

Supplementary Information (SI)

Adjusting the electronic properties and contact types of graphene/F-diamane-like C_4F_2 van der Waals heterostructure: A first principles study

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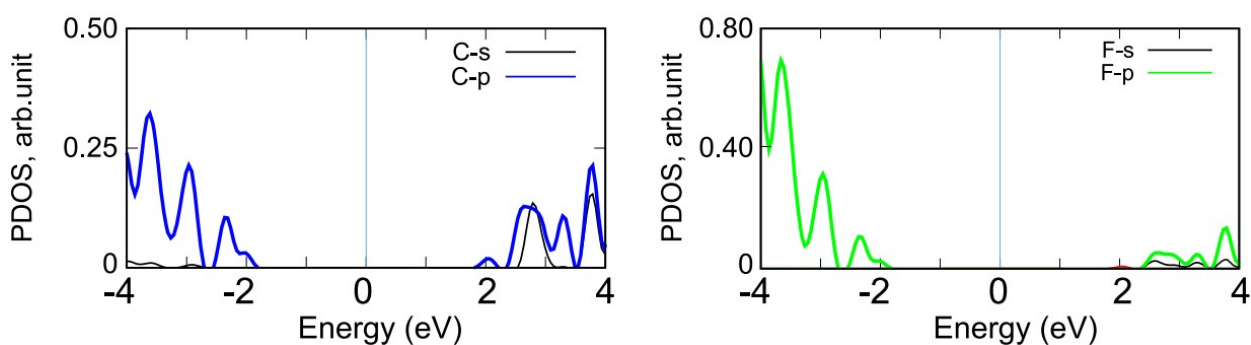


Fig. S1. Partial density of states (PDOS) of carbon and fluorine in C_4F monolayer.

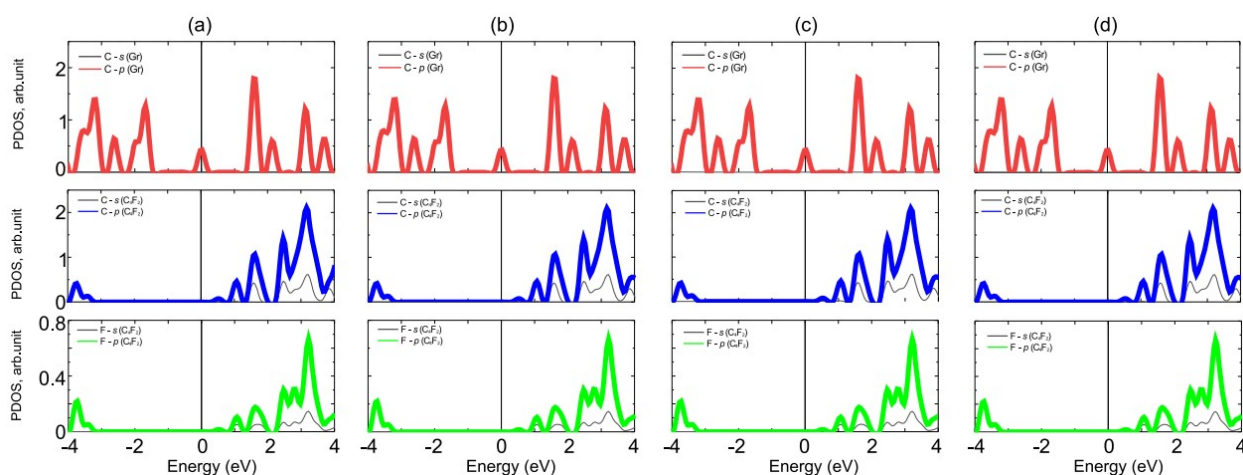


Fig. S2. Partial density of states (PDOS) of carbon in graphene layer and carbon and fluorine in C_4F_2 layer for different stacking configurations of (a) Stacking I, (b) Stacking II, (c) Stacking III and (d) Stacking IV. The Fermi level is set to be zero.

