

Director de tesis: Dr. José Luis Maldonado Rivera

Sinodales: Dr. Bernardo Antonio Frontana Uribe
(Sinodal Externo - Instituto de Química, UNAM y CCIQS-UAEMéx, UNAM; Secretario)

Dra. Ma. Concepción Arenas Arrocena
(Sinodal Externa – ENES UNAM, Vocal)

Dr. José Luis Maldonado Rivera
(Director de Tesis, Presidente del Jurado)

Tesis: **“ANALYSIS THROUGH EQE AND STM OF ORGANIC SOLAR CELLS, BASED ON PTB7, PTB7-TH AND PBDB-T DONORS”**

Resumen:

In the present thesis, external quantum efficiency (EQE or IPCE) technique was implemented. This home-made set up was used as a complementary characterization to better understand solar cell performance and to find optimal fabrication conditions. Organic photovoltaic solar cells (OPVs) were fabricated using commercial electron-donor polymers PTB7, PTB7-Th and PBDBT, and electron-acceptors PC71BM, ITIC and FeS₂, and by means of scanning tunneling microscopy (STM), donor film molecular ordering was analyzed. These measurements indicate that PTB7-Th film chains are somewhat thicker and less spaced than those in PTB7 based OPVs, which could possibly provide better electrical charge transport. Besides, PBDB-T, with a shorter distance between polymer backbone chains, could facilitate a more efficient intramolecular charge separation, and thus improve charge transfer from the active layer to the OPV electrodes. For PTB7 based OPVs, non-toxic iron sulfide (FeS₂) nanocrystals (NCs) were added to the active layer at different weight ratios as a second electron-acceptor, achieving an increase in power conversion efficiency (PCE) of 21%. For PTB7-Th based OPVs (best achieved PCE was 7.65%), optoelectrical analyses were carried out using EQE and internal quantum efficiency (IQE), applying active layer thickness variation (from 40 to 165 nm) by means of the transfer matrix method (TMM). Our results show a significant reduction of IQE (when increasing the active layer thickness above 120 nm), and consequently, also of EQE and PCE, mainly due to the reduction in charge carrier collection probability. A comparison between the experimental measurements and theoretical simulations was discussed in order to have better understanding of the OPVs performance. Finally, PBDB-T:ITIC based OPVs were tested with different hole transport layers (HTLs): PEDOT:PSS, fluorinated reduced graphene oxide (F-rGO)/PEDOT:PSS and just F-rGO. With F-rGO/PEDOT:PSS and PEDOT:PSS as HTLs, average PCEs of 8.3% and 8.7% were achieved, respectively (the highest efficiency reached with PEDOT:PSS was 8.9%), and with FrGO, efficiency decayed to 5.4%. Device stability maintained a similar trend with the use of either F-rGO/PEDOT:PSS or PEDOT:PSS; however, for the F-rGO case, stability showed a faster decay.