Supporting Information

First-principles Study on the Adsorption Properties of Phenylalanine on Carbon Graphitic Structures

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- Fig. S1: Equilibrium atomic structure of a Phe molecule
- Fig. S2: Various Phe adsorption configurations and adsorption energies
- Fig. S3: Electronic band structure of the Phe-adsorbed graphene with respect to external electric fields
- Fig. S4: Electronic band structures of the Phe-adsorbed (10,0) and (5,5) CNTs with respect to external electric fields
- Fig. S5: Electronic band structure of the Phe-adsorbed Mg-B_2-functionalized graphene with respect to external electric fields

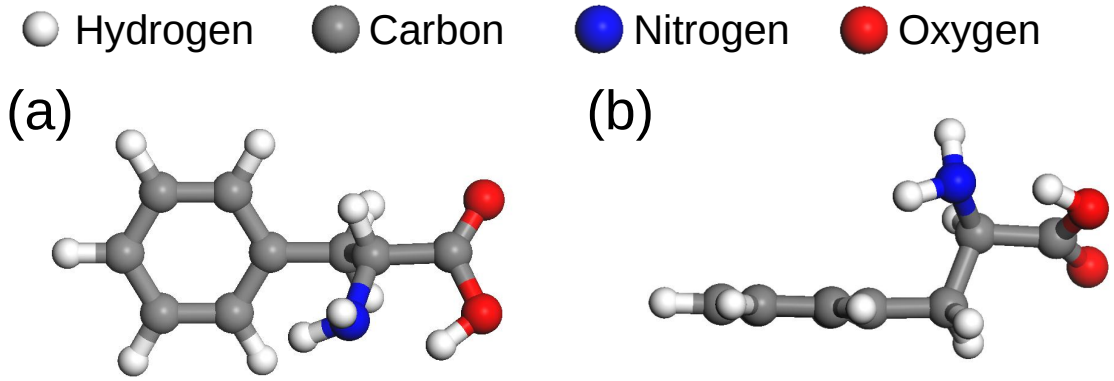

FIG. S1. Equilibrium atomic structure of Phe in (a) top and (b) side views. Different elements in the structure are represented by different colors, as given in the legend.

