Supporting Information

Predicting Two-Dimensional Silicon Carbide Monolayers

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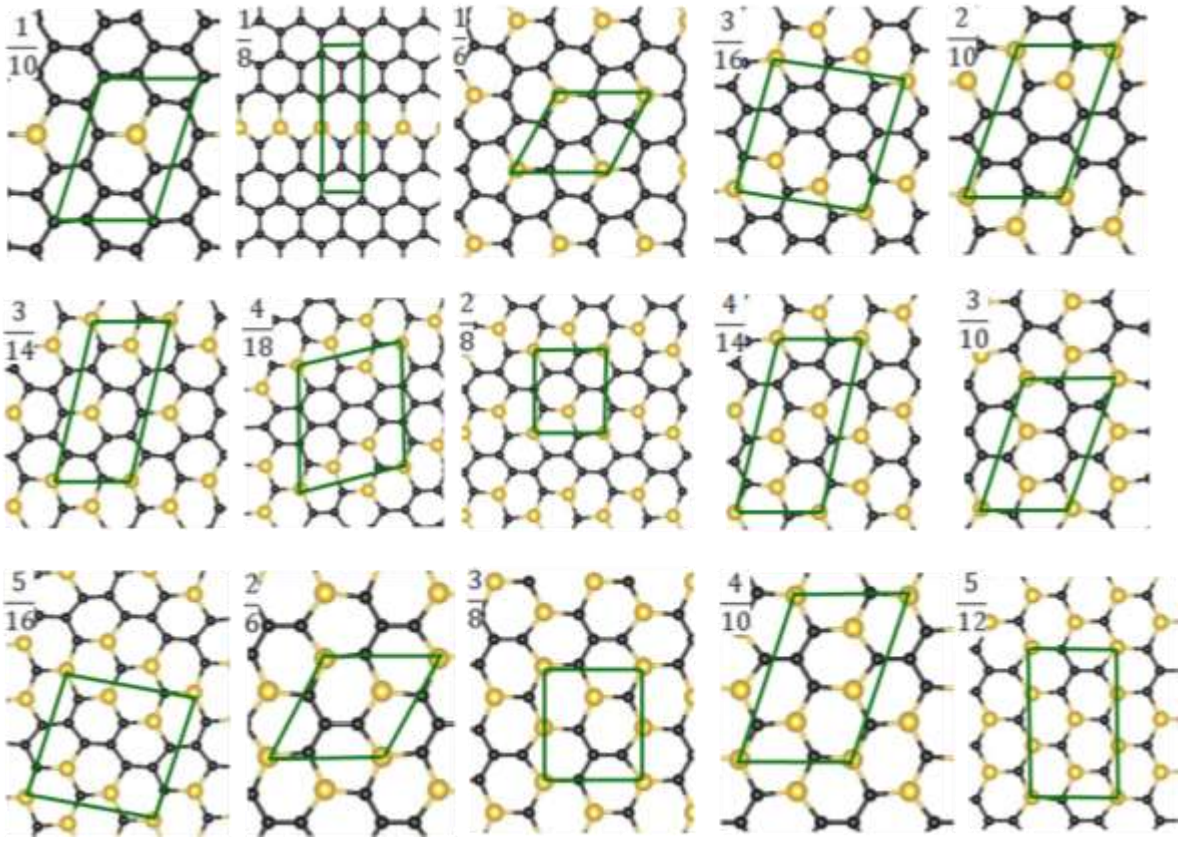

Figure S1. The low-energy structures predicted by CE-1, unit cell have been marked by green solid line. The fraction on left top corner indicate the component in an unit cell, the numerator and denominator represent the number of Si and total atoms in an unit cell.

