Supporting Information

Switchable metal-to-half-metal transition at semi-hydrogenated graphene/ferroelectric interface

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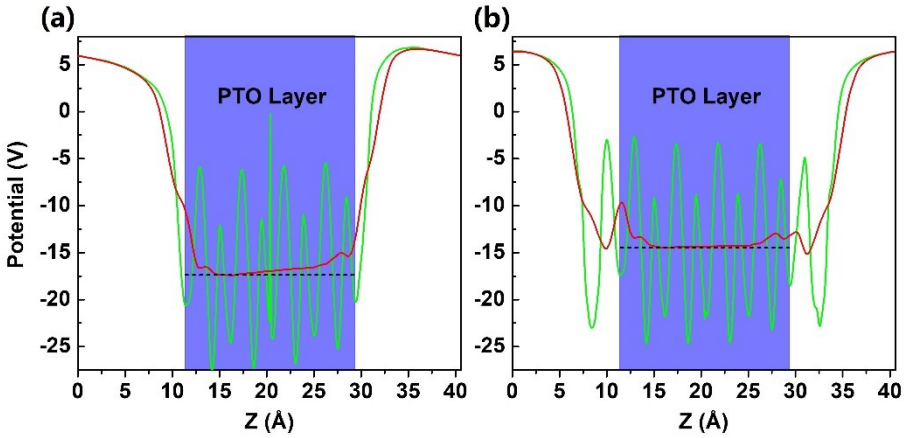

Fig. S1. Planar average (green line) and the macroscopic average (red line) electrostatic potential along (001) direction for (a) $PbTiO_3$ slab and the corresponding Graphone/$(PbO\text{-}TiO_2)_m$PbO/Graphone heterostructures (m = 4).

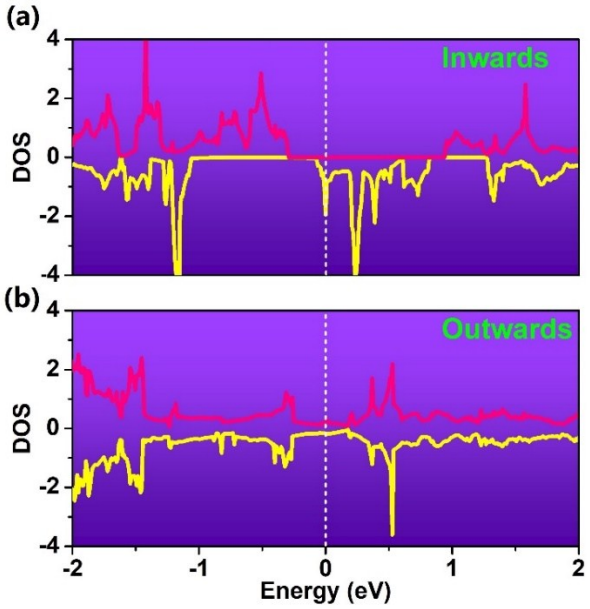

Fig. S2. Density of states of graphone layer with inwards and outwards polarization in Graphone/(PbO-TiO_2)$_m$PbO/Graphone heterostructures with m = 8.