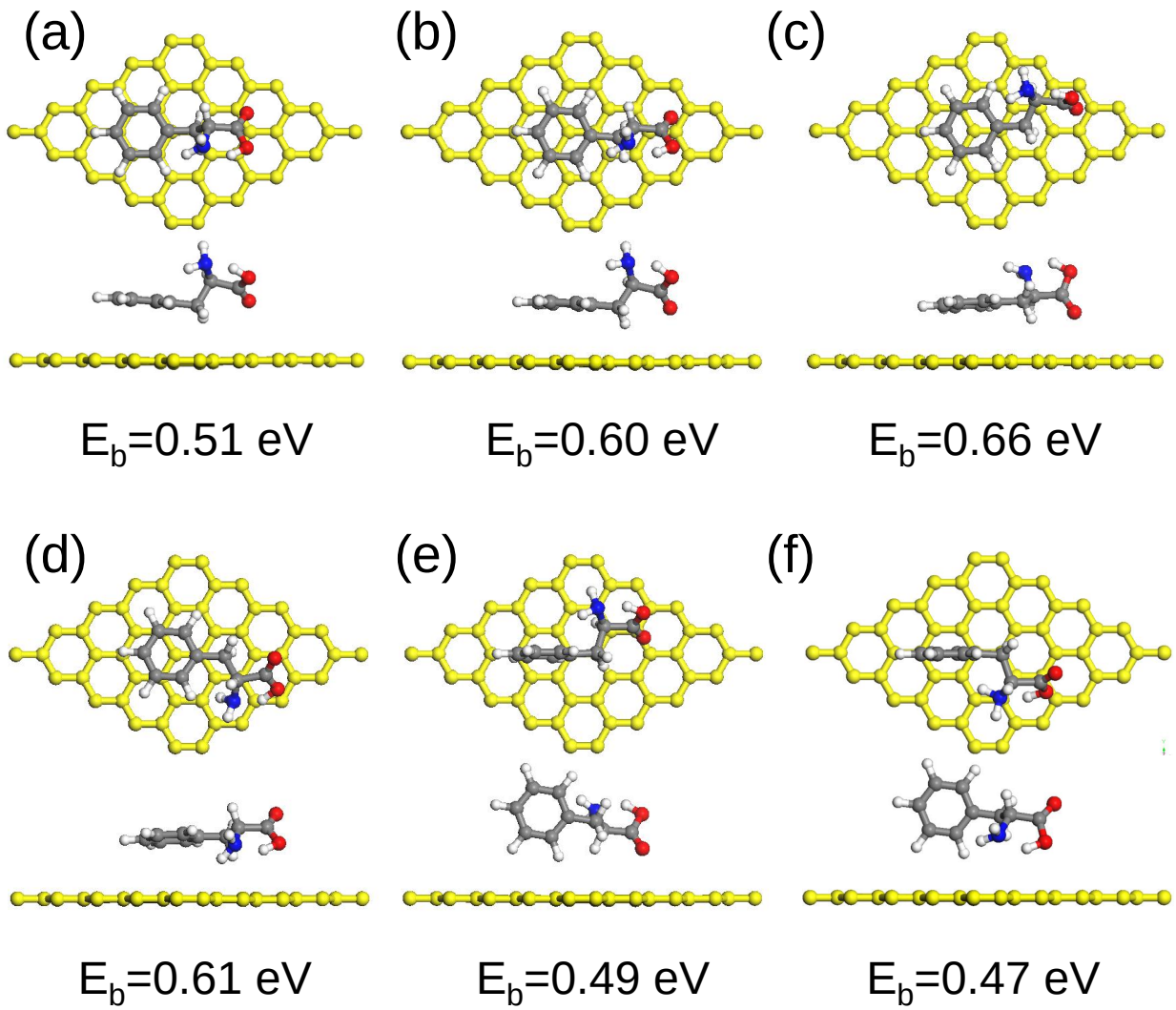

FIG. S2. Various equilibrium configurations with different orientation of a Phe molecule adsorbed on graphene depending on where the amine (–NH_2), carboxyl acid (–COOH), and benzyl ($C_6H_5CH_2$–) groups of Phe are located. The Phe binding energy of each configuration is given below. The same color scheme was used as in Fig. S1 for the respective elements, except for the host materials being yellow-colored for distinction.

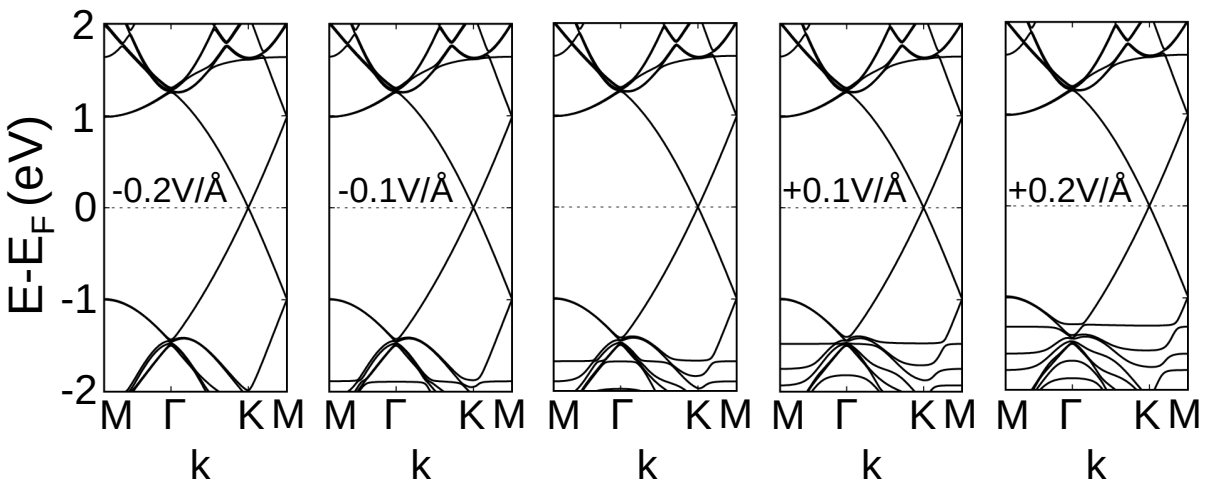

FIG. S3. Electronic band structure $E(k)$ along the high-symmetry lines of the Phe-adsorbed graphene in the absence (middle) and the presence of an electric field from -0.2 V/Å(left) to $+0.2$ V/Å(right) applied along the z direction, which is normal to the graphene sheet.

