

Supporting on-line material for:
Optimizing electronic structure and quantum transport at the
graphene-Si(111) interface: An *ab-initio* density-functional study

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To understand the binding of a graphene monolayer on the Si(111) surface, we considered a large number of candidate structures, which we optimized using the conjugate gradient approach. In the main paper, we focus on the optimum structure with 2×1 unit cells. Other relevant optimized structures are presented in the following.

Wavy graphene on Si(111)

The optimized structure of wavy graphene on the Si(111) surface is presented in Fig. S1 for the 2×1 , 4×1 and 6×1 supercell structures. In our energy discussion in the main paper, we distinguished between the energy needed to buckle initially planar graphene and subsequently to attach the wavy graphene to the substrate. Comparing energy differences per carbon atom of the graphene layer, Fig. S1 illustrates that large graphene supercells require less buckling energy, but are not as well bonded to the substrate.

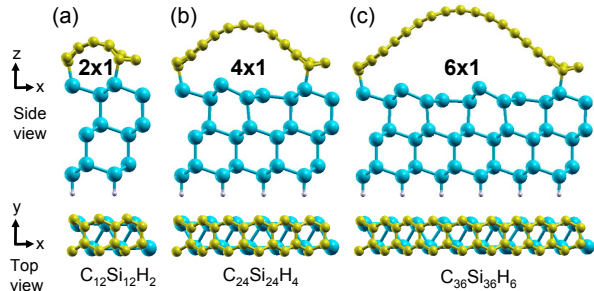


FIG. S1. (Color online) Top and side view of relaxed wavy graphene on the Si(111) surface with (a) 2×1 , (b) 4×1 and (c) 6×1 unit cells.

Relaxation of a free-standing wavy graphene monolayer

To obtain better insight in the relaxation process of a wavy graphene monolayer that is structurally frozen in the optimum adsorption geometry of the 2×1 graphene/Si superstructure, we reproduce the relaxation of the graphene sub-system in different superstructures in Fig. S2. The unit cell nomenclature is taken from Fig. S1.

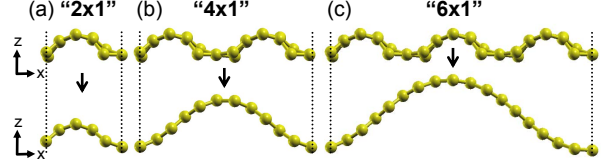


FIG. S2. (Color online) Side view of wavy graphene on the Si(111) surface with (a) 2×1 , (b) 4×1 and (c) 6×1 unit cells, with the nomenclature taken from Fig. S1. Top panels are one-, two- and three-cell replicas of the graphene subsystem in Fig. S1(a). Bottom panels represent the optimized structure of wavy graphene, constrained only by the lateral size of the unit cell.

Effect of chemisorbed hydrogen on the equilibrium structure of 2×1 supercells of graphene on Si(111)

Presence of chemisorbed hydrogen reduces the flexural rigidity of graphene and thus the buckling energy, while affecting to a lesser degree the graphene-Si bonds. The equilibrium structure of the 2×1 graphene overlayer on Si(111) with different numbers of hydrogen atoms per unit cell is presented in Fig. S3.

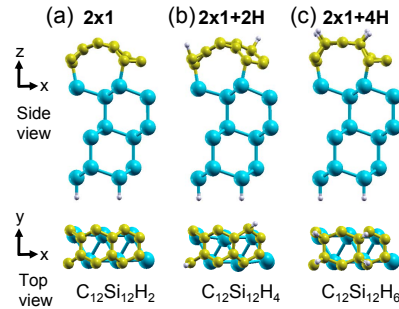


FIG. S3. (Color online) Top and side view of the relaxed geometry of 2×1 supercells of wavy graphene on the Si(111) surface at different H coverages.

Effect of chemisorbed hydrogen on the equilibrium structure of 4×1 supercells of graphene on Si(111)

The equilibrium structure of the 4×1 graphene overlayer on Si(111) with different numbers of hydrogen atoms per unit cell is presented in Fig. S4.

