

# Materials Science and Application of Electrides



## Creating a stable material with anionic electrons for industry use

"Electride" is the general term for a chemical compound in which electrons serve as anions. Electrides are a new concept, and as such, are expected to show intriguing physical properties. In previous studies, electrides have been chemically and thermally unstable and even the best-quality electrides are only stable at -40 degrees Celsius or less, and in a no-air environment, they have been hard to handle and so very little was known about their physical properties.

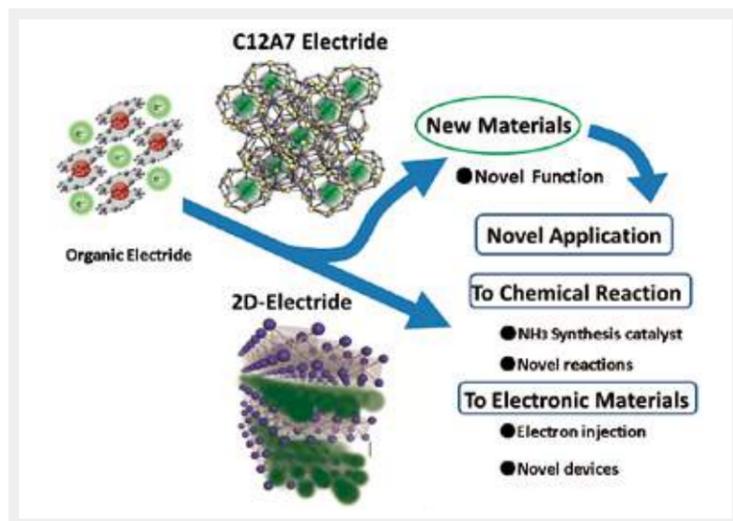
We have succeeded in synthesizing a new material, "C12A7 Electride," which is composed of aluminum oxide and calcium oxide (used in cement) by replacing its oxygen ions with electrons. This gives us what we could call "electrically conductive cement," a material that is stable both in air and at room temperature. We can expect breakthrough applied research for the material such as high-performance catalysts or electronic materials.

## Developing electrides as high-performance catalysts and electronic materials

In the ACCEL project, we aim to develop electrides that include not only the C12A7 electride but also a two-dimensional electride, for industrial use as catalysts or electronic materials.

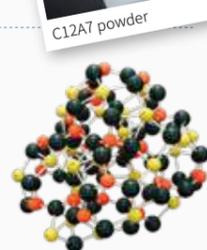
In applications as catalysts, we are aiming to synthesize ammonia at lower pressures and lower temperatures than conventional. We aim to commercialize manufacturing ammonia synthesis that uses less energy and is environmentally friendly.

Ammonia is a raw material for nitrogen-based fertilizers and a common chemical intermediate, and has recently attracted attention as a hydrogen carrier for renewable energy. For electronic material use, we are carrying out research with an eye on applications as an electron-injection layer material to be used for organic EL (OLED) displays.



### Electride

The C12A7 electride has a skeletal structure that looks like a cage some 0.5 nanometers in diameter, and was originally an insulator with cages filled with oxygen ions. The C12A7 which replaces the oxygen ions with anionic electrons becomes very electrically conductive and readily releases electrons. Although it readily releases electrons like alkali metals, it has the unique characteristics of being both chemically and thermally stable.



### Research Director

#### Hideo Hosono

Professor of Laboratory for Materials and Structures, Institute of Innovative Research, and Director of Materials Research Center for Element Strategy, Tokyo Institute of Technology

My research theme has mainly covered the creation of new materials for transparent oxide semiconductors. "IGZO" is a typical example, used in thin-film transistors to drive high-definition liquid crystal displays and large organic EL television screens. This helped create "Better Life," but I didn't want to stop there. I really wanted to create something "Essential for Life". On the assumption that I would be able to make good use of the unique properties of the C12A7 electride discussed above, I began researching the synthesis of ammonia, which is necessary for food production, under mild conditions.

In the ACCEL project, we have succeeded in conducting ammonia synthesis at under 400 degrees Celsius, at atmospheric pressures, and in just a short time. This process used to require high temperatures, between 400 and 500 degrees Celsius, and high pressures, between 100 to 300 atmospheres. If this synthesis process is achieved at lower energy levels, ammonia will be able to be manufactured in small batches and in a variety of locations, contributing to solve the food problem.

To succeed in research that can be linked to actual applications, it is important to understand the true nature of the material and to create a bird's-eye view in your mind. A catalyst and a semiconductor may seem to be two completely different subjects, but are similar in terms of the control of electrons in a solid.

### Program Manager

#### Toshiharu Yokoyama

ACCEL Program Manager, Japan Science and Technology Agency

Electride is a new material that has great potential for industry. The issue how its superior functions and properties should be brought out and put into practical use.

In the ACCEL project, we are advancing research integrally, from the fundamental to the application study phases, supporting it as we pave the way to commercialization. For catalyst use, we will study the issues, expecting further developments, after aiming for the construction of a compact ammonia manufacture plant. For electronic material use, we are developing materials with superior properties to use for electron injection layers and transport layers that will allow us to achieve a low electric voltage drive for and increase the life of large OLED displays. In addition, we are working to expand applications, considering a variety of possibilities such as recycling and chemical synthesis using low temperature decomposition of carbon dioxide, which has provided interesting results. Through this research, we would like to train researchers who will be responsible for the next generation.

Forerunners who put innovative research outcomes into practical use always feel uneasy. However, I will make my way towards our great goal with convictions based on my experience.

The variety of possibilities  
the electride provides,  
such as food production,  
renewable energy,  
and large televisions,  
will encourage technological  
innovation.

### PROFILE

**HIDEO HOSONO**  
1982: Ph.D. (Engineering), Tokyo Metropolitan University; 1999: Professor, Materials and Structures Laboratory (currently Institute for Innovative Research), Tokyo Institute of Technology after Nagoya Institute of Technology and Institute for Molecular Science; 2012: appointed concurrently to Director, Materials Research Center for Element Strategy. Fields of expertise: Inorganic material science, transparent oxide semiconductors, new superconductive materials, and magnetic resonance.

### PROFILE

**TOSHIHARU YOKOYAMA**  
1971: Graduated from the Department of Industrial Chemistry, National Institute of Technology, Gunma College. Joined Mitsubishi Chemical Industries, Ltd. (currently Mitsubishi Chemical Corporation). Field of expertise: Catalytic chemistry. Research into the development of catalysts for petrochemicals and fine chemicals and the development of manufacturing processes. Ph.D. (Engineering)