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Surface Modification of TiO2 Layer with Phosphonic Acid Monolayer in Perovskite Solar Cells: Effect of Chain Length and Terminal Functional Group

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Abstract : In this study, charge extraction characteristics at the perovskite/TiO2 interface in the conventional perovskite solar cell is studied by interface engineering. Self-assembled monolayers of phosphonic acids with different chain length and terminal functional group were used to modify mesoporous TiO2 surface to modulate the surface property and interfacial energy barrier to investigate their effect on charge extraction and transport from the perovskite to the mp-TiO2 and then the electrode. The chain length introduces a tunnelling distance and the end group modulate the energy level alignment at the mp-TiO2 and perovskite interface. The work function of these SAM-modified mp-TiO2 varied from −3.89 eV to −4.61 eV, with that of the pristine mp-TiO2 at −4.19 eV. A correlation of charge extraction and transport with respect to the modification was attempted. The study serves as a guide to engineer ETL interfaces with simple SAMs to improve the charge extraction, carrier balance and device long term stability. In this study, a maximum PCE of ~16.09% with insignificant hysteresis was obtained, which is 17% higher than the standard device.

Keywords : Energy level alignment, Interface engineering, Perovskite solar cells, Phosphonic acid monolayer, Tunnelling distance
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