Origin of Unusual Electronic and Atomic Structures of Epitaxial Graphene on SiC

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On the basis of first-principles calculations, we report that a novel interfacial atomic structure occurs between graphene and the surface of silicon carbide, destroying the Dirac point of graphene and opening a substantial energy gap there. In the calculated atomic structures, a quasiperiodic 6×6 domain pattern emerges out of a larger commensurate $(6\sqrt{3} \times 6\sqrt{3})R30^\circ$ periodic interfacial reconstruction, resolving a long standing experimental controversy on the periodicity of the interfacial superstructures. Our theoretical energy spectrum shows a gap and midgap states at the Dirac point of graphene, which are in excellent agreement with the recently observed anomalous angle-resolved photoemission spectra.

[1] S. Kim, J. Ihm, H.J. Choi and Y-W Son, Phys. Rev. Lett. **100**, 176802 (2008).