Supplementary Material

Interface and interaction of graphene layers on SiC(000$\bar{1}$) covered

with TiC(111) intercalation

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Table S1. Total energy (eV) of 1L-TiC/SiC, 2L-TiC/SiC, and 3L-TiC/SiC with the (a, b, c) C/C-, (d, e) C/Ti/C-, and (f) C/Ti-terminated interfaces.

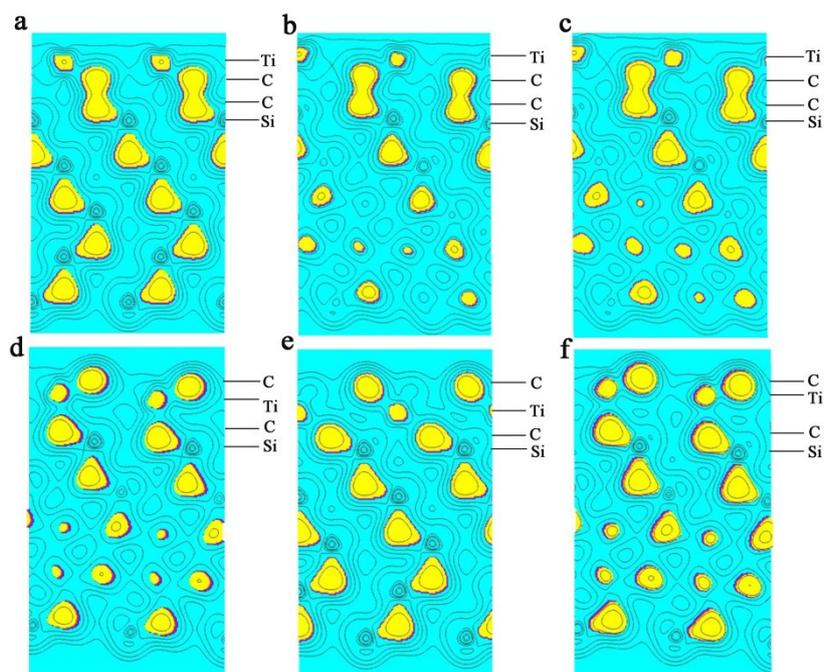| System	a	b	c	d	e	f
1L-TiC/SiC	-274.34	-273.87	-273.53	-273.21	-273.10	-272.51
2L-TiC/SiC	-284.32	-284.09	-282.13	-	-	-
3L-TiC/SiC	-295.99	-295.83	-	-	-	-

Fig. S1 Valence electron density for 1L-TiC/SiC: with (a, b, c) C/C-, (d, e) C/Ti/C-, and (f) C/Ti-terminated interfacial configurations.
