

Ultraviolet Photoelectron Spectra of Two Ti Atoms Encapsulated Metallofullerenes

Shojun Hino, Takema Miyazaki and Kentaro Iwasaki,
Faculty of Engineering, Chiba University
Inage-Ku, Chiba 263-8522 Japan
Daisuke Yoshimura
Institute for Molecular Science,
Okazaki 444-8585 Japan
Baopeng Cao, Toshiya Okazaki and Hisanori Shinohara
Graduate School of Science, Nagoya University
Chikusa-Ku, Nagoya, 464-8602 Japan

Fullerenes are able to accommodate metal atoms inside their cage, and encapsulation of the metal atoms induces electron transfer from the metal atoms to the cage. Determination of the amounts of transferred electrons is one of the important issues concerning with the science of metallofullerenes. Recently two Ti atoms encapsulated metallofullerenes $Ti_2@C_{80}$ [1] and $Ti_2@C_{84}$ [2] have been isolated. Since Ti is a group IV element, an estimation of the amounts of transferred electrons from its chemical nature is difficult. Therefore, experimental and theoretical determination of the amounts of transferred electrons is strongly desired from a view point of both scientifically and implicational purposes. Photoelectron spectroscopy is one of methods to estimate the amounts of transferred electrons.

We have succeeded to measure ultraviolet photoelectron spectra (UPS) of $Ti_2@C_{80}$. The spectra have been measured at BL8B2 of Ultraviolet Synchrotron Orbital Radiation (UVSOR) Facility at Institute for Molecular Science. The specimen for the measurement was a vacuum deposited $Ti_2@C_{80}$ film sublimed from a quartz crucible. Sublimation temperature of $Ti_2@C_{80}$ was around 450 C. Thickness of the deposited film was about 12 nm.

The UPS of $Ti_2@C_{80}$ are shown in the figure. The spectra are referred to the Fermi level (E_F) of the spectrometer and plotted as a function of binding energy. Spectral onset is about 0.7 eV below the E_F , which indicates semi-conductive nature of $Ti_2@C_{80}$. There are 7 distinct structures in this spectral region. Their intensity changes when the incident photon energy is tuned. This is a characteristic behavior for the photoelectron spectra of fullerenes and this finding is another evidence that C_{80} containing two Ti metal atoms has a cage structure. It should be noted that a structure located at about 2.4 eV is clearly observed only in the spectra obtained with 45 eV and a structure at about 4.6 eV is clearly observed only when the specimen was irradiated with 25 -30 eV photon.

Present specimen of $Ti_2@C_{80}$ is a mixture of isomers having symmetry of I_h and D_{5h} . The ratio of I_h to D_{5h} is 1 : 3. Because of this we cannot distinguish the contribution of each isomer from the whole spectra. Molecular orbital (MO) calculation is under the way to distinguish the origin of each structure. At the conference assignment of the spectra will be presented.

We are planning to measure the UPS of another Two Ti metal atom encapsulated metallofullerene $Ti_2@C_{84}$. Its result will also be presented at the conference.

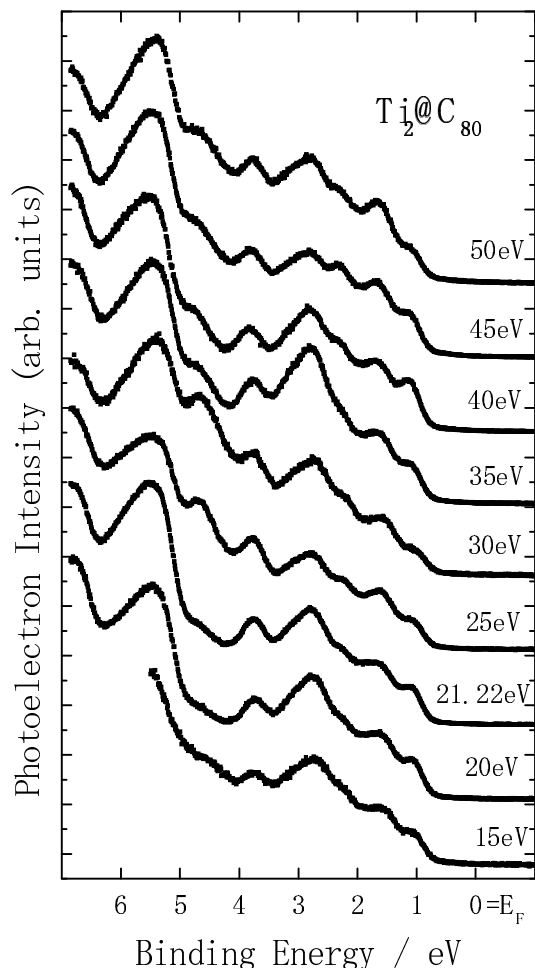


Figure Ultraviolet photoelectron spectra of $Ti_2@C_{80}$.

References

- 1) B.-P. Cao, M. Hasegawa, K. Okada, T. Tomiyama, To Okazaki, K. Suenaga, H. Shinohara, J. Ame. Chem. Soc. 123, 9679 (2001).
- 2) B.-P. Cao et al. private communication and to be published.