Supporting Information

Identifying Effects of TiO$_2$ Nanowires inside Bulk Heterojunction Organic Photovoltaics on Charge Diffusion and Recombination


In the FTIR spectrum of PCBAcid, the double peaks at 708 and 765 cm$^{-1}$ correspond to the C-H bonds, the peaks at 1608 and 1099 cm$^{-1}$ are from C=O and C-O bonds on the side chain, respectively, and the C$_{60}$ in the PCBAcid has two peaks in the FTIR spectrum at 520 and 1378 cm$^{-1}$.

Conversely, the TiO$_2$-NW exhibits only one broad band from 900 to 450 cm$^{-1}$ with a peak position at 491 cm$^{-1}$. After 20 h coating, a slight shift in peak position from 491 cm$^{-1}$ to 495 cm$^{-1}$ was observed and two new peaks were found at 1611 and 1410 cm$^{-1}$. With longer coating (40 h), these peaks were further shifted, and several new peaks appeared at 1102 cm$^{-1}$. Surface modification causes the shift in the main peak of TiO$_2$-NW from 491 to 499 cm$^{-1}$, as well as the new peak at 1416 cm$^{-1}$. The new peaks at 1614 and 1102 cm$^{-1}$ on the coated TiO$_2$-NW are from C=O and C-O in the carboxylic acid connecting the C$_{60}$ and TiO$_2$-NW. The slight shifting of the peaks from these two bonds indicates formation of new bonds in adjacent atoms. Therefore, the FTIR spectrum shows that a self-assembled monolayer from PCBAcid was formed on the surface of TiO$_2$-NW.

Reference