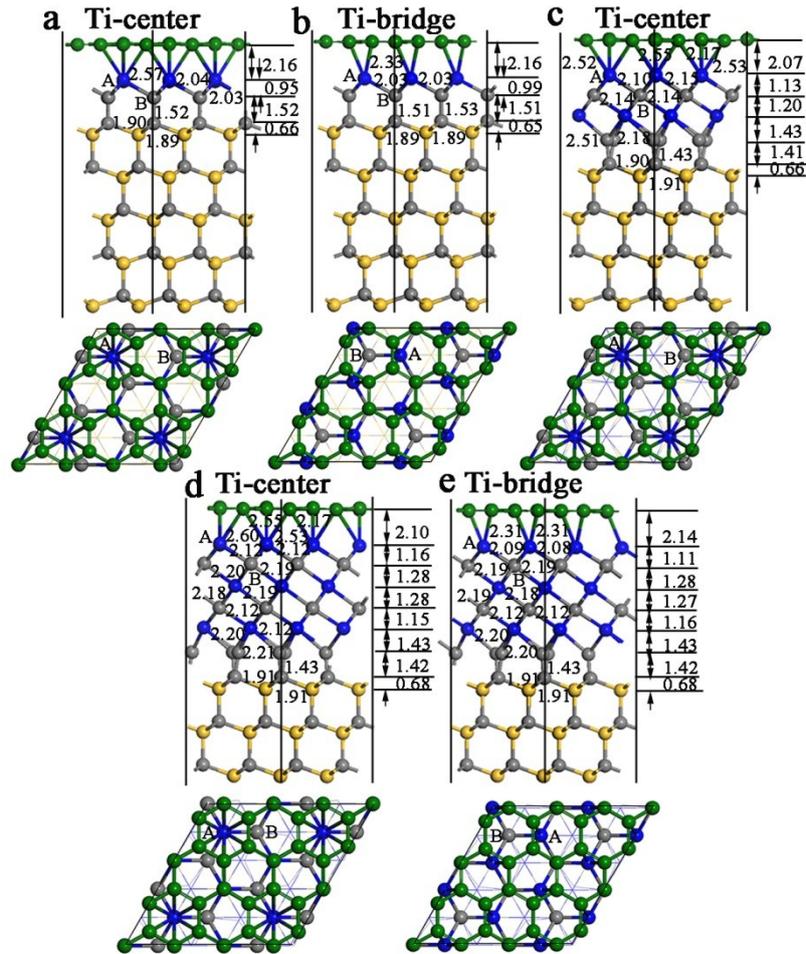
Fig. S2 Optimal structures of monolayer graphene adsorbed on (a, b) 1L-TiC/SiC, (c) 2L-TiC/SiC, and (d, e) 3L-TiC/SiC substrates. There are two stable configurations of graphene on TiC(111)/SiC(000$\bar{1}$) surfaces: (i) Ti-center-site (A site) and (ii) Ti-bridge-site staking (B site). Green, blue, gray, and yellow spheres represent graphene C atoms, Ti, C, and Si atoms in the TiC(111)/SiC(000$\bar{1}$) substrate, respectively. The unit cell is highlighted by grey solid lines.
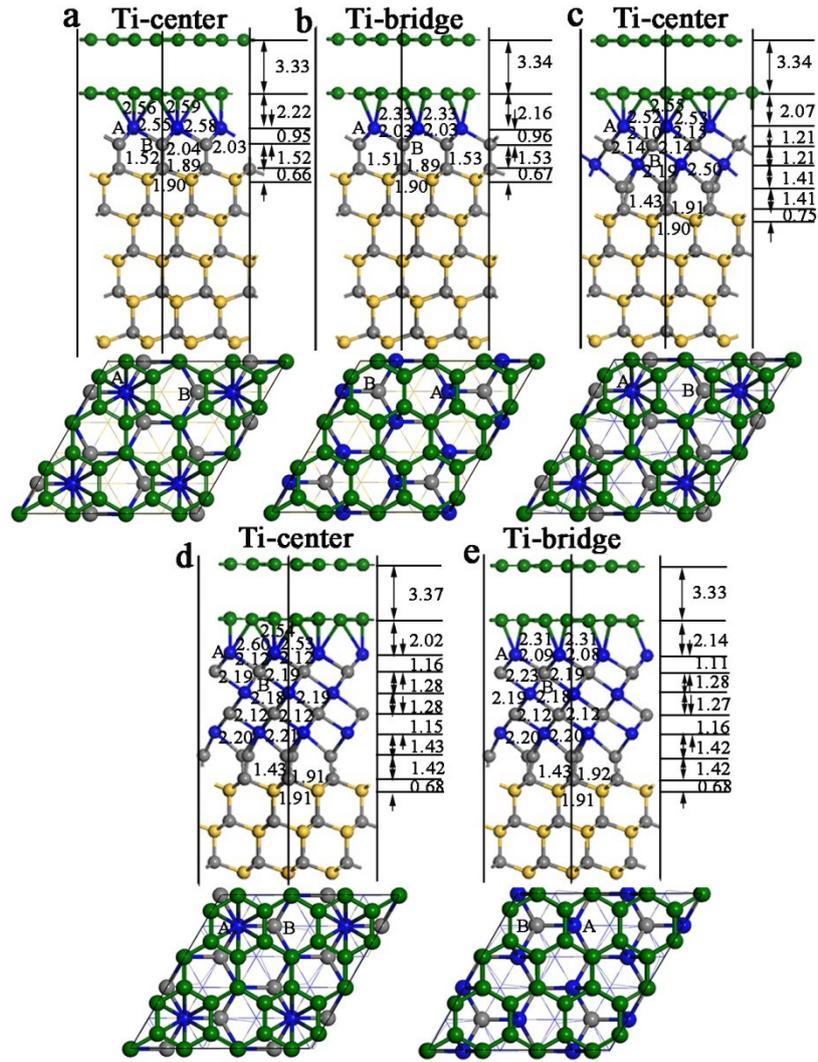
