Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Tunable band gap and high carrier mobility in stanene by small organic molecule adsorption and external electric field

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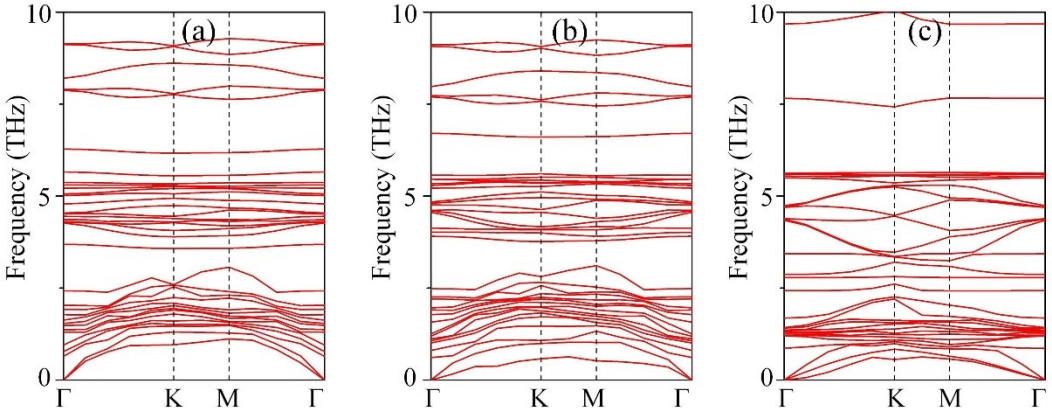

Fig. S1 Phonon band structures of (a) C_6H_6/stanene with B–2 configuration, (b) C_6F_6/stanene with T–4 configuration and (c) $C_6H_4F_2$/stanene with B–2 configuration.

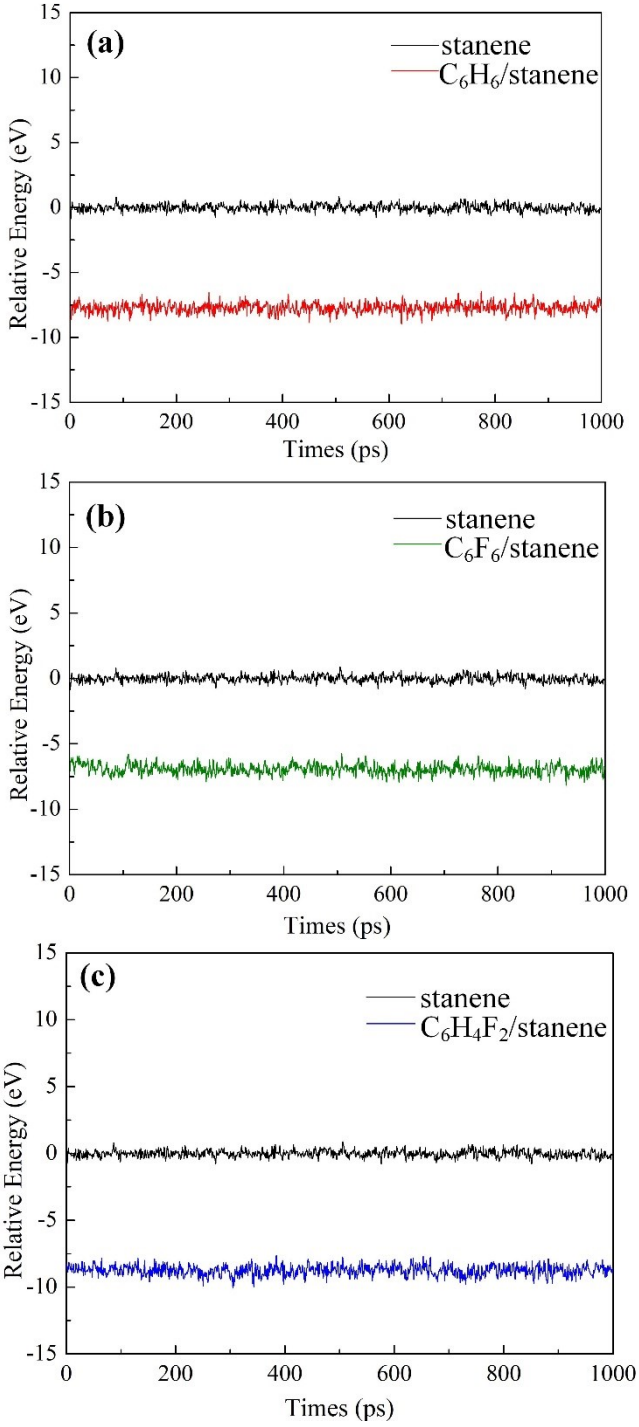

Fig. S2 Relative energies of (a) C_6H_6/stanene with B–2 configuration, (b) C_6F_6/stanene with T–4 configuration and (c) $C_6H_4F_2$/stanene with B–2 configuration as a function of time at T = 300 K.

