

## Surface Modification of TiO<sub>2</sub> 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/TiO<sub>2</sub> 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 TiO<sub>2</sub> 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-TiO<sub>2</sub> and then the electrode. The chain length introduces a tunnelling distance and the end group modulate the energy level alignment at the mp-TiO<sub>2</sub> and perovskite interface. The work function of these SAM-modified mp-TiO<sub>2</sub> varied from -3.89 eV to -4.61 eV, with that of the pristine mp-TiO<sub>2</sub> 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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