Fig. S3 Optimal structures of bilayer graphene adsorbed on (a, b) 1L-TiC/SiC, (c) 2L-TiC/SiC, and (d, e) 3L-TiC/SiC substrates. Green, blue, gray, and yellow spheres represent graphene C atoms, Ti, C, and Si atoms in the TiC(111)/SiC(000$\bar{1}$) substrate, respectively. The unit cell is highlighted by grey solid lines.
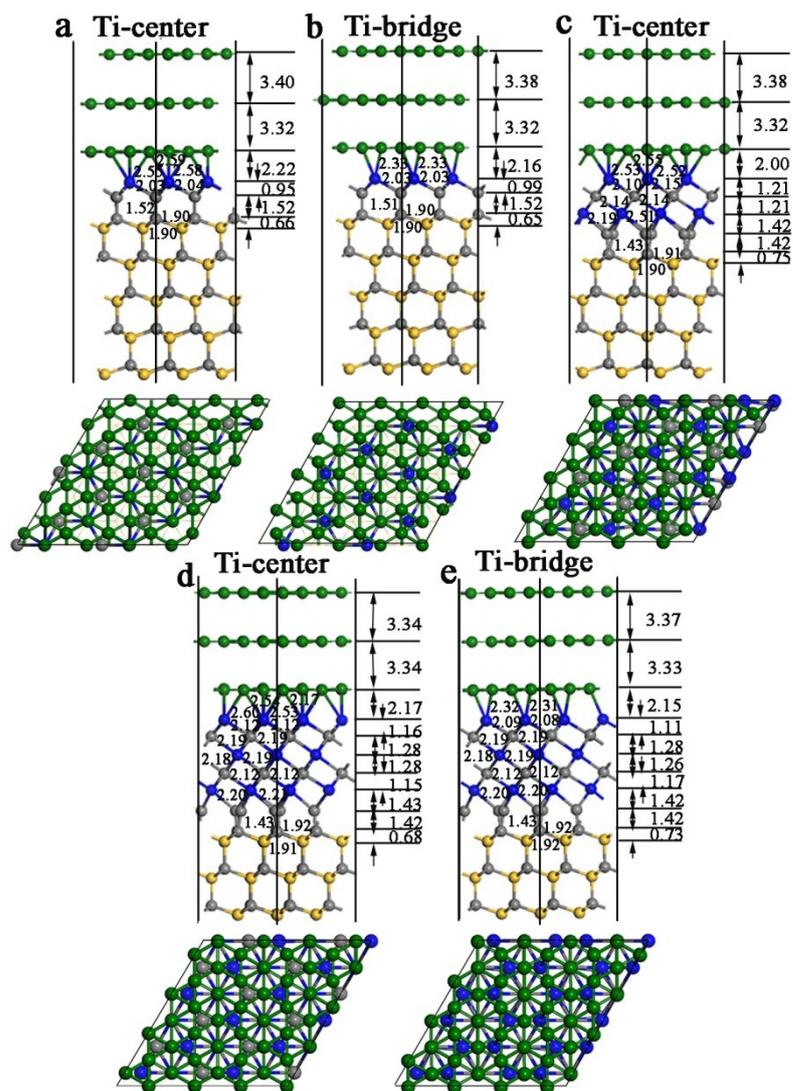
Fig. S4 Optimal structures of trilayer graphene adsorbed on (a, b) 1L-TiC/SiC, (c) 2L-TiC/SiC, and (d, e) 3L-TiC/SiC substrates. Green, blue, gray, and yellow spheres represent graphene C atoms, Ti, C, and Si atoms in the TiC(111)/SiC(000$\bar{1}$) substrate, respectively. The unit cell is highlighted by grey solid lines.
