Photoelectron spectroscopy of anionic electron in inorganic electride C12A7:e^-

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$12CaO \cdot 7Al_2O_3$ (C12A7) has a nano-porous structure consisting of positively charged cage framework and free oxygen ions in cages (Fig.1). It is possible to substitute all of the free oxygen ions with electrons, resulting in the formation of so-called electride. Electride is an exotic ionic crystal in which electrons behave like anions. C12A7 based electride (C12A7:e^-), which is the only stable electride in air at room temperature, exhibits high electronic conductivity (1). In theoretical studies, the entrapped electrons of C12A7:e^- are s-orbital like and form metallic additional density of states in the band gap formed by the cage framework as shown in Fig.1 (2).

In this present study, we measured hard X-ray photoelectron spectra (H-XPS) of C12A7:e^- at BL47XU(hν=8keV) of SPring-8. "The framework valence band" composed of O 2p and Al 3s-p orbitals and "electronic states of the substituted electrons entrapped in the cages" were clearly observed in the cage framework band gap as shown in Fig.2. The result relies heavily on the advantage of H-XPS: high sensitivity to s-orbital electrons in bulk states. This observation provides solid evidence that the entrapped electrons form "cage conduction band" in the band gap, which is responsible for the high electronic conductivity in C12A7:e^-.

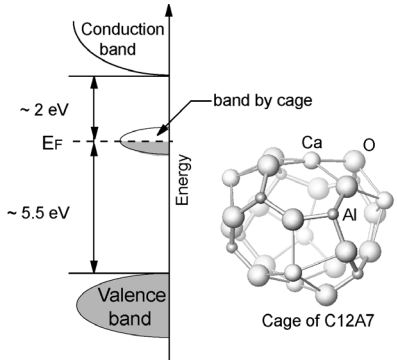

Fig.1 Electronic structure of C12A7:e^- & Crystallographic cage of C12A7

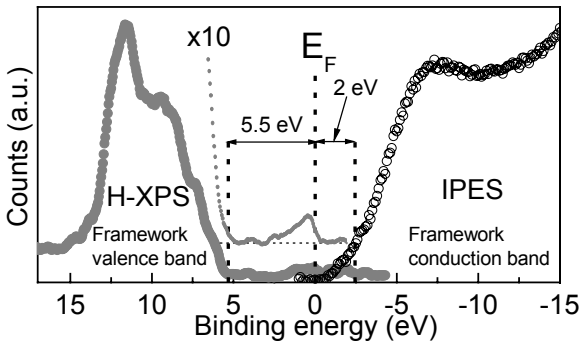

Fig.2 H-XPS & IPES of C12A7:e^- (Framework valence, conduction band and near E_F)

(1) S. Matsuishi et al., *Science* **301**, 626 (2003)
(2) P. V. Sushko et al., *Phys. Rev. Lett.* **91**, 126401 (2003)