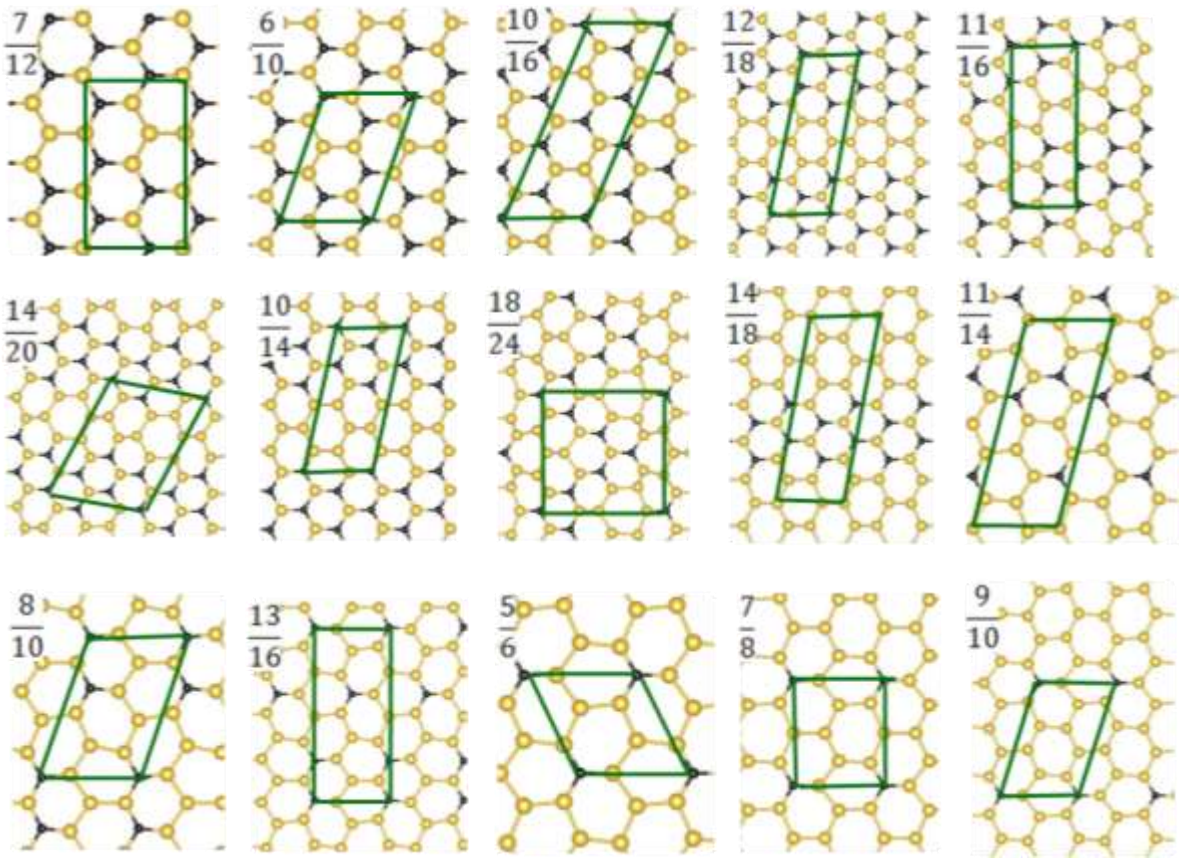

Figure S2. The low-energy structures predicted by CE-2, unit cell have been marked by green solid line. The fraction on left top corner indicate the component in an unit cell, the numerator and denominator represent the number of Si and total atoms in an unit cell.