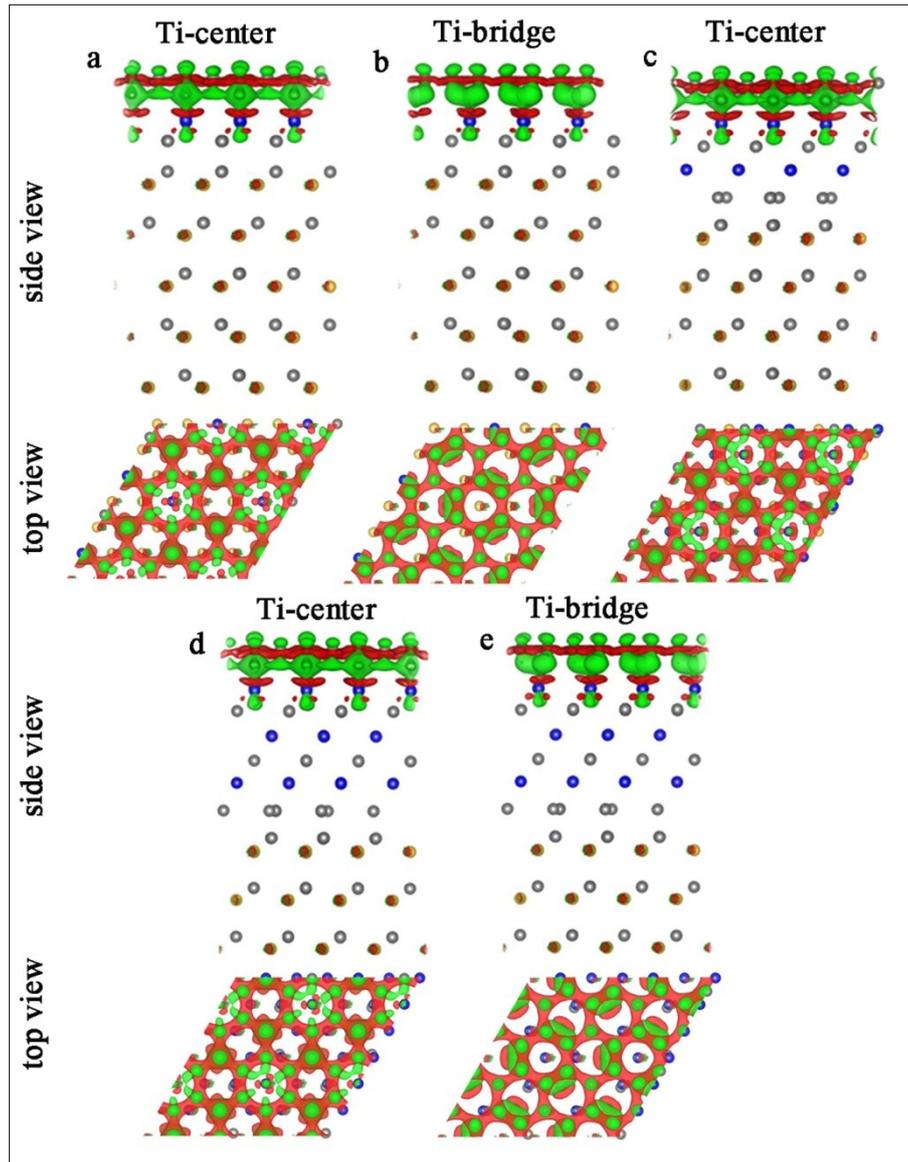
Fig. S5 Charge density difference plots of monolayer graphene on (a, b) 1L-TiC/SiC, (c) 2L-TiC/SiC, and (d, e) 3L-TiC/SiC substrates. The charge density difference refers to the variance between the total charge density of graphene/TiC(111)/SiC(000$\bar{1}$) systems and the sum of the charge density of the separated graphene and TiC(111)/SiC(000$\bar{1}$). The geometric structures of separated graphene and TiC(111)/SiC(000$\bar{1}$) were kept the same as those in graphene–TiC(111)/SiC(000$\bar{1}$) systems. The red and green color regions mark the depletion and accumulation of electronic charges, respectively. The top views show the charge density difference at interface of the graphene/TiC(111)/SiC(000$\bar{1}$) systems.
