

Edge functionalized germanene nanoribbons: Impact on electronic and magnetic properties

Received 00th January 20xx,
Accepted 00th January 20xx

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DOI: 10.1039/x0xx00000x

www.rsc.org/

Electronic Supplementary Information

Table S1 Formation energy E_f (eV), band gap E_g (eV), magnetic state, the energy difference between the FM and AFM state ΔE_{FM-AFM} (eV), and spin-polarized band gap (eV) for N- and B-doped armchair edge GeNRs functionalized with hydrogen and fluorine.

Edge Type	Edge Atom	Dopant	E_f (eV/A)	Band gap (eV)	Magnetic State	Magnetic Edge State	
						ΔE (meV)	Band gap (eV)
a_{11}	H	N	-0.522	0.0	FM	-0.08	-
	H	B	-4.163	0.0	NM	-	-
	F	N	+2.654	0.0	AFM-S	+0.01	Up (0.1362) (in) – Down (0.4392) (d)
	F	B	-4.737	0.0	FM-S	-0.01	Up (0.4254) (d) – Down (0.3932) (d)
a_{22}	H	N	+0.142	0.00	NM	-	-
	H	B	-4.663	0.00	NM	-	-
	F	N	-0.473	0.00	NM	-	-
	F	B	-4.043	0.389 (d)	NM	-	-

Table S2 Edge formation energy E_{edge} (eV), band gap E_g (eV), magnetic state, the energy difference between the FM and AFM state ΔE_{FM-AFM} (eV), total magnetic moment M_{total} (μ_B), and spin-polarized band gap (eV) for z_{11} and z_{22} zigzag edge GeNRs functionalized with hydrogen and halogens.

Edge Type	Edge Atom	E_{edge} (eV/Å)	Band Gap (eV)	Magnetic State	Magnetic Edge State		
					ΔE (meV)	Band Gap (eV)	Moment (μ_B)
z_{11}	Bare	+0.243	0.00	AFM-S	+14.98	0.3274(d)	-
	H	+0.127	0.00	AFM-S	+11.36	0.2626 (d)	0.00
	F	-0.730	0.00	AFM-S	+7.73	0.2325 (d)	0.00
	Cl	-0.351	0.00	AFM-S	+2.49	0.2226 (d)	0.00
z_{22}	Bare	+0.243	0.00	AFM-S	-	-	-
	H	+0.107	0.00	AFM-S	+0.023	0.2833 (in)	0.00
	F	-1.665	0.00	NM	0.0	0.00	0.00
	Cl	-0.843	0.00	NM	0.0	0.00	0.00

a : armchair, z : zigzag, subscripts: the number of functional atoms attached to Ge edge atom, NM: non-magnetic, FM: ferromagnetic, AFM: antiferromagnetic, S: semiconductor, d: direct band gap, in: indirect band gap, ΔE : $E_{FM}-E_{AFM}$

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Table S3 Edge formation energy E_{edge} (eV), band gap E_g (eV), magnetic state, the energy difference between the FM and AFM state $\Delta E_{\text{FM-AFM}}$ (eV), and spin-polarized band gap (eV) for different N- and B-doped zigzag edge GeNRs with hydrogen and fluorine.

Edge Type	Edge Atom	Dopant	E_{edge} (eV/Å)	Band gap (eV)	Magnetic State	Magnetic Edge State	
						ΔE (meV)	Band gap (eV)
Z_{11}	H	B	-4.33	0.00	AFM-S		Up (0.314) (d) – Down (0)
	H	N	-0.625	0.00	AFM-S		Up (0) (d) – Down (0.3329) (d)
	F	B	-4.646	0.00	AFM-S		Up (0) (d) – Down (0.1461) (in)
	F	N	+2.59	0.00	AFM-S		Up (0.3081) (d) – Down (0.1318) (d)
Z_{22}	H	B	-3.954	0.00	AFM-S		Up (0.3505) (d) – Down (0) (in)
	H	N	-0.02	0.00	AFM-S		Up (0.3379) (d) – Down (0.1189) (d)
	F	B	-4.62	0.00	FM-S		Up (0.2071) (d) – Down (0.0988) (d)
	F	N	-1.05	0.00	AFM-S		0.0

a : armchair, z : zigzag, subscripts: the number of fictional atoms attached to Ge edge atom, NM: non-magnetic, FM: ferromagnetic, AFM: antiferromagnetic, S: semiconductor, d: direct band gap, in: indirect band gap, ΔE : $E_{\text{FM}} - E_{\text{AFM}}$