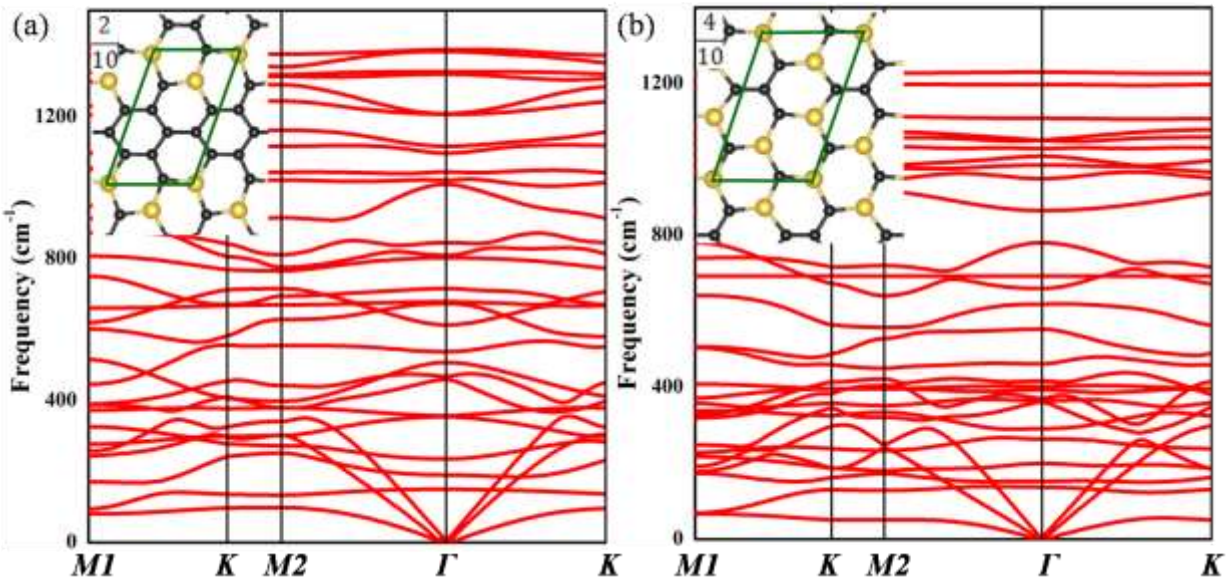

Figure S3. Computed phonon band structures of (a) SiC_4 and (b) Si_2C_3.

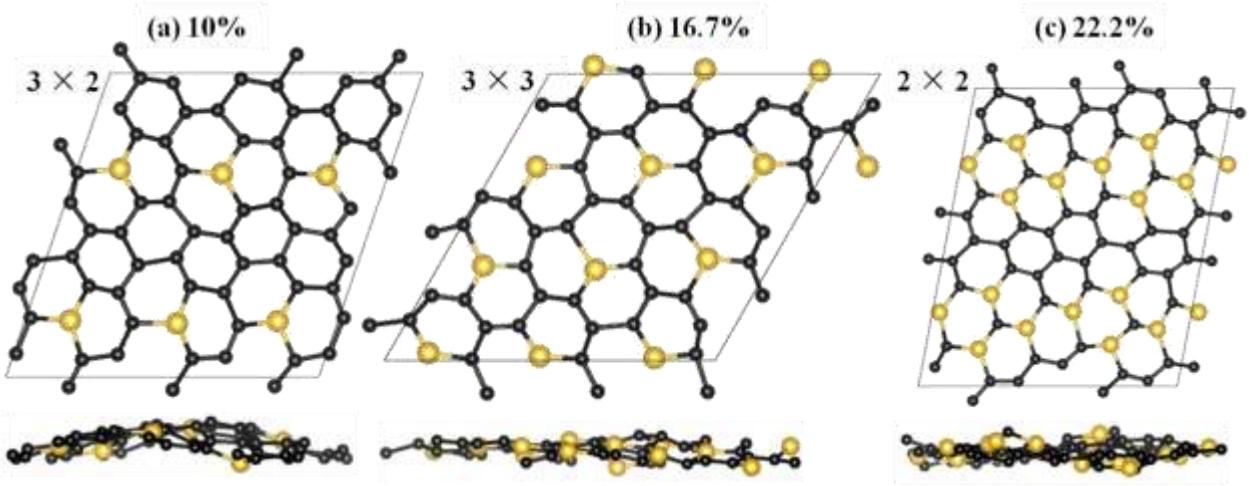

Figure S4. Top and side view of snapshots of the Si_xC_{1-x} sheets for (a) x=0.1, (b) x=0.167 and (c) x=0.222 at 10 ps of the ab initio molecular dynamics simulation in the NVT ensemble at 2500 K.