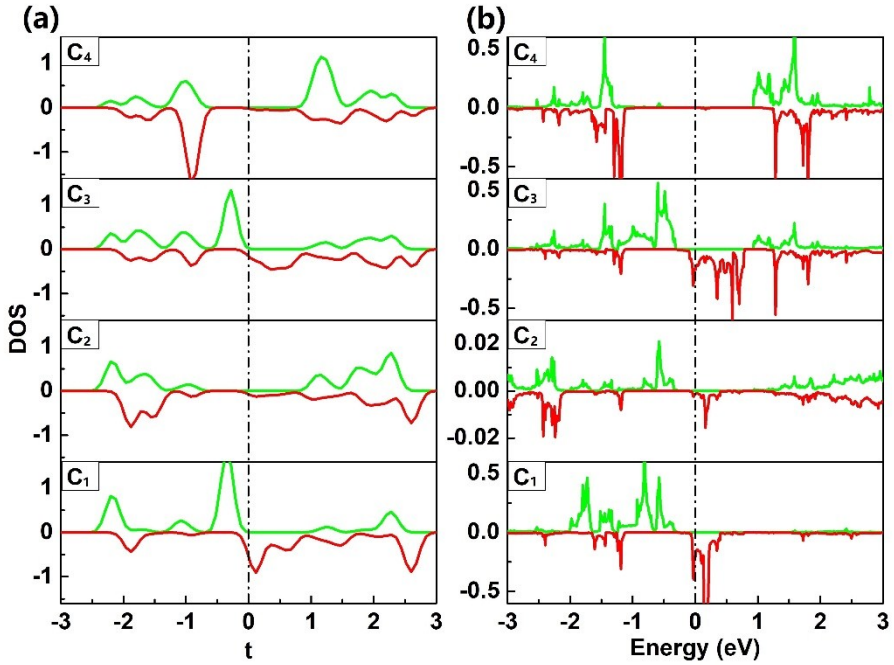

Fig. S3. Comparison of the density of states for C atoms from C_1 to C_4 between results from (a) Hubbard model and (b) first-principles calculations.

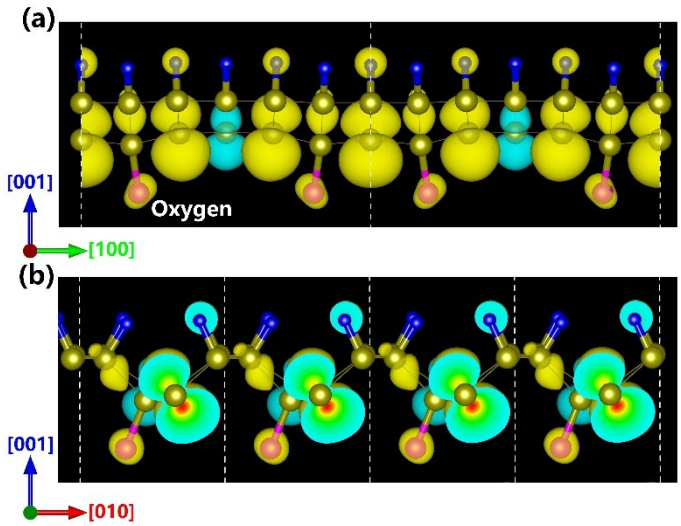

Fig. S4. Spin charge density at the interface of graphone/(PbO-TiO2)$_m$-PbO/graphone heterostructures with outwards polarization in the (a) (010) and (b) (100) plane, respectively, the yellow (cyan) color indicates isosurfaces of spin-up (spin-down) densities of 0.005 μ_B/ bohr^3.

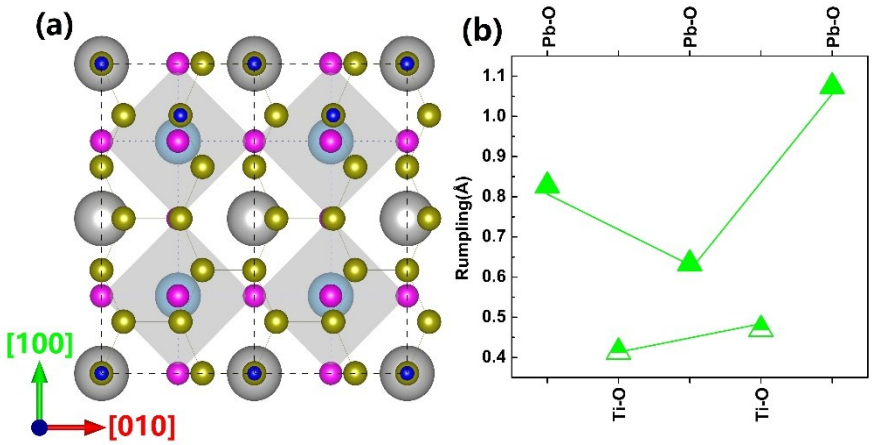

Fig. S5. (a) Top view of graphene/$PbTiO_3$ heterostructures with one H atom per PTO unit cell area absorbed on top of graphene, (b) rumpling of the heterostructures with two layers $PbTiO_3$.