Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.


**Supporting Information**

# Insights into the passivation effect of atomic layer deposited hafnium oxide for efficiency and stability enhancement in organic solar cells

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**Additional Figures**

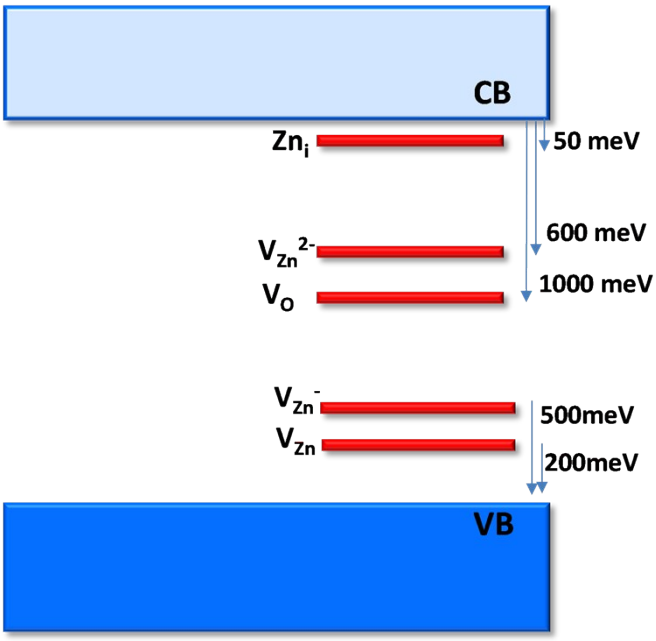



**Figure S1** Schematic diagram depicting the various defect states in ZnO.[1-4]

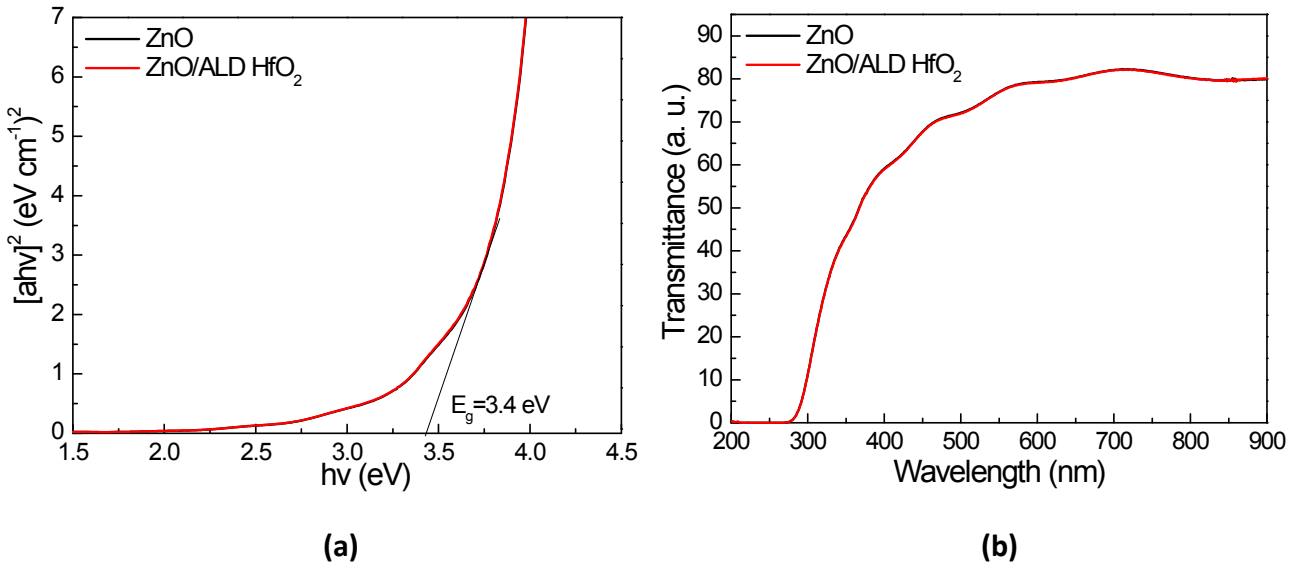



**Figure S2** (a) Tauc plots as derived from UV-vis absorption measurements and (b) transmittance spectra of ~50 nm either as-deposited or passivated with 6 cycles of ALD $HfO_2$ ZnO films on glass/FTO substrates.

