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Rich essential properties of silicon-substituted graphene nanoribbons: A comprehensive computational study

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Table S1: bandgap (eV), magnetic moment (μB), and magnetism of the 6AGNR configurations

GNR	Configuration	Bandgap E_g (eV)	Magnetic moment (μ_B)	Magnetism
6AGNR	Pristine N6	PBE: 0.91	0	nonmagnetic semiconductor
	$(1Si)_{edge}$	PBE: 0.84	0	nonmagnetic semiconductor
	$(2Si)_{meta}$	PBE: 1.16	0	nonmagnetic semiconductor
	$(2Si)_{para}$	PBE: 0.22	0	nonmagnetic semiconductor
	(6Si)/100% Si	PBE: 2.36	0	nonmagnetic semiconductor

Table S2: bandgap (eV), magnetic moment (μB), and magnetism of the 8AGNR configurations

GNR	Configuration	Bandgap E_g (eV)	Magnetic moment (μ_B)	Magnetism
8AGNR	Pristine N8	PBE: 0.43	0	nonmagnetic semiconductor
	$(1Si)_{edge}$	PBE: 0.41	0	nonmagnetic semiconductor
	$(2Si)_{meta}$	PBE: 0.52	0	nonmagnetic semiconductor
	$(2Si)_{para}$	PBE: 0.54	0	nonmagnetic semiconductor
	(8Si)/100% Si	PBE: 2.28	0	nonmagnetic semiconductor

Table S3: bandgap (eV), magnetic moment (μB), and magnetism of the pristine and single Si-substituted 7AGNRs under (2x1x1) supercells

Configuration	Bandgap E_g (eV)	Magnetic moment (μ_B)	Magnetism
Pristine 7AGNR supercell	PBE: 1.57	0	nonmagnetic semiconductor
$(1Si)_{edge}$ (2x1x1) supercell	PBE: 1.46	0	nonmagnetic semiconductor
$(1Si)_{non\text{-}edge}$ (2x1x1) supercell	PBE: 1.27	0	nonmagnetic semiconductor

Table S4: Magnetic energies of the pristine 6ZGNR configuration (configuration 1), including the antiferromagnetic (AFM), ferromagnetic (FM), and nonmagnetic (NM).

Configuration 1	AFM	FM	NM
Energy	-117.050	-117.039	-116.981

Table S5: Magnetic energies of the (1Si)edge-substituted 6ZGNR configuration (configuration 2), including the antiferromagnetic (AFM), ferromagnetic (FM), and nonmagnetic (NM).

Configuration 2	AFM	FM	NM
Energy	-110.039	-110.054	-110.019

Table S6: Magnetic energies of the (1Si)non-edge-substituted 6ZGNR configuration (configuration 3), including the antiferromagnetic (AFM), ferromagnetic (FM), and nonmagnetic (NM).

Configuration 3	AFM	FM	NM
Energy	-110.080	-110.089	-110.046

Table S7: Magnetic energies of the (6Si)-substituted 6ZGNR configuration (configuration 4)