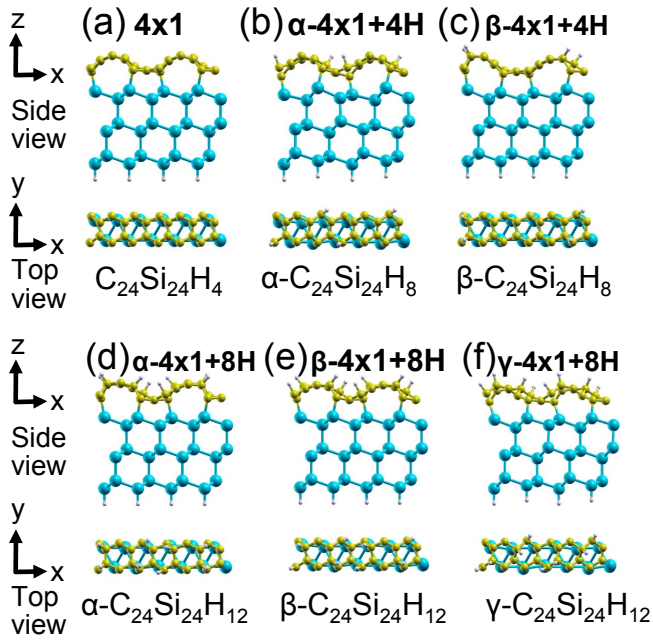


FIG. S4. (Color online) Top and side view of the relaxed geometry of 4×1 supercells of wavy graphene on the Si(111) surface at different H coverages. The Greek characters in structure names distinguish between different stable geometries at a given coverage.

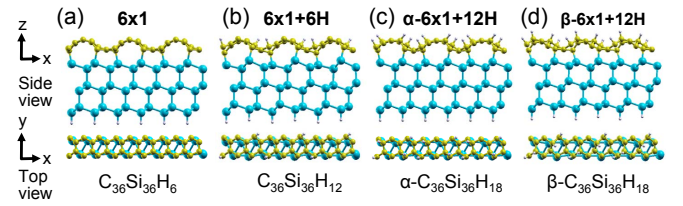


FIG. S5. (Color online) Top and side view of the relaxed geometry of 6×1 supercells of wavy graphene on the Si(111) surface at different H coverages. The Greek characters in structure names distinguish between different stable geometries at a given coverage.

Effect of chemisorbed hydrogen on the equilibrium structure of 6×1 supercells of graphene on Si(111)

The equilibrium structure of the 6×1 graphene overlayer on Si(111) with different numbers of hydrogen atoms per unit cell is presented in Fig. S5.

Electronic band structure of graphene on Si(111)

The electronic band structure of the 2×1 graphene overlayer on Si(111), corresponding to the electronic density of states shown by the solid line in Fig. 1(d) of the main manuscript, is presented in Fig. S6.

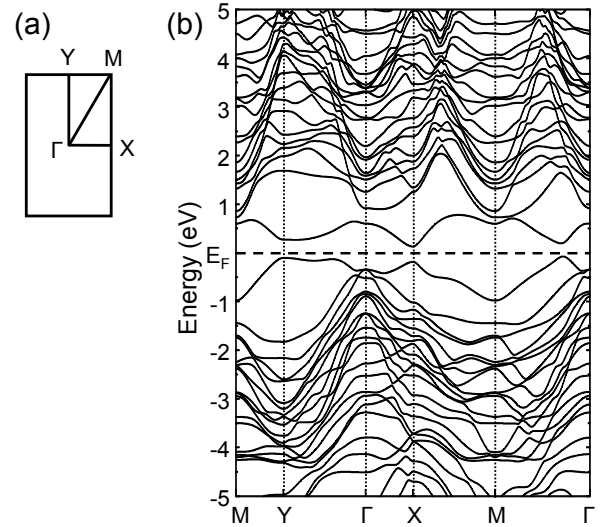


FIG. S6. (a) Surface Brillouin zone and (b) electronic band structure of the graphene overlayer on Si(111) with a 2×1 unit cell.