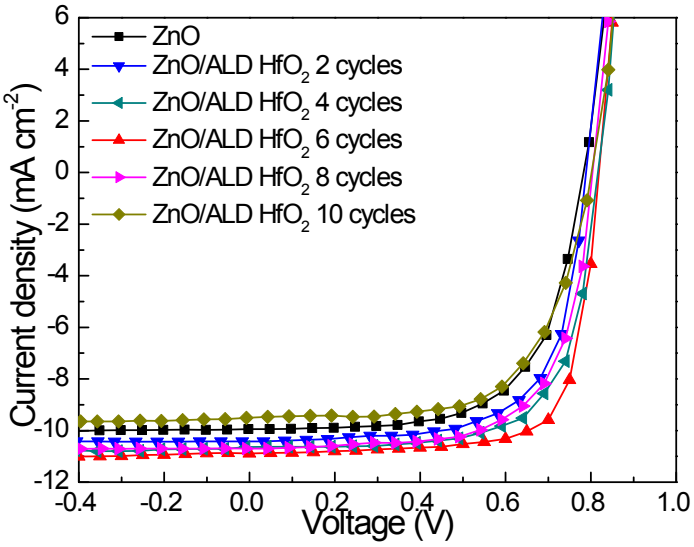
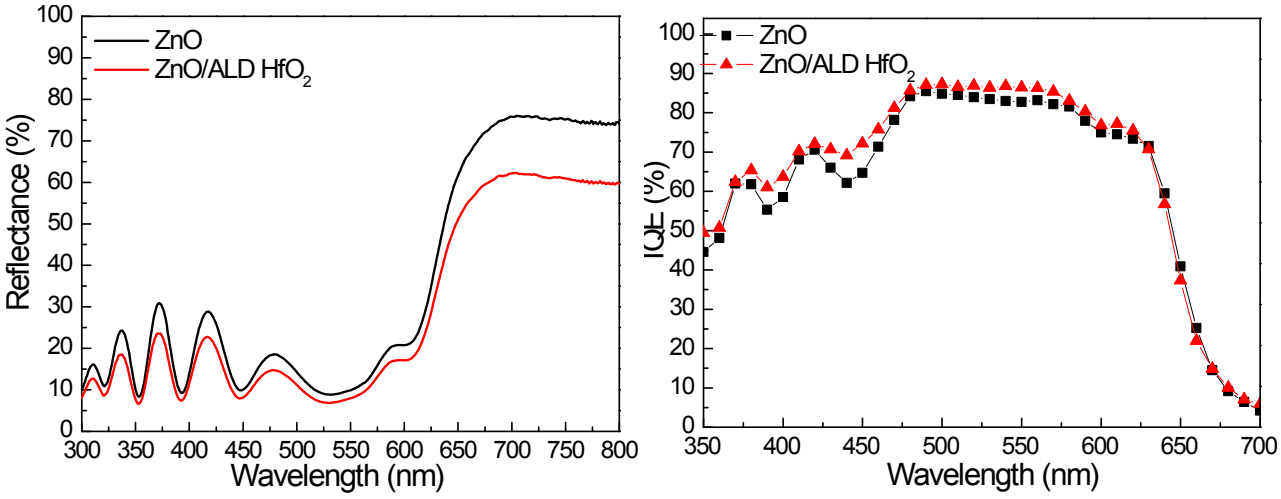



**Figure S3** J-V characteristics under 1.5 AM illumination of P3HT:$IC_{60}BA$-based devices containing different cycles of ALD $HfO_2$ passivation interlayers.