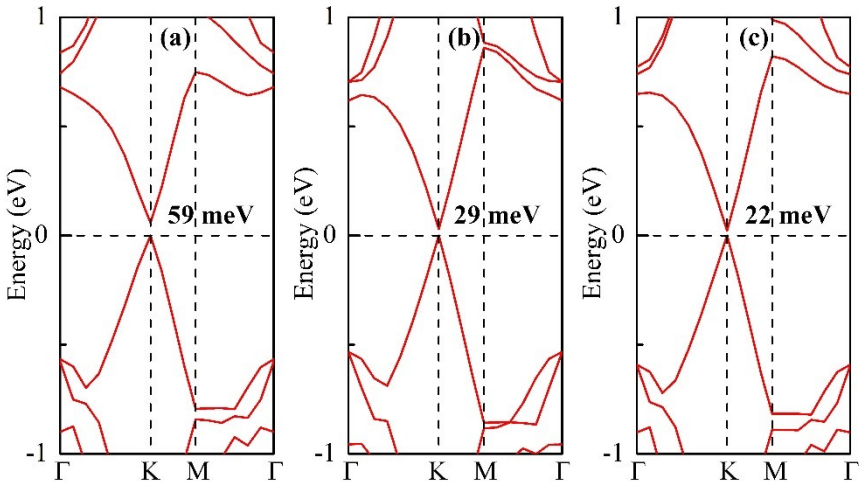

Fig. S3 Band structures of (a) C_6H_6/stanene with B–2 configuration, (b) C_6F_6/stanene with T–4 configuration and (c) $C_6H_4F_2$/stanene with B–2 configuration with HSE06, respectively.

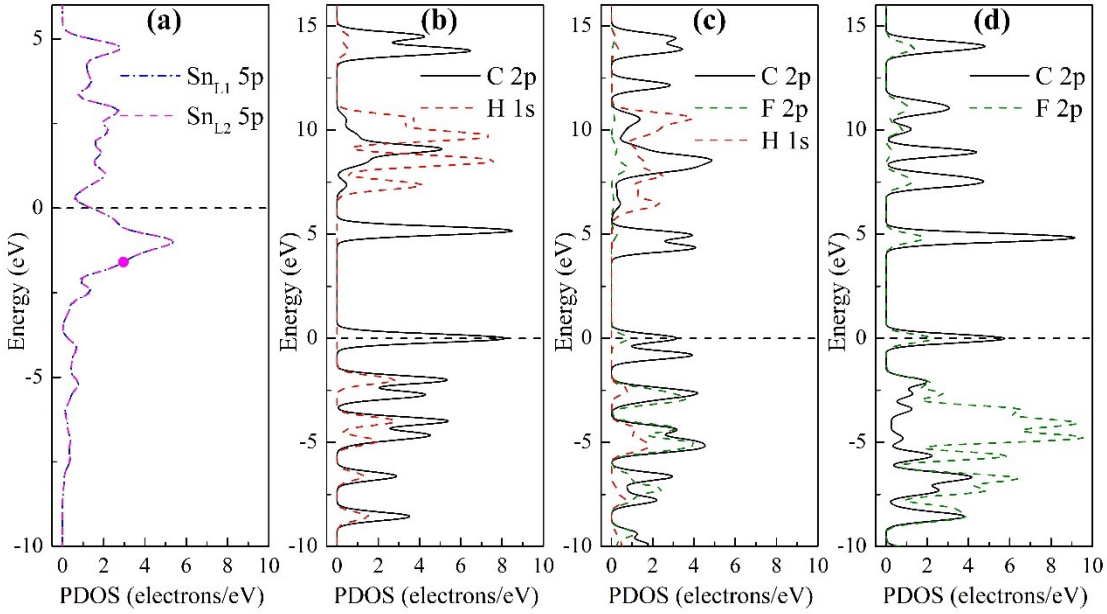

Fig. S4 PDOS of (a) free-standing stanene, (b) C_6H_6, (c) C_6F_6 and (d) $C_6H_4F_2$, respectively.