Configuration 4	AFM	FM	NM
energy	-90.140	-90.148	-90.118

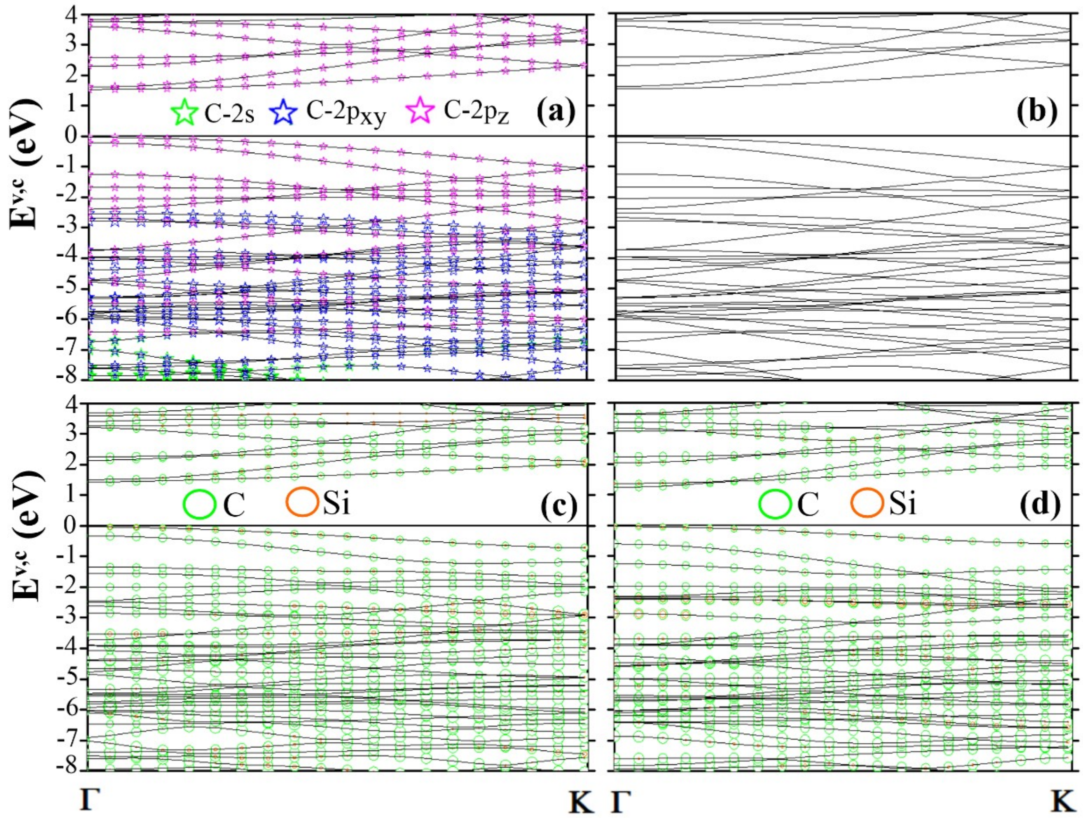

Figure S1: (a) orbital-projected and (b) total band structures of 7AGNRs under (2x1x1) supercell; atom-dominated band structures of (c) single Si edge- and (d) single Si non-edge-substituted AGNRs under (2x1x1) supercell. The green, blue, and magenta stars are responsible for the C-2s, C-2p_{xy}, and C-2p_z orbitals, while the green and orange circles display the carbon and silicon dominations, respectively.

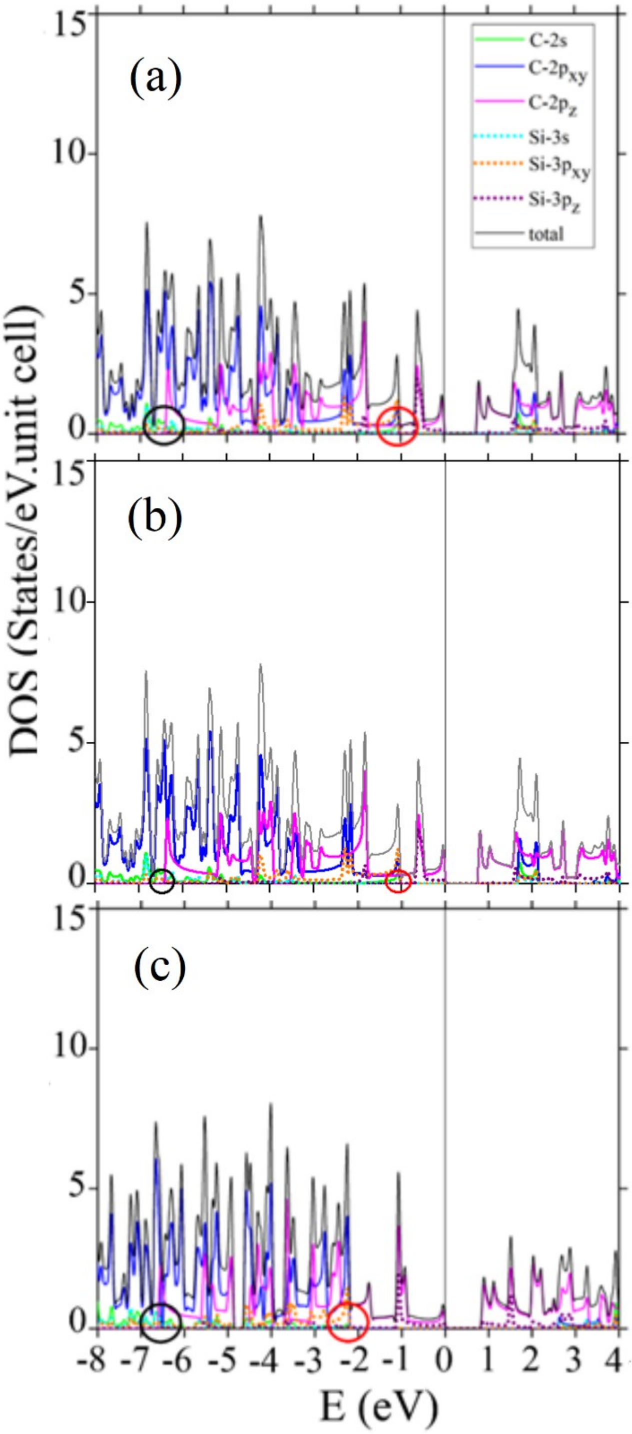

Figure S2: Orbital-projected density of states of (a) single Si non-edge- (b) double Si ortho-, and (c) double Si para-substituted 7AGNR configurations, in which the black and red circles display the termination of C-2p_z and C-2p_{xy} orbitals, respectively.