy security and achieve a technical breakthrough to facilitate the dissemination of hydrogen energy infrastructure without an excessive economic burden.

To economically realize a carbon-free society, we design functional materials and related new processes that particularly explore the quantum effect occurring at the hydrogen-functional materials interface. The functionality of the designed materials and related processes are verified experimentally both microscopically and macroscopically.

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Branching Reactions in Melanogenesis
- Mechanism and Design Guidelines -

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Hideaki Kasai. Professor Hideaki Kasai is currently the President of the National Institute of Technology, Akashi College, Hyogo, Japan. He is also a professor emeritus at Osaka University. He pioneered studies in ultra-fast quantum processes, elementary processes in excitations and reactions on surfaces/interfaces, and quantum-based design of nanomaterial devices. He is a recipient of several awards including the Minister of Education, Culture, Sports, Science and Technology of Japan award in 2012, the GanesaWidya Jasa Adiutama of the Institute of Technology Bandung, Indonesia in 2014, and an honorary doctorate of the De La Salle University, Philippines in 2017.

Abstract

Our skin color is essentially controlled by melanogenesis, which is the production of natural pigments called melanin. Melanogenesis can be generally defined as a cascade of multiple reactions, which is triggered by oxidation of *p*-substituted phenols or catechols like tyrosine or dopa. Oxidation of these phenols or catechols results in formation of reactive *o*-quinones. Some *o*-Quinones can spontaneously undergo cyclization, which is a ring-closure reaction by bonding between a benzene ring carbon and *p*-substituent. On the otherhand, *o*-quinones can also react with thiols (R-SH). As the final product, the cyclization results in formation of black to brown eumelanin whereas the binding of cysteine results in formation of yellow to reddish brown pheomelanin. This can be said as the first branching of melanogenesis.

The cyclization is followed by a redox exchange between the cyclized molecule and a remaining *o*-quinone. A molecule resulting from the redox exchange is still unstable and undergoes further conversion. This conversion involves intramolecular proton rearrangements. In addition, this conversion can also undergo a decarboxylation, which is a desorption of -COOH, if the melanogenic substrate has a carboxyl group (-COOH) in *p*-substituent. Two types of monomers of eumelanin are directly generated by the decarboxylative and non-decarboxylative pathways, respectively. Thus, this conversion process can be said as the second branching of melanogenesis.

In this Asia CMD® workshop, we will deepen the mechanistic understanding of the branching reactions and provide guidelines for design of the properties and functions of melanin.

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