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$Ti_3C_2T_X$ MXene Hole Transport Layer for Polymer Non-Fullerene Solar Cells

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Conjugated polymers have been intensively studied due to their unique properties including having a light weight and mechanical flexibility, being environmentally friendly, and having easily tunable energy levels which make these materials very attractive for several optoelectronic applications, such as solar cells [1]. Significant improvement in power conversion efficiency (PCE) of polymer solar cells (PSCs) has been realized when polymers are blended with non-fullerene acceptors (NFA) as NFAs have several advantages namely high absorption coefficient and highly tunable molecular energy levels [2, 3]. To date, the PCE of solar cells based on polymer donor and non-fullerene acceptor has surpassed 17% [4]. The charge transport layer is an essential component of efficient polymer non fullerene solar cells as it plays the crucial role in charge transport and recombination [5]. The charge transport layer poly (3,4-ethylene dioxythiophene): poly(styrenesulfonate) (PEDOT:PSS) has been used as an effective hole transport layer in PSCs for over a decade. However, the hygroscopic nature of PEDOT:PSS usually limits the stability and efficiency of PSCs, and therefore the exploration of efficient materials for the hole transport layer remains a critical challenge. . In this work, we used the two-dimensional Ti_3C_2 MXene as an efficient hole transport layer to study the charge transport properties in PSCs. MXenes have unique properties including high electrical conductivity, high transparency in the visible range, hydrophilicity, and structural diversity. We used poly[(2,6-(4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)-benzo[1,2-b:4,5-b0]dithiophene))-alt-(5,5-(10,30-di-2-thienyl-50,70-bis(2 ethylhexyl)benxo[10,20-c:40,50-c0]dithiophene-4,8-dione))](PBDB-T):3,9-bis(2-methylene-(3-(1,1-dicyanomethylene)-indanone))-5,5,11,11-tetrakis(4-hexylphenyl)-dithieno[2,3-d:20,30-d0]-s-indaceno[1,2-b:5,6-b0]-dithiophene (ITIC) blend as an active layer and studied the impact of charge transport layer on morphology and charge transport of this blend using Atomic Force Microscopy (AFM).

The donor polymer PBDB-T and non -fullerene acceptor ITIC were purchased from 1-Materials and used as received without further purification. PEDOT:PSS was purchased from Sigma Aldrich and $Ti_3C_2T_X$ MXene was synthesized by selectively etching the aluminum (A-layer) of the commercially-available Ti_3AlC_2 MAX phase with a LiF/HCl solution for 24 hours at ambient temperature. Blend solution of PBDB-T:ITIC (1:1 w/w) was prepared by dissolving in chlorobenzene and stirring at 80^0 C for 12 hours. The concentration of blend solution was 10 mg/ml. The indium tin oxide (ITO) glass substrates were cleaned ultrasonically using deionized water, acetone, and isopropanol for 15 min per cleaning solvent before spin casting. PEDOT:PSS and MXene were spin coated at 3000 rpm on ITO and annealed at 130^0 C for 10 minutes. Blend films were prepared by spin casting the PBDB:ITIC solution on PEDOT:PSS and MXene at 1000 rpm for 60 s.

Morphology of PBDB:ITIC on PEDOT:PSS layer shows root mean square (RMS) roughness of 15.7 nm and maximum height of 101 nm (**Figure 1a**) whereas PBDB:ITIC prepared on MXene layer has shown the RMS roughness 6.2 nm and maximum particle size up to 72.4 nm (**Figure 1b**). Our results indicate that the charge transport layer underneath the active layer impacts the nanomorphology of PBDB-T:ITIC blend. This difference in morphology can cause differences in performance of these solar cells. The current sensing atomic force microscopy (CSAFM) image showed a maximum current of 2.48

pA (**Figure 2a**) for PBDB-T:ITIC blend on PEDOT:PSS whereas it is at a level of 45 pA (**Figure 2b**) for PBDB-T:ITIC blend on MXene indicating that higher current is observed with MXene interface. This study will provide important information about the enhancement of current in MXene-based polymer solar cells [6].

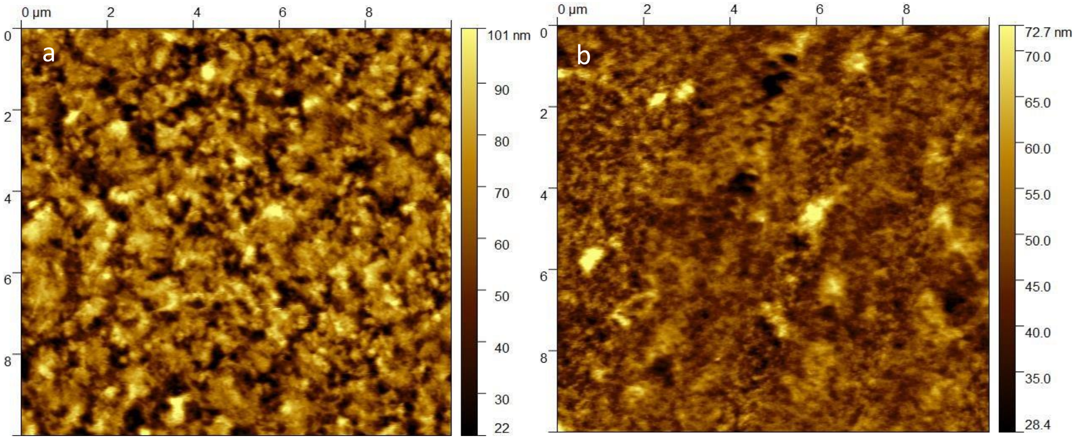

Figure 1. Atomic force microscopy topography image of (a) PBDB-T:ITIC film on PEDOT:PSS (b) PBDB-T:ITIC film on MXene.

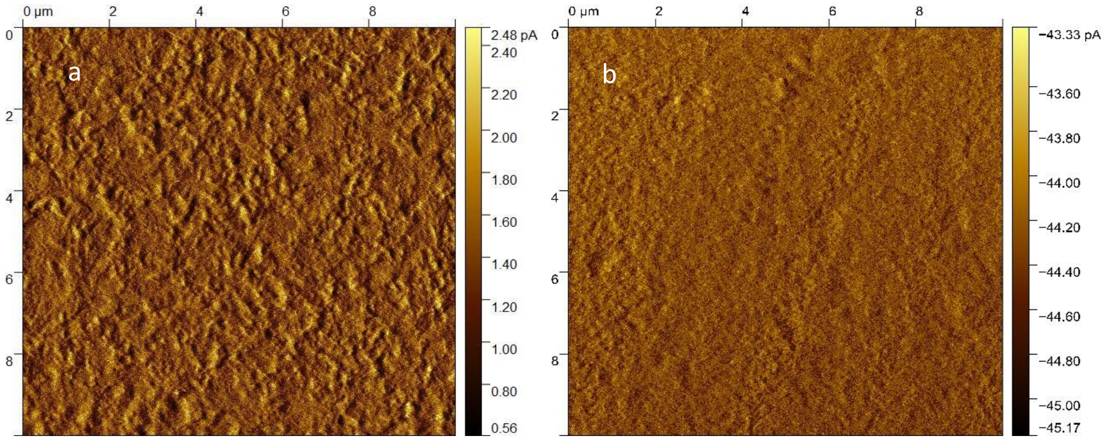

Figure 2. Current sensing atomic force microscopy image of (a) PBDB-T:ITIC film on PEDOT:PSS (b) PBDB-T:ITIC film on MXene.

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