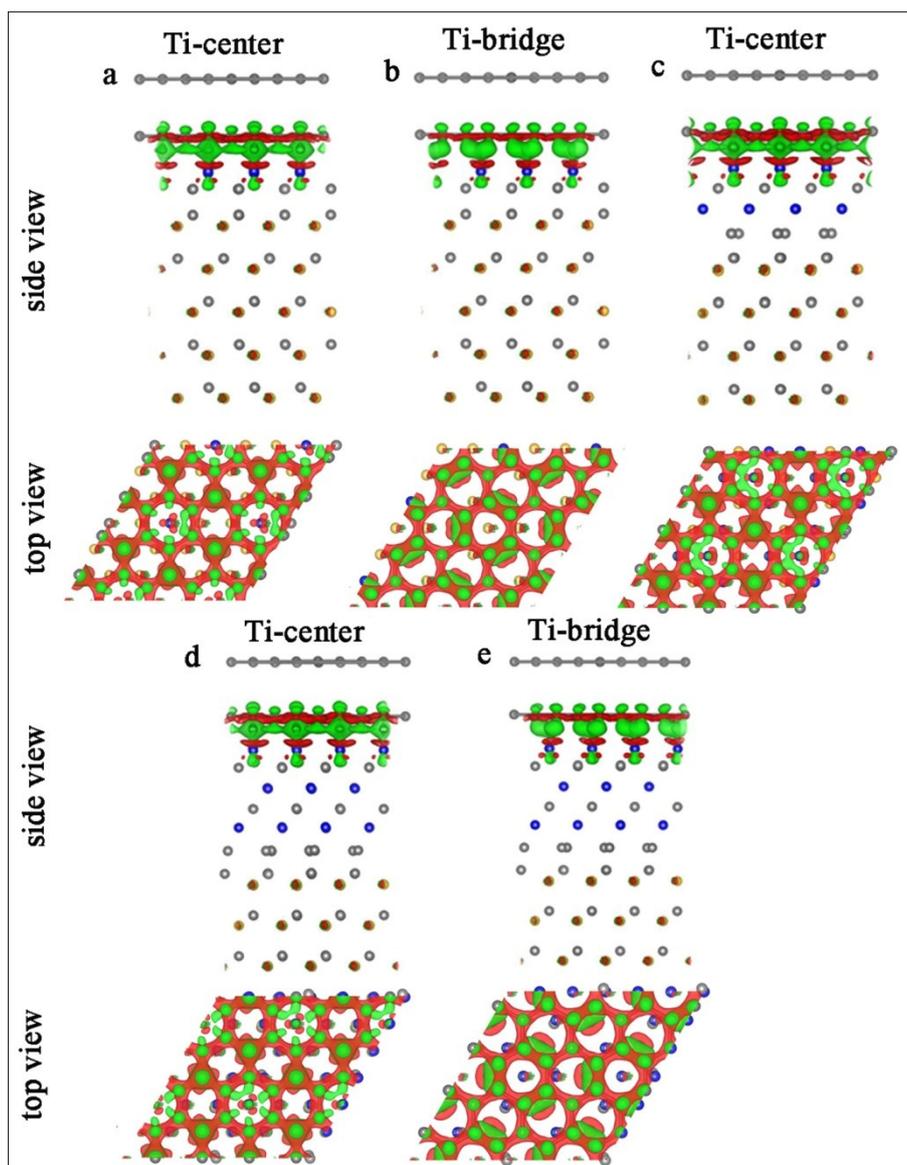
Fig. S6 Charge density difference plots of bilayer graphene on (a, b) 1L-TiC/SiC, (c) 2L-TiC/SiC, and (d, e) 3L-TiC/SiC substrates. The red and green color regions mark the depletion and accumulation of electronic charges, respectively. The top views show the charge density difference at interface of the graphene/TiC(111)/SiC(000$\bar{1}$) systems.