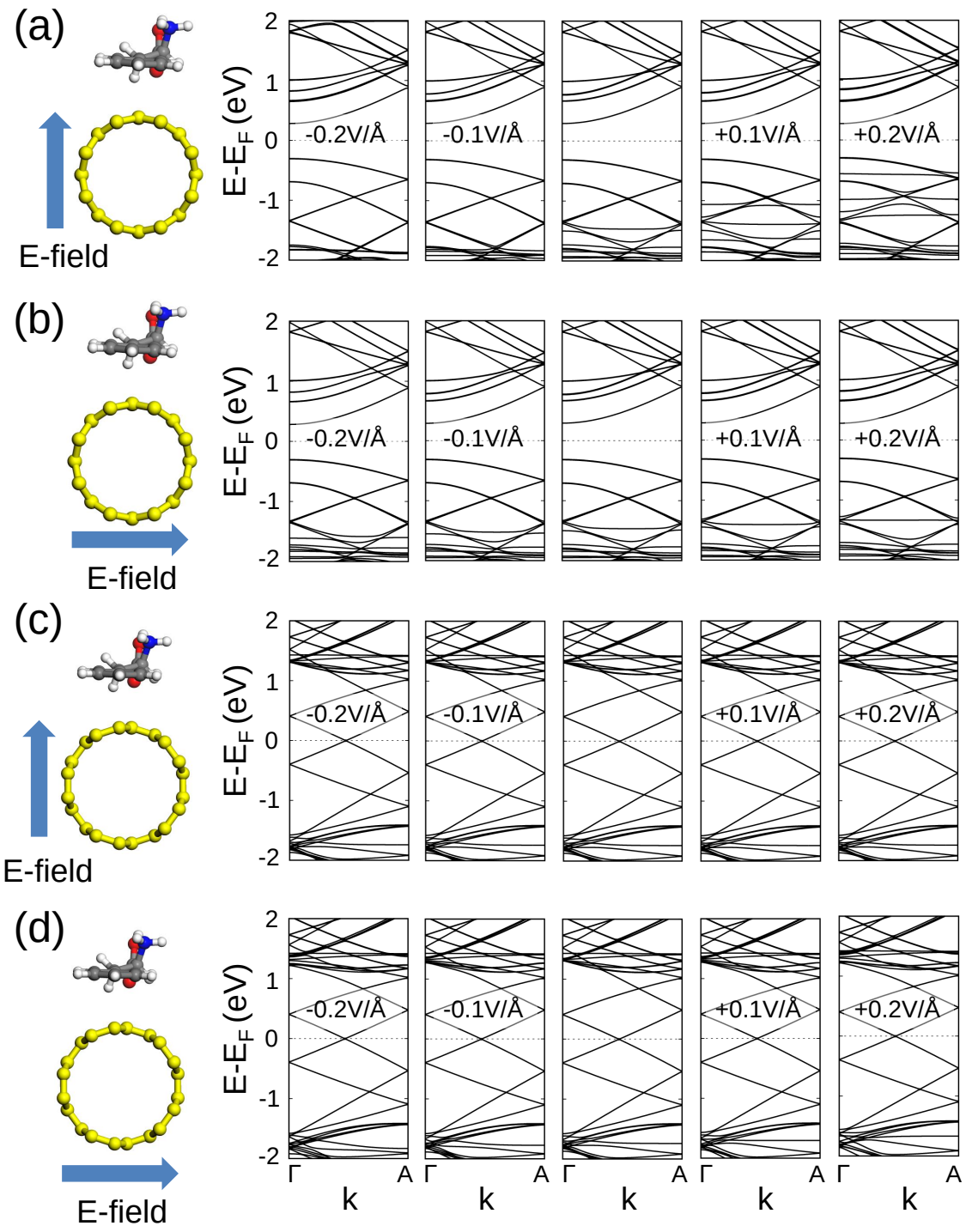

FIG. S4. Schematics of Phe-adsorbed (a, b) (10,0) and (c, d) (5,5) CNTs and their electronic band structure $E(k)$ along the axial direction, Γ–A, for two opposite electric field directions and different strengths.

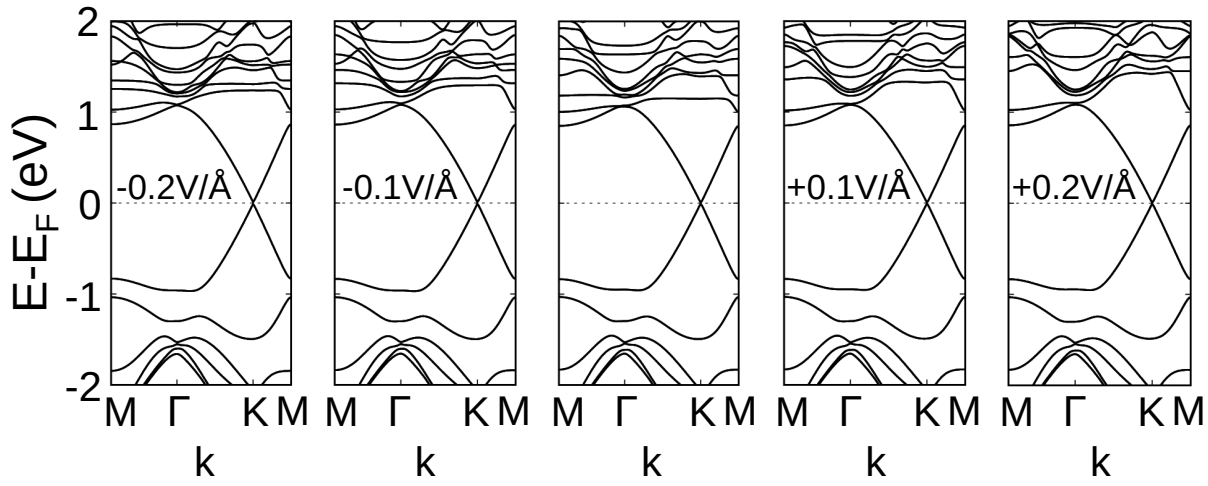

FIG. S5. Electronic band structure $E(k)$ along the high-symmetry lines of the Phe-adsorbed Mg-B_2-functionalized graphene in the absence (middle) and the presence of an electric field from -0.2 V/Å(left) to $+0.2$ V/Å(right) applied along the z direction, which is normal to the graphene sheet.