

SUPPORTING INFORMATION

Halogen-substituted Fullerene Derivatives for Interface Engineering in Perovskite Solar Cells

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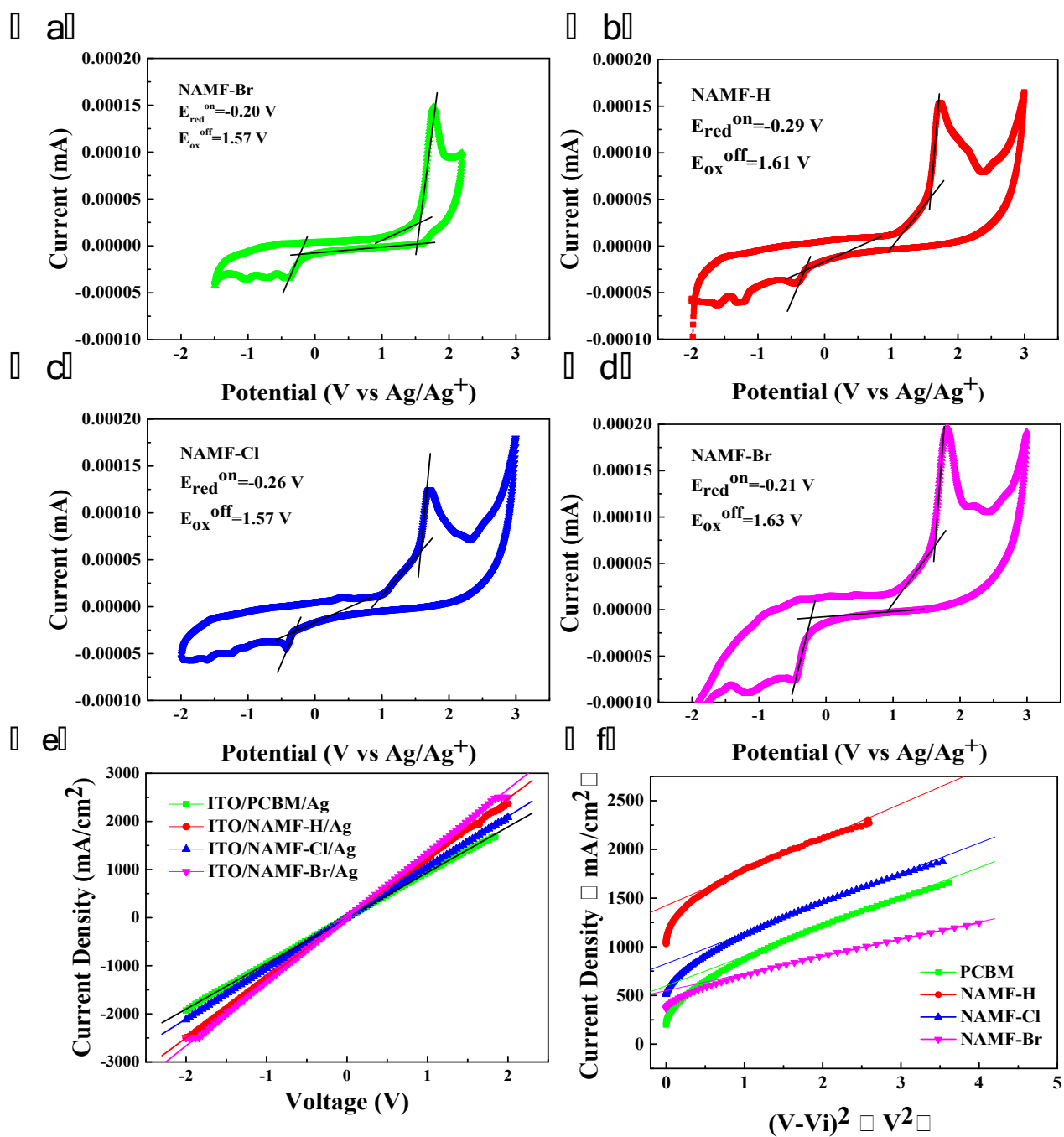


Fig. S1. Cyclic voltammograms of (a) PCBM, (b) NAMF-H, (c) NAMF-Cl and (d) NAMF-Br films. The dark $J-V$ curves to calculate (e) conductivity and (f) mobility of fullerene derivatives.