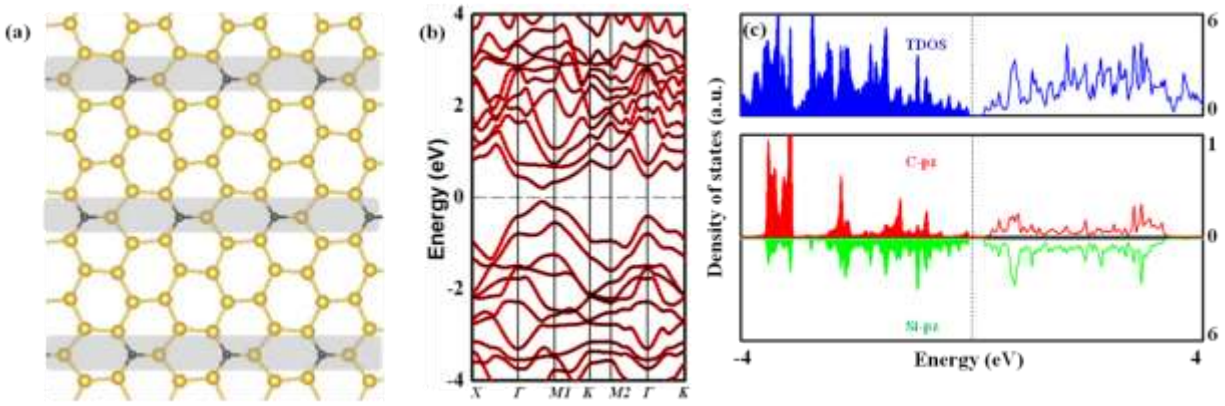

Figure S5. Mechanism for semiconducting properties in inhomogeneous distribution Si_xC_{1-x}.The (a) geometric structure (b) PBE-based band structure, (c) total and partial density of states (DOS) of the $Si_{0.9}C_{0.1}$. The green shadow in (a) covered the SiC chain which separated silicene into nanoribbons.

