**Supporting Information:**

# Strong interactions and charge transfers between a charged benzene molecule and multilayer graphenes

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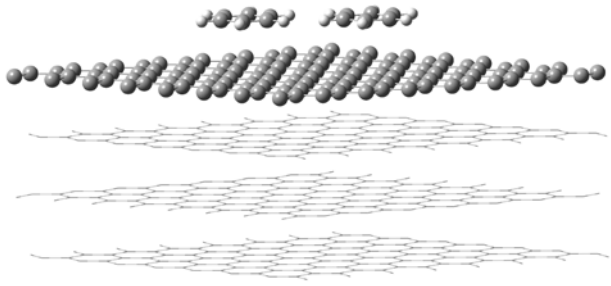

**Figure 1S**. Adsorption models of two benzene molecules on the periodic graphene surfaces of one and four layers in AB stacking.

**Table 1S**. The charge distributions at ionic states of two benzene molecules on the single layer and four-layer graphenes. (Unit: e):

| Component / Structure | Benzene | Layer 1 | Layer 2 | Layer 3 | Layer 4 |
|---|---|---|---|---|---|
| Gra1+Ben*2 | 0.002 | 0.999 | | | |
| Gra4+Ben*2 | 0.0 | 0.353 | 0.146 | 0.147 | 0.353 |

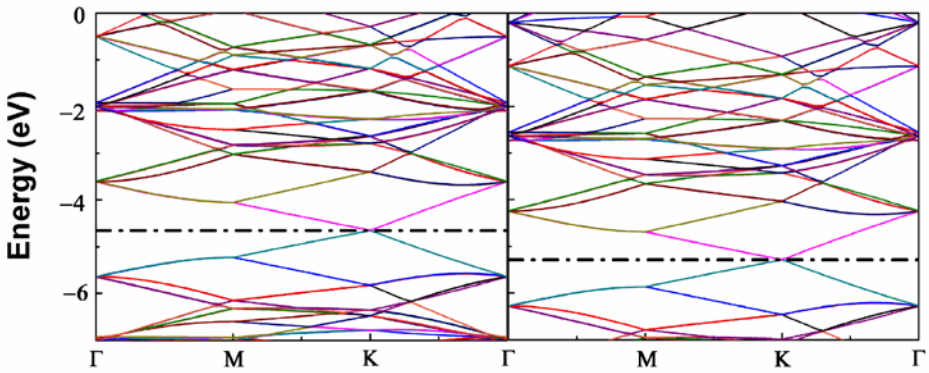


**Figure 2S**. The band structures of neutral and ionic single layer graphene. Left: neutral; right: ionic.

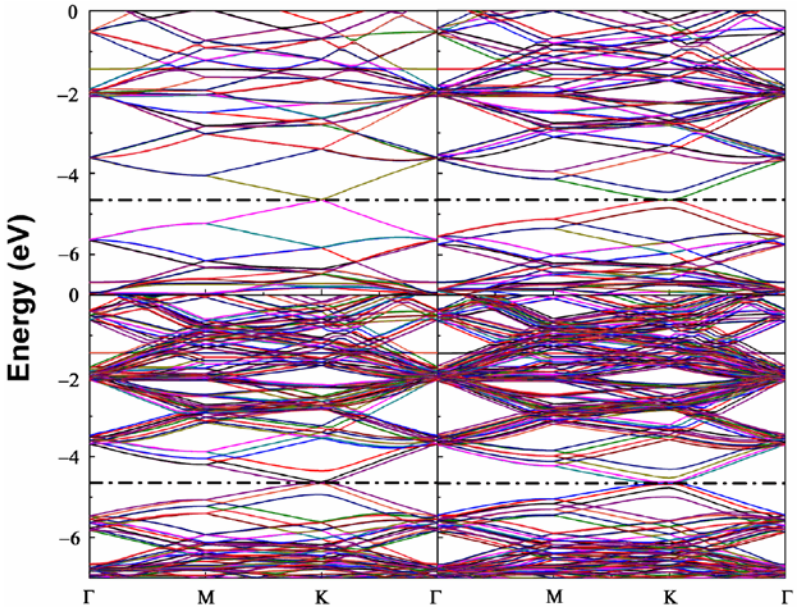

**Figure 3S**. The band structures of four neutral adsorption systems of the benzene molecule adsorbed on multilayer graphenes. Top left: single layer graphene; top right: double layer graphenes; bottom left: three layer graphenes; bottom right: four layer graphenes.