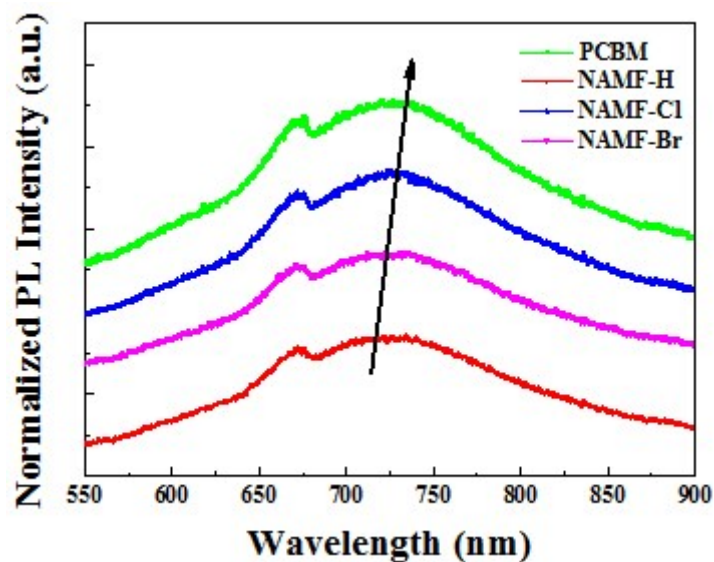


Fig. S2. The PL spectra of thin films of different fullerene derivatives.

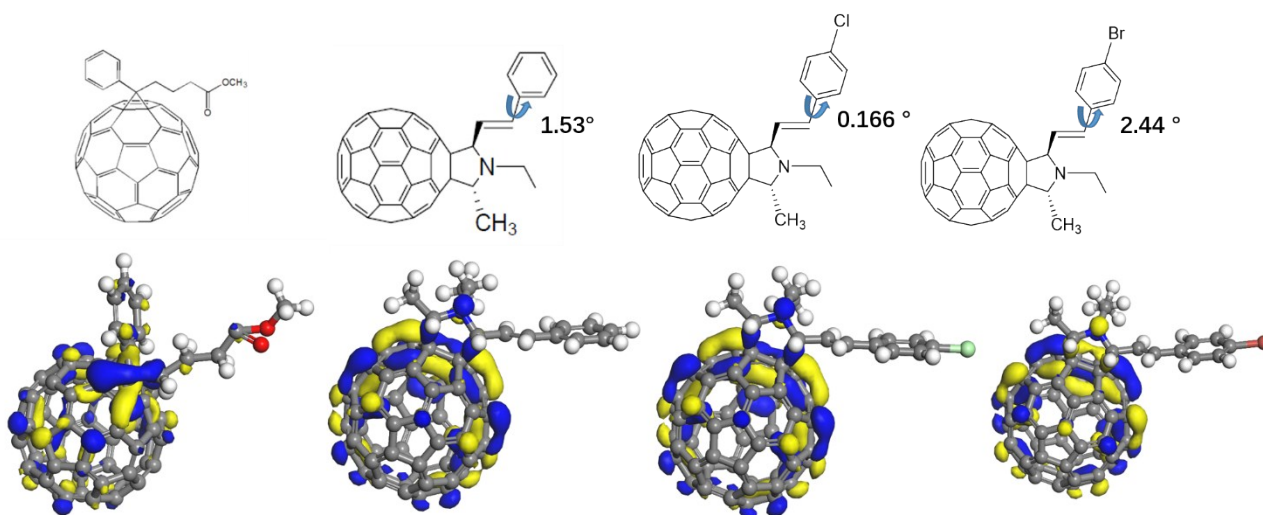


Fig. S3. Computed orbit profiles of NAMF-H, NAMF-Cl, NAMF-Br and PCBM. Quantitative values of LUMO orbit and dihedral angle are in arbitrary unit.

