Near Infrared Emission Property Variation of Chemically Functionalized Single-walled Carbon Nanotubes Based on Structures of Chemical Modifiers

([1]*Department of Applied Chemistry, Kyushu University,* [2]*International Institute for Carbon-Neutral Energy Research (I2CNER), Kyushu University,* [3]*Center for Molecular Systems (CMS), Kyushu University*) ○ Tomohiro Shiraki[1,2], Haruka Aoki[1], Keita Hayashi[1], Tsuyohiko Fujigaya[1,2,3]

Keywords: Carbon Nanotube, Photoluminescence, Near Infrared Light, Chemical Modification, Defect

Local chemical functionalization of single-walled carbon nanotubes (SWCNTs) has been developed to enhance their photoluminescence (PL) properties in the near infrared (NIR) region.[1-4] In this functionalization, local defects such as sp^3 carbon are doped to the semiconducting crystalline sp^2 carbon networks of SWCNTs based on chemical bond formation between modifier molecules and the tube walls. As a result, emissive doped sites that have narrower bandgaps and exciton trapping features are created in the locally functionalized SWCNTs (lf-SWCNTs). Accordingly, new E_{11}* PL appears with red-shifted wavelengths and increased PL quantum yields compared with original E_{11} PL of pristine SWCNTs. To date, chemical modifiers such as aryldiazonium salts and halogenated compounds have been used and the molecular functionalization has allowed to modulate E_{11}* PL emission properties of lf-SWCNTs.

Here, organic azide compounds are used for a [2+1] cycloaddition reaction with SWCNTs, which aims for the synthesis of lf-SWCNTs (lf-SWCNTs>N). The local chemical functionalization was conducted by mixing solubilized SWCNTs in an aqueous micelle solution and an azide compound under light irradiation. Fig. 1 shows PL spectra of SWCNTs before and after the functionalization. For the lf-SWCNTs>N, a new PL peak appeared at 1116 nm that was observed in the longer wavelength region than E_{11} PL at 977 nm. In the XPS measurements of the lf-SWCNTs>N, N1s peak was clearly observed around 400 eV. Therefore, azide compounds could offer new series of defect doping modifiers to produce E_{11}* PL characters for lf-SWCNTs.

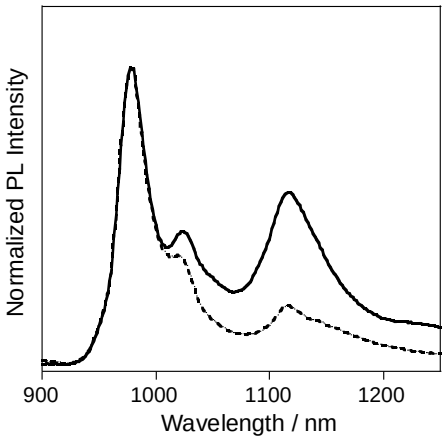

Fig. 1 Normalized PL spectra of lf-SWCNTs>N (solid line) and pristine SWCNTs (dashed line), λ_{ex} = 570 nm.

1) T. Shiraki, *Chem. Lett*., **2021**, *50*, 397. 2) T. Shiraki *et al*., *Acc. Chem. Res.*, **2020**, *53*, 1846. 3) S. Tretiak *et al*., *Acc. Chem. Res.*, **2020**, *53*, 1791. 4) Y. Wang *et al*., *Nat. Rev. Chem.*, **2019**, *3*, 375.