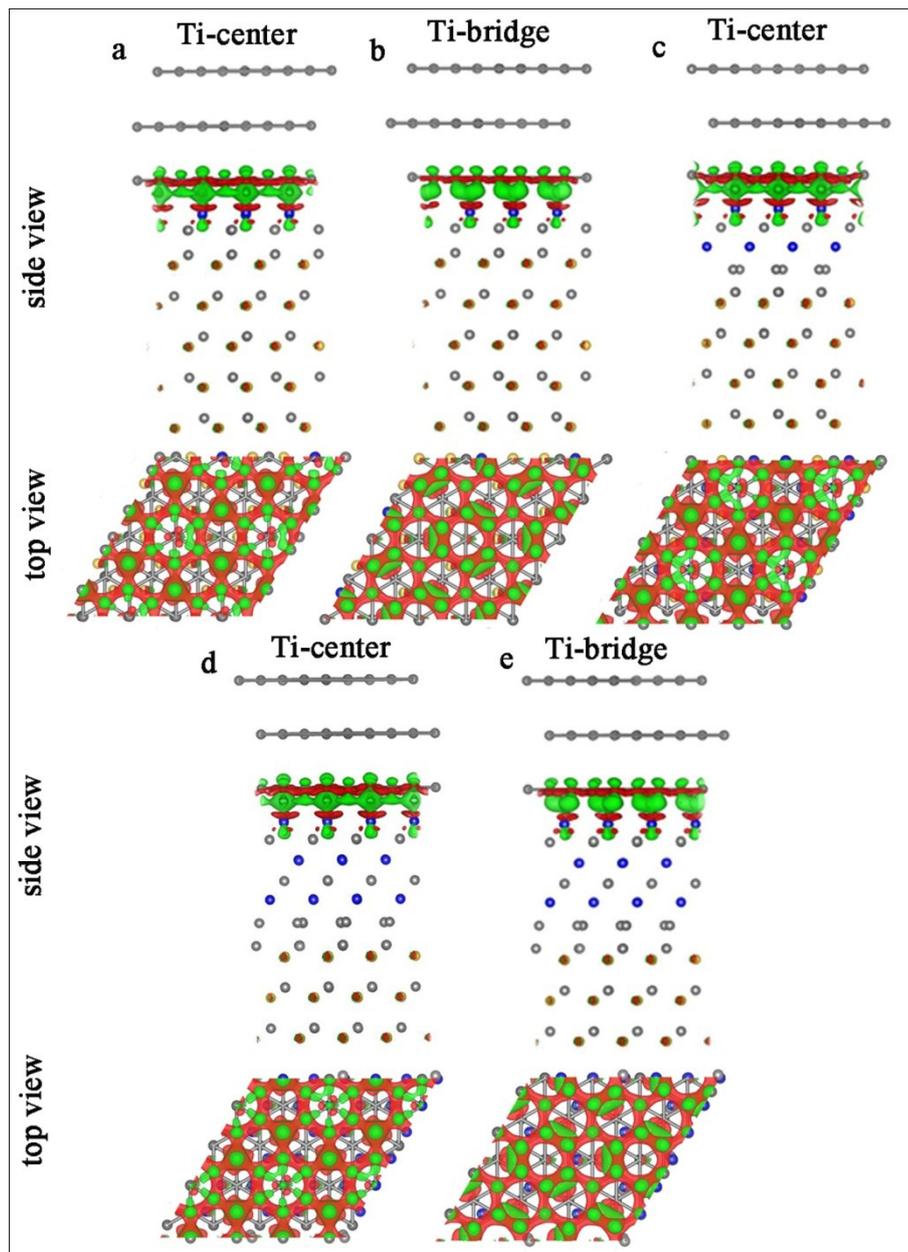
Fig. S7 Charge density difference plots of trlayer graphene on (a, b) 1L-TiC/SiC, (c) 2L-TiC/SiC, and (d, e) 3L-TiC/SiC substrates. The red and green color regions mark the depletion and accumulation of electronic charges, respectively. The top views show the charge density difference at interface of the graphene/TiC(111)/SiC(000$\bar{1}$) systems.