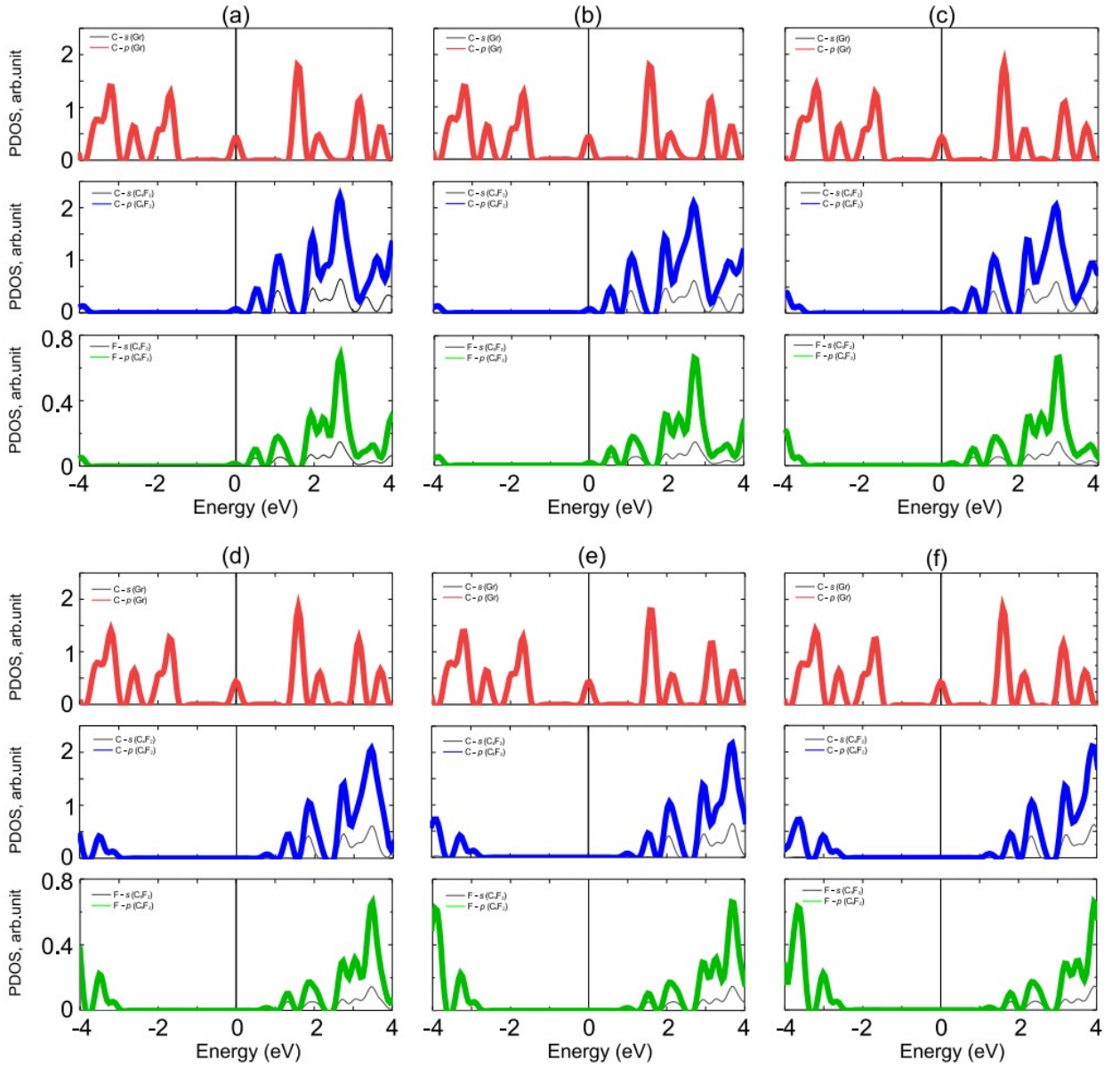


Fig. S3. Partial density of states (PDOS) of carbon in graphene layer and carbon and fluorine in C_4F_2 layer for different strength of electric field, ranging from (a) -3 V/nm, (b) -2 V/nm, (c) -1 V/nm, (d) +1 V/nm, (e) +2 V/nm and (f) +3 V/nm. The Fermi level is set to be zero.