# [Grant-in-Aid for Scientific Research (S)]

Science and Engineering (Engineering)



# Title of Project : New evolution of materials concept and application of electrides

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Research Project Number : 17H06153 Researcher Number : 30157028 Research Area : Inorganic Materials Materials Property

#### Keyword : Novel Inorganic Materials, Electrides [Purpose and Background of the Research]

Electride is a compound in which electrons anions be regarded serve as and may as the crystal of solvated electrons. First electride materials were synthesized by dissolving alkali metal into crown ether solutions in 1983. Although these organic electrides attracted attention as an exotic material as cited in university textbooks of inorganic chemistry, their property research remained almost uncultivated due primarily to extremely high sensitivity to heat and oxidation. We realized the first RT-stable electride C12A7:e in 2003 by replacing O<sup>2-</sup> ions as counter anions in  $12CaO \cdot 7Al_2O_3(C12A7)$  with electrons, and found several unique properties such as insulator-metal-superconductor transition and very small work function. Subsequently, we found 2-dimensional electride, Ca2N, in which anionic electrons are sandwiched by cationic [Ca<sub>2</sub>N]<sup>+</sup> slabs. These works stimulated the condensed matter community, leading to rapid growth of research on electride materials worldwide, recently. However, electride research so far has been restricted to anion deficient-type crystalline materials.

Our objective in the project is to cultivate new area of electride materials and their applications based on the recent findings of new crystalline and amorphous electrides.



Fig.1. New electrides reported by our group

## [Research Methods]

Focused fundamentals : Focuses are low dimensional electride materials in electron deficient type, neutral electrides and surface electride materials. Material systems for exploration expand to intermetallic compounds. Applications: Thin film fabrication is examined for electric device applications. In particular, amorphous C12A7:e thin films are focused as an electron-injection layer in the inverted OLEDs which are difficult to fabricate the devices with a good performance.



Figure 2. Inverted OLED

#### [Expected Research Achievements and Scientific Significance]

It is expected that materials concept for electrides is expanded and opportunity of applications based on the intrinsic nature is rather increased. Since amorphous electride is a novel class of amorphous semiconductors, research on this subject would open a new frontier. In device application, inverted OLEDs with performance comparable/superior to the normal type would be realized. We expect the good catalytic activity for new electride materials.

## [Publications Relevant to the Project]

• H.Hosono et al. Superconductivity in room-temperature stable electride and high-pressure phases of alkali metals; Phil. Trans. R. Soc. A373, 20140450-62(2015).

• E. Johnsona, P.V. Sushko, Y.Tomota, and H.Hosono: Electron anions and the glass transition temperature; Proc. Natl. Acad. Sci. USA, 113, 10007-10012(2016).

**Term of Project** FY2017-2021

[Budget Allocation] 134,600 Thousand Yen [Homepage Address and Other Contact Information] http://www.msl.titech.ac.jp/~hosono/