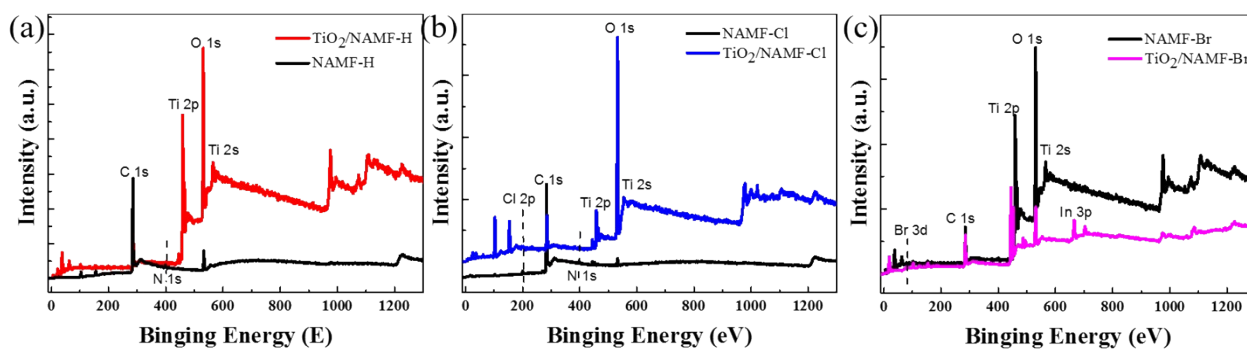


Fig. S4. (a-c) XPS spectra of the fullerene derivatives and TiO₂/fullerene derivative bilayers.

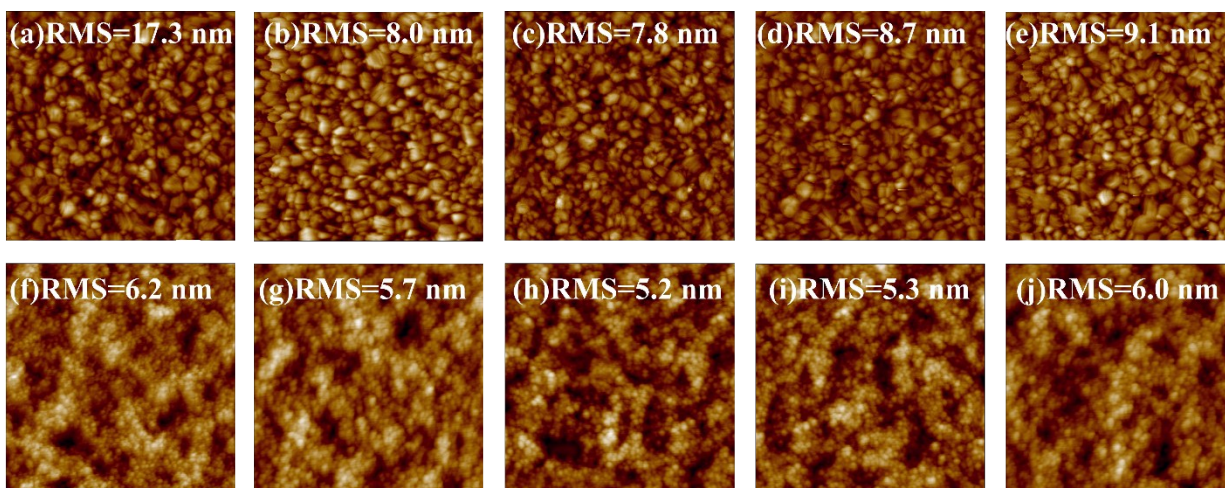


Figure S5. Images from scanning probe microscope (SPM) showing the surface morphology for (a) TiO_2 /perovskite, (b) TiO_2 /PCBM/perovskite, (c) TiO_2 /NAMF-H/perovskite, (d) TiO_2 /NAMF-Cl/perovskite, (e) TiO_2 /NAMF-Br/perovskite, (f) TiO_2 , (g) TiO_2 /PCBM, (h) TiO_2 /NAMF-H, (i) TiO_2 /NAMF-Cl and (j) TiO_2 /NAMF-Br/perovskite.

