

Crystal Structure Analysis of Cationic Lithium
Endohedral Fullerene under Electric Field

Shinobu Aoyagi,¹ Yuki Sado,^{1,2} Kunihisa Sugimoto,³
Ryo Kitaura,² Hisanori Shinohara²

¹*Department of Information and Biological Sciences,
Nagoya City University, Nagoya 467-8501, Japan*

²*Department of Chemistry and Institute for Advanced
Research, Nagoya University, Nagoya 464-8602, Japan*

³*SPring-8/JASRI, Kouto, Sayo, Hyogo 679-5198, Japan*

Metallofullerenes encapsulating metal atoms within the hollow carbon cage are promising materials for molecular devices such as a single molecular memory. Recently, we have achieved the macroscopic synthesis and structure determination of metallofullerenes encapsulating a lithium cation, $\text{Li}^+@\text{C}_{60}$.^[1] The cationic $\text{Li}^+@\text{C}_{60}$ has a high tendency to form ion-pair states with an anion such as SbCl_6^- . The PF_6^- salt, $[\text{Li}^+@\text{C}_{60}](\text{PF}_6)^-$, that forms a rock-salt-type cubic structure has also been obtained.^[2]

The electrostatic attraction between the off-centered Li^+ and anions through the carbon cage implies that the position of the encapsulated Li^+ can be switched by an external electric field. To reveal the effects of external electric fields to the position and thermal motion of the Li^+ inside the carbon cage, the synchrotron-radiation X-ray structure analyses of $[\text{Li}^+@\text{C}_{60}](\text{PF}_6)^-$ under electric fields were performed in this study. The results are shown in this presentation.

[1] S. Aoyagi, E. Nishibori, H. Sawa, K. Sugimoto, M. Takata, Y. Miyata, R. Kitaura, H. Shinohara, H. Okada, T. Sakai, Y. Ono, K. Kawachi, K. Yokoo, S. Ono, K. Omote, Y. Kasama, S. Ishikawa, T. Komuro, H. Tobita, *Nature Chem.*, **2** (2010) 678-683.

[2] S. Aoyagi, Y. Sado, E. Nishibori, H. Sawa, H. Okada, H. Tobita, Y. Kasama, R. Kitaura, H. Shinohara, *Angew. Chem. Int. Ed.*, **51** (2012) 3377-3381.