Design of Novel D-π-A Organic Dyes for Dye-Sensitized Solar Cells

Japan Advanced Institute of Science and Technology[1], China University of Petroleum (Beijing)[2],

Chunmeng Liu[1,2], Zhenqing Yang[2], Changjin Shao[2], Yoshifumi Oshima[1]

E-mail: s1720432@jaist.ac.jp

Dye sensitizer was recognized as the most important part for dye-sensitized solar cells (DSSC) to get high power conversion efficiency (PCE). However, to obtain the dyes with good performance is still a challenge. It is necessary to design highly efficient sensitizers with broad absorption spectra and good electron transfer mechanism for improving PCE of DSSC.

We designed novel donor-π-acceptor (D-π-A) structure dyes SPL101-SPL108[1] based on the experimentally synthesized C217 dye (which exhibited a high PCE of 9.8%, under AM1.5G full sunlight) by modifying π-conjugated bridge and acceptor. For selecting the highly efficient dyes, we obtained their energy levels, absorption spectra, frontier molecular orbital and optimized geometrical structures by using density functional theory (DFT) and time-dependent DFT (TDDFT). And we further estimated light harvesting efficiency, driving force of injection and regeneration which influence the PCE of DSSC. Firstly, we modified π-conjugated bridge of C217 and obtain SPL101-104. We found that the dyes with coplanar structure π-conjugated bridge (SPL103, SPL104) have larger absorption peak redshift, higher molar extinction coefficient and efficient electron transfer from donor to acceptor group. Then we further modified the acceptor based on SPL103 and SPL104 and obtain SPL105-108. we found that the dyes SPL106 and SPL108 with coplanar structure group as π-conjugated bridge and dicyanovinyl sulfonic acid group as acceptor have broader extent of absorption spectra (which covering entire visible range up to the near-IR region of 1200nm compared to C217 dye as shown in Figure 1), smallest energy gaps, improved light harvesting efficiency and faster electron injection and regeneration mechanism. Therefore, we think SPL106 and SPL108 are better candidates among all the new designed dyes for improving PCE of DSSC.

It is expected that this work can provide a new strategy for the design and synthesize of new dyes with excellent performance for highly effective DSSC.

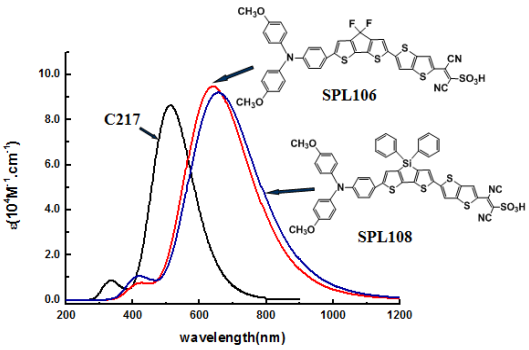

Figure 1. Absorption spectra of dyes SPL106, SPL108 and C217

(1) Yang Z, Liu C, Shao C, et al. Journal of Physical Chemistry C, 2015, 119 (38): , 21852−21859.

© 2018年 応用物理学会