

# Material Science toward achieving Carbon Neutrality

Takayuki Ichikawa

*Graduate School of Advanced Science and Engineering, Hiroshima University, 1-4-1 Kagamiyama  
Higashi-Hiroshima, 739-8527, Japan*

Growing global energy demand and exhaustion of fossil fuels are gradually becoming a big concern for all the people on the Earth. Meanwhile, the deteriorating environmental pollution and global warming with the emergence of recent extreme weather make us re-recognize the importance of the usage of renewable resources with carbon-free emission and energy storage with high efficiency. A secondary battery to store the fluctuating renewable energy attracts a lot of attention and seems to fulfill the requirements of human beings. Since these battery technologies are only suitable for short-term energy storage daily or weekly due to their high cost, and cannot be used for leveling seasonal fluctuations. Due to economic requirement, it is important to establish hydrogen utilization technology as a countermeasure against long-term fluctuations in renewable energy. Therefore, in order to achieve carbon neutrality, it is impossible to avoid the development of high-performance secondary batteries and the establishment of a hydrogen-utilizing society.

Our group has so far focused on various kind of metal hydrides and focused on exploring their functions to solve the above problems. As an example, metal hydrides are considered to be a potential anode material for all-solid-state Li-ion batteries, because of its high theoretical Li storage capacity, relatively low volume expansion, and suitable working potential with very small polarization by the “hydride conversion reaction”. On the other hand, as characteristic properties related to hydrogen gas, not only for high capacity hydrogen storage but also for obtaining high pressure H<sub>2</sub>, producing heat by control of H<sub>2</sub> pressure, and absorbing NH<sub>3</sub> with relatively low pressure, we focused on various kinds of hydrides related materials, such as MgH<sub>2</sub>, TiFe intermetallic compound, TiH<sub>2</sub>, and LiBH<sub>4</sub>. And then, for high performance properties, “nano-composite techniques” played an important role. Of course, material modification to achieve required performance can only be accelerated by precise and accurate characterizations based on materials science.

The synthesis of hydrogen gas from renewable energies is also quite important technology to be developed with a reasonable cost (in Japan, target cost for hydrogen production is about 2 USD/kg). To achieve this economic requirement, thermochemical method to produce hydrogen is attracting a significant attention. The reaction cycles for water-splitting based on redox reactions of metallic phase of Na are focused in our group, which is composed of three reactions, that is hydrogen generation by solid-liquid reaction, metal separation by thermolysis, and oxygen generation by hydrolysis, where we are able to expect to have the effect of mass production. As is well known that sodium oxides, Na<sub>2</sub>O and Na<sub>2</sub>O<sub>2</sub> show highly reactive properties to any kind of metals and ceramics at high temperature conditions around 500 °C, it is quite difficult to control the target reaction, which lead to serious corrosion of the vessel materials. In this work, thermodynamic analyses are performed by using the parameters such as operating temperature and partial pressures of the products obtained by the experiments to determine that the Na metal redox cycle is potential hydrogen production technique as thermochemical energy storage. And some suitable way to control this promising reaction by minimizing the corrosion effect would be demonstrated.