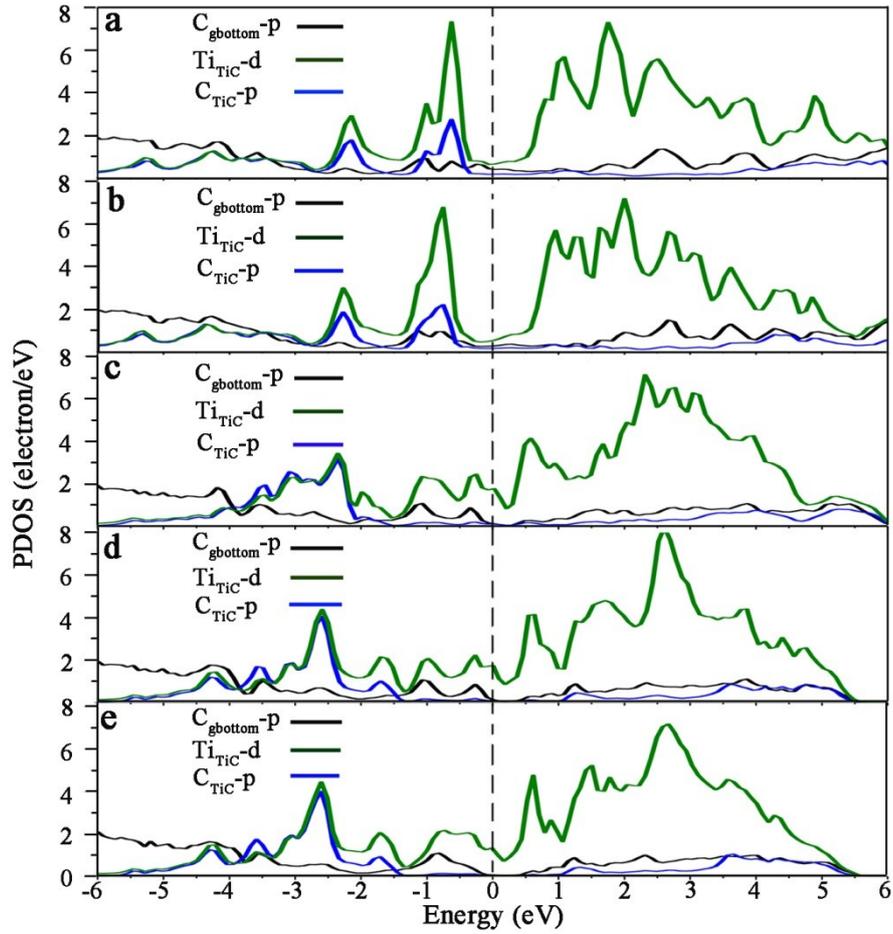
Fig. S8 The PDOS of bilayer graphene on (a, b) 1L-TiC/SiC with the Ti-center and Ti-bridge site stacking, (c) 2L-TiC/SiC, and (d, e) 3L-TiC/SiC with the Ti-center and Ti-bridge site stacking. The dash lines indicate the Fermi level, which is taken as zero.