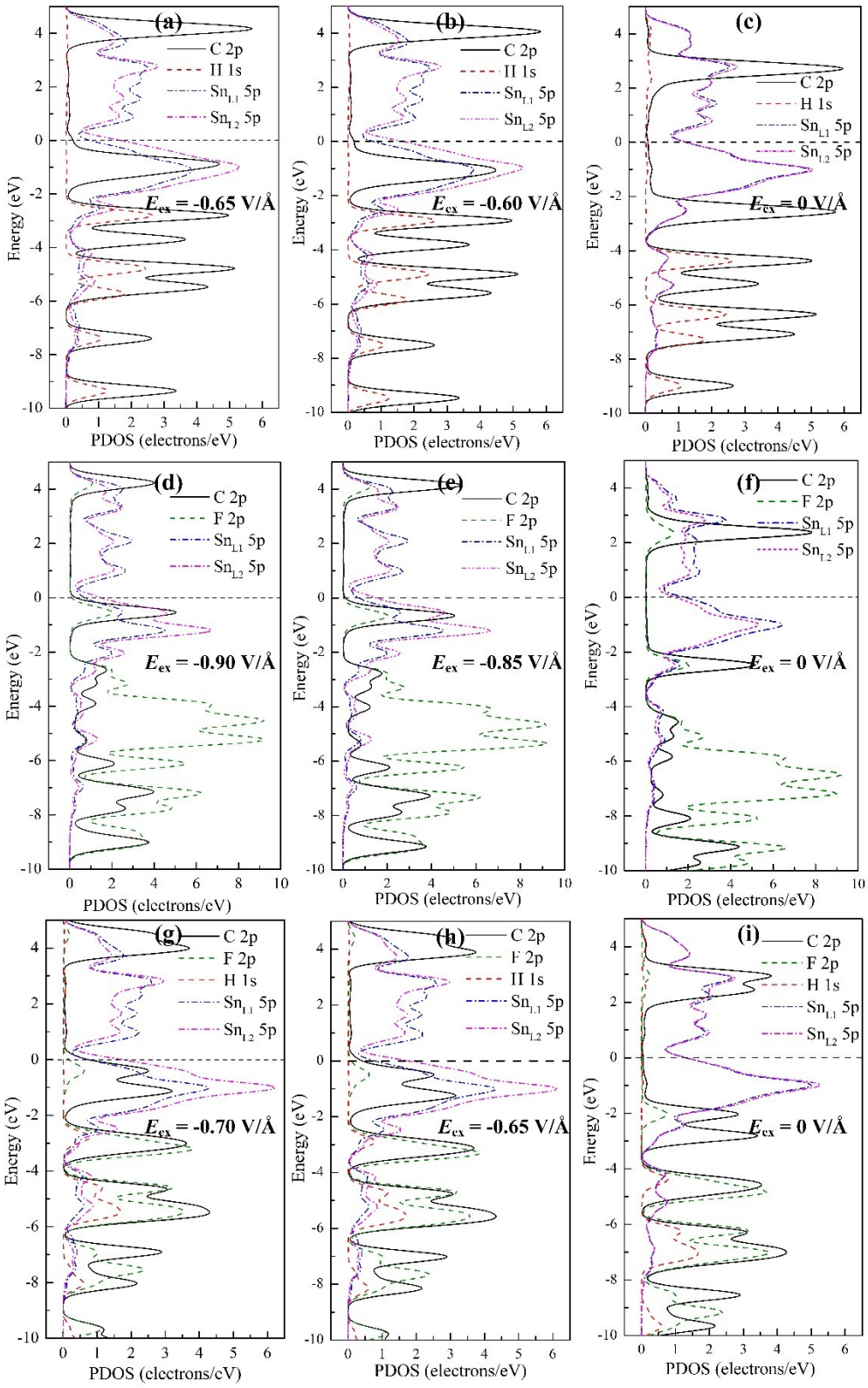

Fig. S5 Under external electric fields, the PDOS of C_6H_6/stanene with B–2 configuration at (a) E_{ex} = -0.65 V/Å, (b) E_{ex} = -0.60 V/Å and (c) E_{ex} = 0 V/Å, C_6F_6/stanene with T–4 configuration at (d) E_{ex} = -0.90 V/Å, (e) E_{ex} = -0.85 V/Å and (f) E_{ex} = 0 V/Å, $C_6H_4F_2$/stanene with B–2 configuration at (g) E_{ex} = -0.70 V/Å, (h) E_{ex} = -0.65 V/Å and (i) E_{ex} = 0 V/Å, respectively.