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Photoemission Spectra of C_{60} Fullerene-Peapod

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Introduction

Hybrid carbon material consisting of single-walled carbon nanotubes (SWNTs) and C_{60} fullerenes, known as C_{60} peapod (C_{60} PPD), has been intensively studied both theoretically and experimentally because of its exotic nano-scale structure. Okada *et al.* [1] and Otani *et al.* [2] performed the local density approximation calculation; the orbital mixing between the nearly-free-electron states of SWNTs and the π orbitals of C_{60} fullerenes leads to the intersection of the lowest unoccupied molecular orbital (LUMO) band of the C_{60} fullerene with the Fermi level (E_F). In this study, we have measured the photoemission spectra of SWNT and C_{60} PPD samples [3].

Experimental

The photoemission experiments were performed using synchrotron radiation at the beam line BL-11D of the Photon Factory, High Energy Accelerator Research Organization (KEK) at the beam line BL-1 of the Hiroshima synchrotron radiation research center (HiSOR), Hiroshima University. The inverse photoemission spectra were measured in Tokyo Metropolitan University. SWNT samples were prepared by the laser vaporization method [4]. The mean diameters of SWNTs in the C_{60} PPD-A and PPD-B samples were estimated to be 1.40 and 1.28 nm, respectively.

Results and Discussion

We measured the photoemission spectra of the SWNT and C_{60} PPD samples at $h\nu$= 65 eV. The photoemission spectra of the C_{60} PPD are, as a whole, similar to those of the SWNT [4]. The spectrum of the C_{60} fullerenes inside the SWNT was obtained by subtracting the empty SWNT spectrum from the C_{60} PPD spectrum. The spectra near E_F obtained for the PPD-A and PPD-B samples are shown in Fig. 1, together with the spectra of a C_{60} fcc solid obtained by Weaver [5]. The overall spectral features are very similar to those of the C_{60} solid spectrum [5]. The peak at the binding energy of 2.3 eV is derived from the highest occupied molecular orbital (HOMO) with h_u symmetry with fivefold degeneracy. The peak is derived from the next HOMO (NHOMO) with g_g and h_g symmetry with ninefold degeneracy. The peak located at −1.1 eV can be assigned to a LUMO level with t_{1u} symmetry with threefold degeneracy.

According to the theoretical calculation [1, 2], the t_{1u} level intersects with E_F when the SWNT diameter is larger than 1.28 nm. As shown in the figure, however, there is no structure in binding energies ranging from the onset of the HOMO peak to E_F; the t_{1u} peak stays above E_F. These results are consistent with the experimental results of the potassium and electrochemical doping effect [6]. It is concluded that the t_{1u} level of the C_{60} fullerenes inside the SWNT stays above E_F even when the SWNT mean diameter is larger than 1.4 nm.

References

[1] S. Okada et al., Phys. Rev. Lett. 86, 3835 (2001).
[2] M. Otani et al., Phys. Rev. B 68, 125424 (2003).
[3] H. Shiozawa et al.: Phys. Rev. B 73, 075406 (2006).
[4] H. Ishii et al., Nature 426, 540 (2003).
[5] J. H. Weaver et al., Phys. Rev. Lett. 66, 1741 (1991).
[6] T. Pichler et al., Phys. Rev. B 67, 125416 (2003).

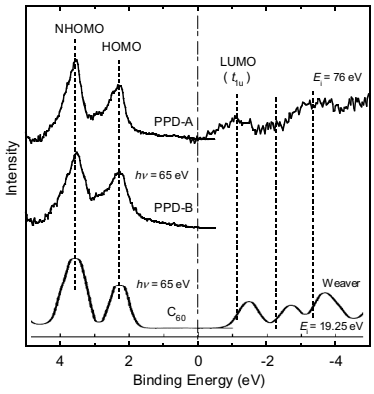

Figure1: Photoemission and inverse photoemission spectra of the C_{60} fullerene in SWNT together with the spectra of a C_{60} solid taken from Ref. 5. The inverse photoemission spectra were measured with tunable photon energy mode using the incident electron beam with the constant energy (E_i).

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