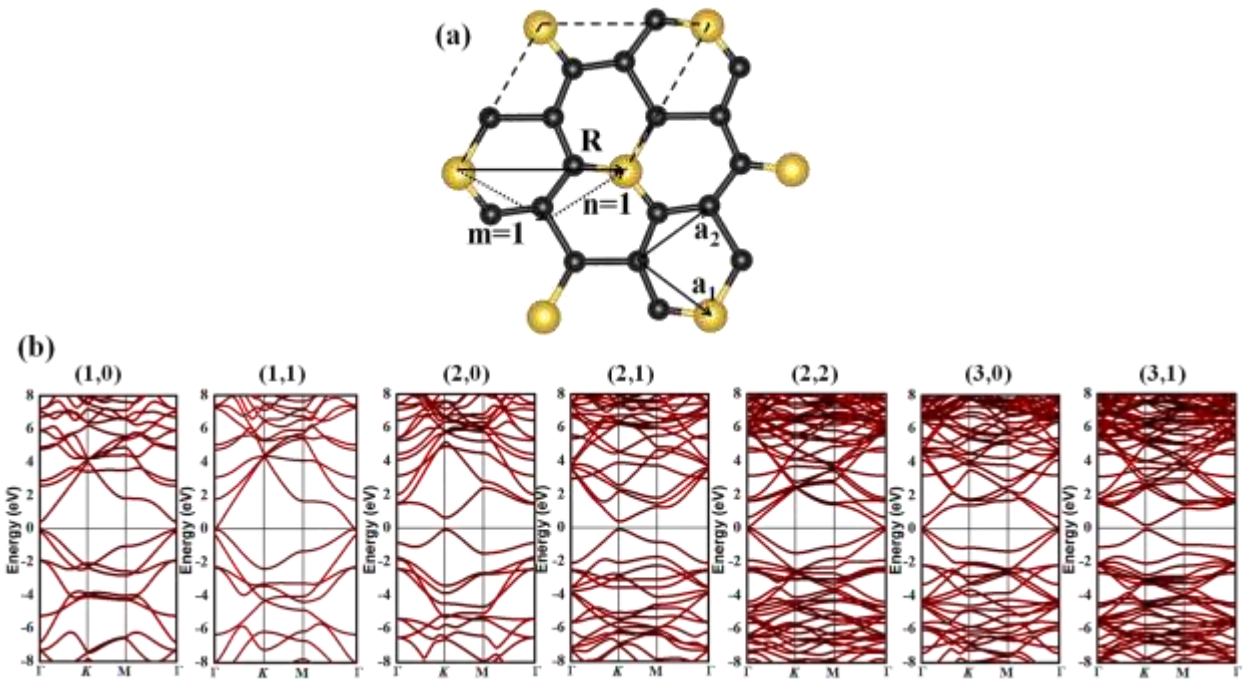

Figure S6. Atomic configurations and electronic band structures of the Si doped graphene homogenous Si_xC_{1-x} structures. (a) The (1,1) characterized by the superlattice vector $\mathbf{R}=1\mathbf{a_1}+1\mathbf{a_2}$. (b) The band structures of for Si doped graphene homogenous Si_xC_{1-x} structures ranging from (1,0) to (3,1)