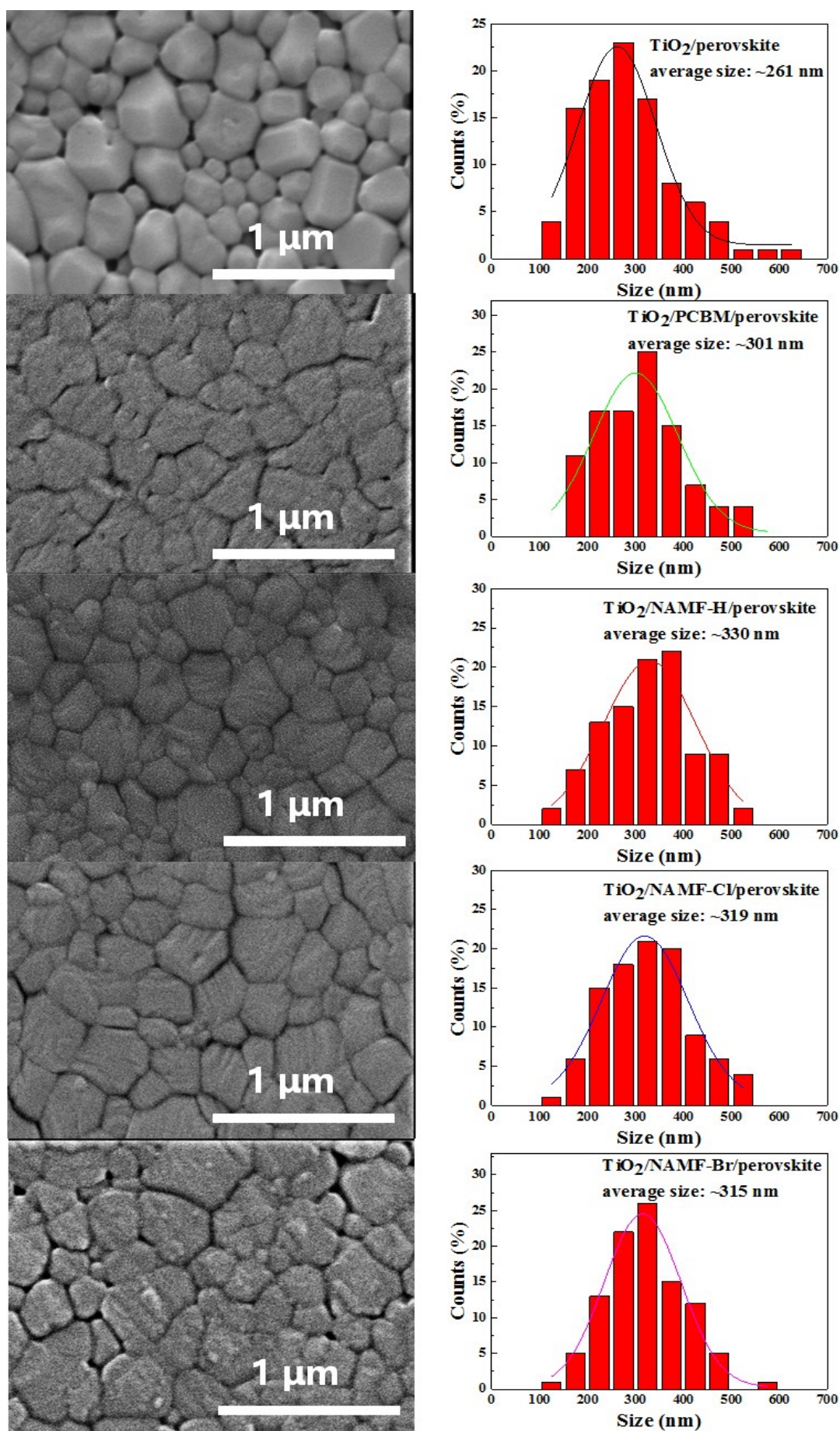


Fig. S6. SEM images of perovskite films cast on different fullerene derivative surfaces: (a) pure TiO_2 ; (b) TiO_2/PCBM ; (c) $\text{TiO}_2/\text{NAMF-H}$; (d) $\text{TiO}_2/\text{NAMF-Cl}$; (e) $\text{TiO}_2/\text{NAMF-Br}$.

