Density Functional Theory-Guided Design of Boronic Acid-Based Self-Assembled Monolayers for ITO Modification in Organic Solar Cells

Çisem Kırbıyık Kurukavak[1], Merve Yurdakul[1], Mütahire Tok[2], Hakan Fidan[3], Mustafa Can[4], Mahmut Kuş[1]

[1] Department of Chemical Engineering, Konya Technical University, 42075, Konya, Turkey
[2] Department of Pharmacy Services, Vocational School, Yuksek Ihtisas University, 06291 Ankara, Turkey
[3] Department of Forest Industry Engineering, Forest Faculty, İzmir Katip Çelebi University, İzmir, Türkiye
[4] Department of Engineering Sciences, Faculty of Engineering and Architecture, İzmir Katip Çelebi University, İzmir, Türkiye

Abstract

Organic solar cells (OSCs) are gaining attention in the field of photovoltaic technology because of its low-cost fabrication, easy processability, flexibility and modulation properties. Currently, interfacial modification is one of the most effective strategies for enhancing the performance of OSCs. Among the various interfacial modification approaches, self-assembled monolayers (SAMs) have emerged as particularly promising materials for tailoring the electrical and morphological properties of indium tin oxide (ITO). Here, we studied the properties of 4,4'-[(N,N'-Bis(4-methylphenyl)-1,4-phenylenediamine)]bis(benzene-1,3-diyl)diboronic acid (BA-25) and (4-(bis(4-(hexyloxy)phenyl)amino)phenyl)boronic acid (BA-27) SAMs theoretically through density-functional theory (DFT) and utilized them as novel SAMs to modify ITO surfaces in OSCs. It was aimed to increase the power conversion efficiency (PCE) of OSCs with the ITO/SAM/PEDOT:PSS/P3HT:PCBM/LiF/Al configuration. According to photovoltaic characterization results, the introduction of BA-25 and BA-27 SAMs resulted promising device performances of 2.52% and 2.33%, respectively, which were higher than control device performance (1.98%). We report that the integration of both BA-25 and BA-27 into the device structure successfully tune the work function of ITO and improves the coverage of the overlying layers, thereby enhancing the photovoltaic performance of the resulting devices.