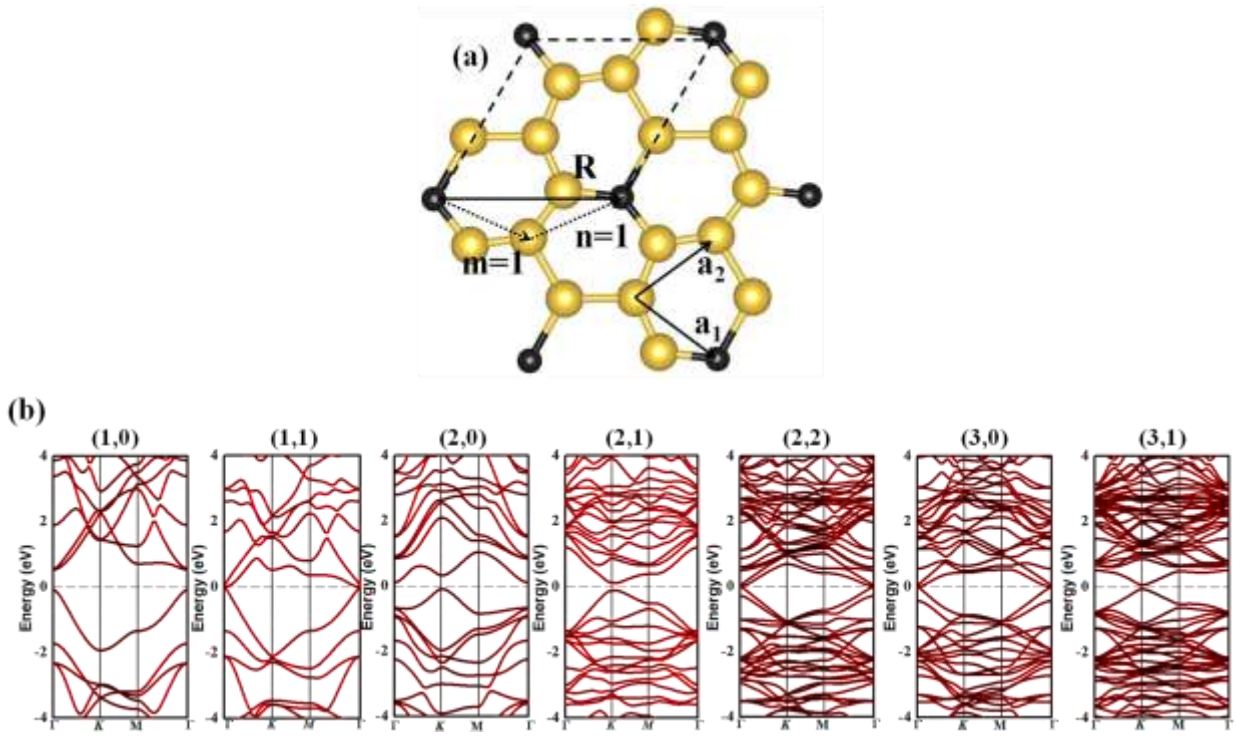

Figure S7. Atomic configurations and electronic band structures of the C dopoed silicene homogenous Si_xC_{1-x} structures. (a) The (3,1) characterized by the superlattice vector $\mathbf{R}=1\mathbf{a_1}+1\mathbf{a_2}$. (b) The band structures of for C doped silicene homogenous Si_xC_{1-x} structures ranging from (1,0) to (3,1)

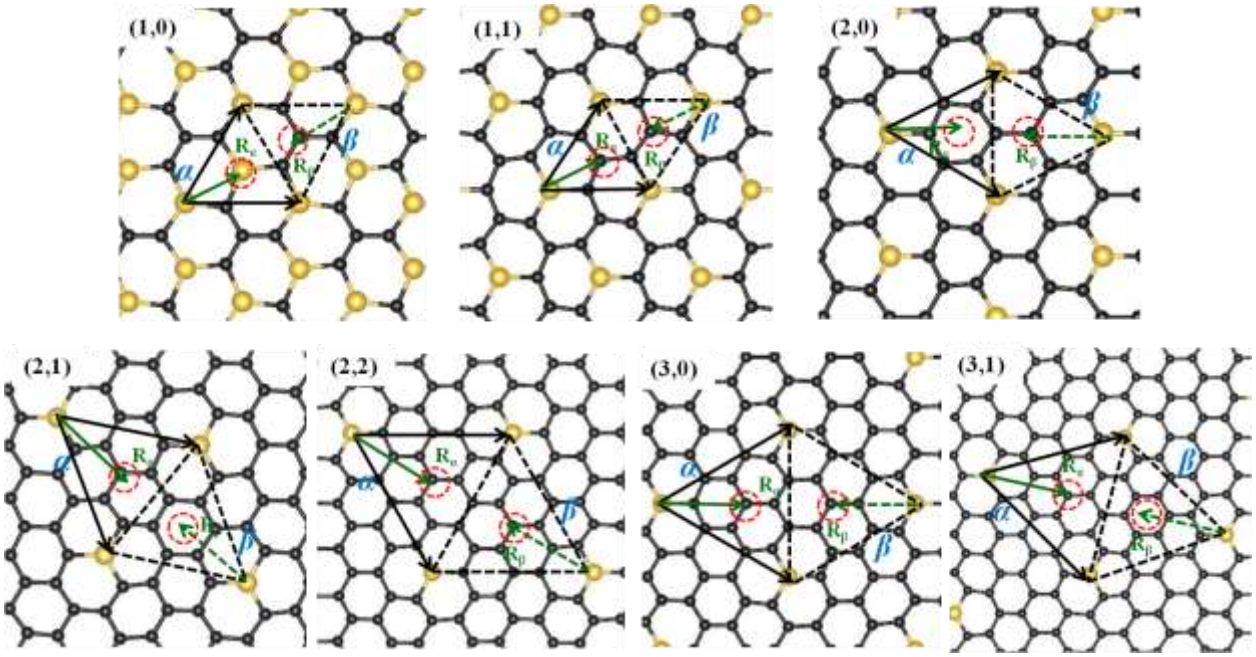

Figure S8. The superatom models of the Si dopoed graphene homogenous Si_xC_{1-x} structures, the two sublattice are differentiated by the solid (α) and dashed (β) triangle. The green arrows are the vector connecting the vertex and the center of each sublattice, and the red circle mark the center of each sublattice.