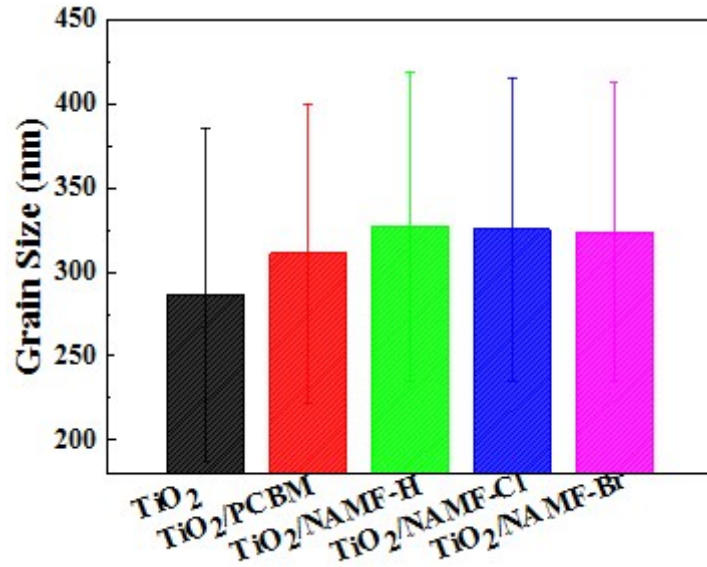


Fig. S7. Grain size evaluation of MAPbI₃ cast on different fullerene interlayers from SEM surface images: The histogram represents the mean value, and the error bar stands for the standard deviation.

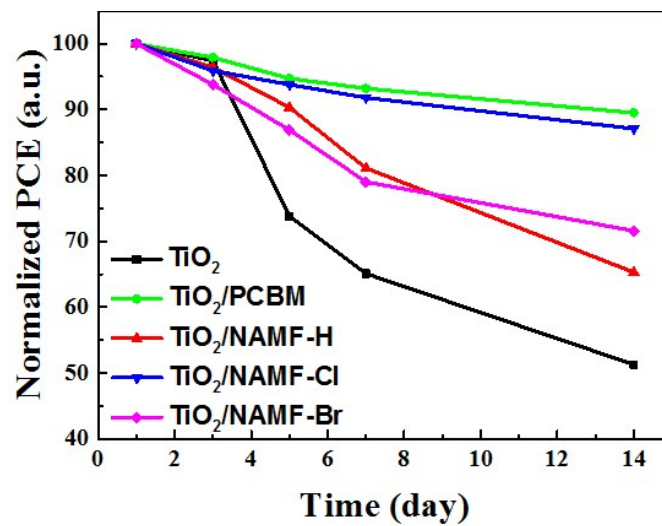


Fig. S8. The evolution of device PCE obtained by storing unencapsulated devices in ambient conditions having a relative humidity of $40 \pm 5\%$ and an average temperature of 25 °C.

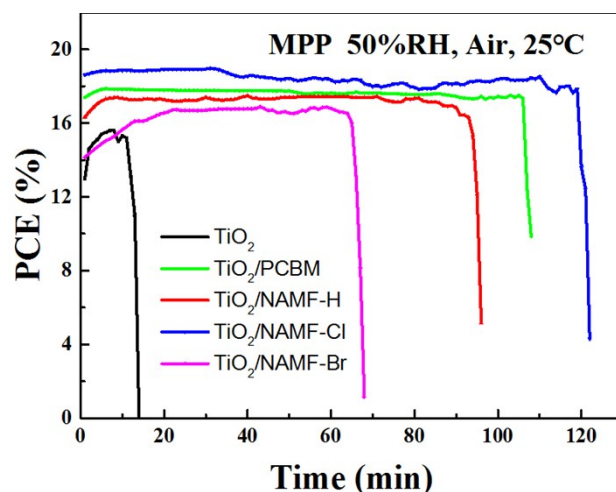


Fig. S9. Operational lifetimes of PSCs at the maximum power point (MPP) and ambient condition.