**(a)** **(b)**

**Figure S4** (a) Reflectance spectra and (b) IQE measurements of organic solar cells without and with ALD $HfO_2$.

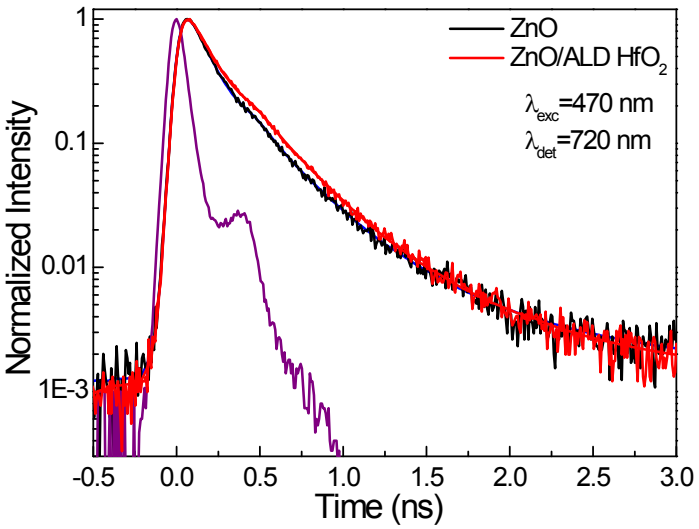



**Figure S5** Transient PL dynamics of P3HT on ZnO and ZnO/ALD $HfO_2$ layers detected at 720 nm.

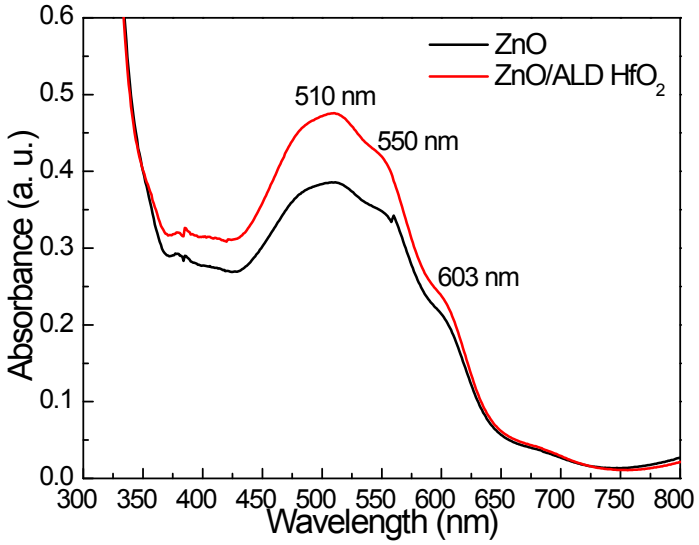



**Figure S6** UV-vis absorption spectra of P3HT:$IC_{60}BA$ blends on ZnO without and with ALD $HfO_2$.

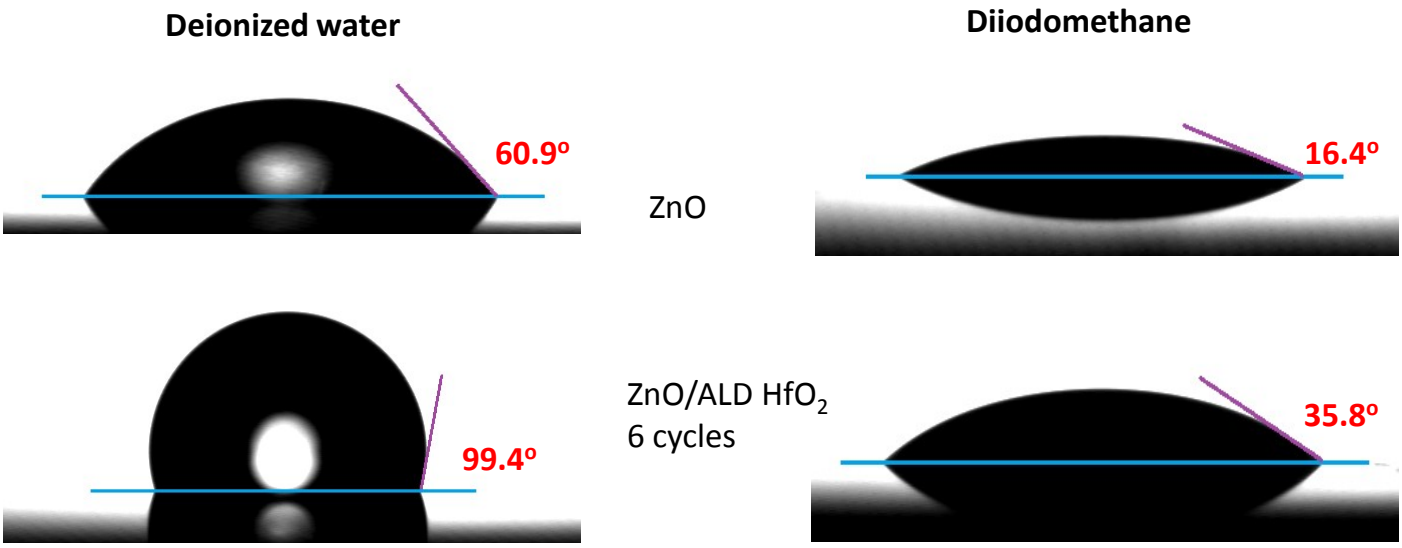



**Figure S7** Contact angle measurements of deionized water and diiodomethane drops on ZnO without and with ALD $HfO_2$.

**Additional Tables**

**Table S1** PL fitting parameters, obtained for P3HT 20 nm thick films (excitation wavelength: 470 nm) deposited on ZnO substrates without and with ALD $HfO_2$.

| Substrate | $\lambda_{det}$ (nm) | $A_1$ | $\tau_1$ (ns) | $A_2$ | $\tau_2$ (ns) | $A_3$ | $\tau_3$ (ns) | $<\tau>$ (ns) |
|---|---|---|---|---|---|---|---|---|
| **ZnO** | 650 | 0.81 | 0.09 | 0.18 | 0.31 | 0.01 | 1.41 | 0.14 |
| **ZnO** | 720 | 0.81 | 0.09 | 0.18 | 0.31 | 0.01 | 1.11 | 0.14 |
| **ZnO/ALD $HfO_2$** | 650 | 0.68 | 0.11 | 0.31 | 0.34 | 0.01 | 1.20 | 0.19 |
| **ZnO/ALD $HfO_2$** | 720 | 0.71 | 0.09 | 0.28 | 0.29 | 0.01 | 1.10 | 0.16 |

**Table S2** Surface energy as derived from contact angle measurements of ZnO substrates without and with ALD $HfO_2$

| Substrate | $\theta_w$ (°) | $\theta_i$ (°) | $\gamma_{sp}$ (mJ $m^{-2}$) | $\gamma_{sd}$ (mJ $m^{-2}$) | $\gamma$(mJ $m^{-2}$) |
|---|---|---|---|---|---|
| **ZnO** | 60.9 | 16.4 | 10.87 | 42.83 | 53.70 |
| **ZnO/ALD $HfO_2$** | 99.4 | 35.8 | 0.0002 | 42.85 | 42.85 |

**Additional References**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