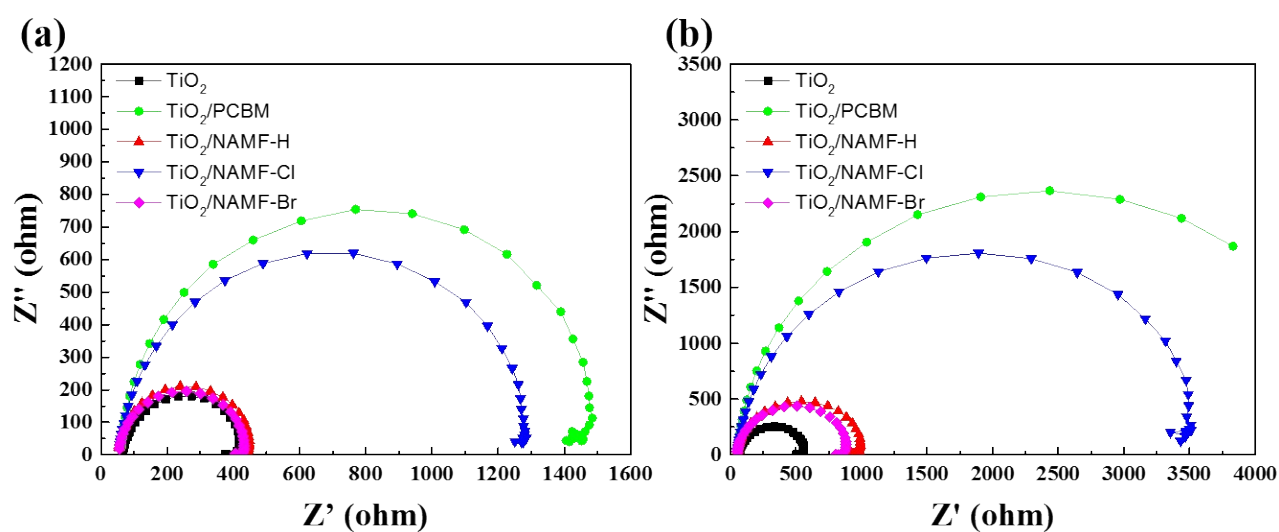


Figure S10. Electrochemical impedance spectroscopy (EIS) measurements. Nyquist plots for the PSCs with and without fullerene derivative interlayers at an applied bias of (a) 0.8V and (b) 0.2V.

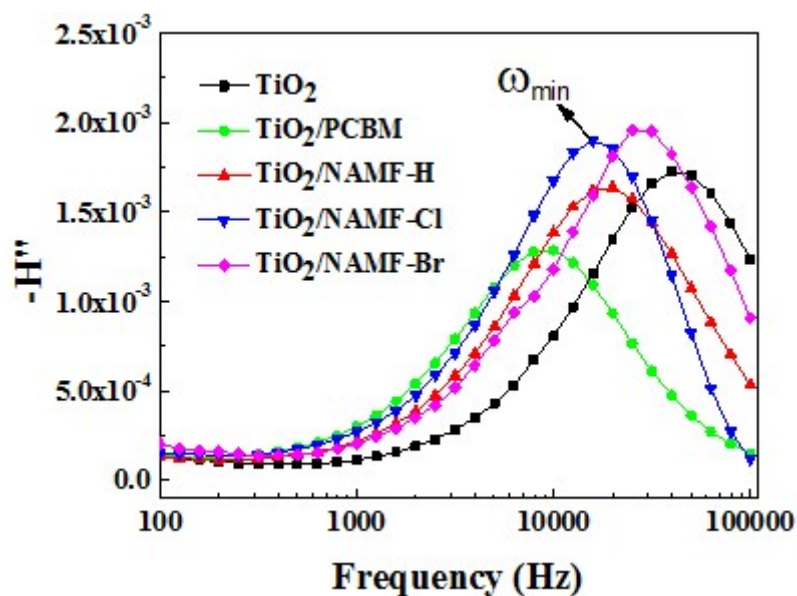


Figure S11. IMVS measurements of PSCs with and without fullerene derivative interlayers.