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# Edge Functionalization and Doping Effects on Stability, Electronic and Magnetic Properties of Silicene Nanoribbons

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## Electronic Supplementary Information

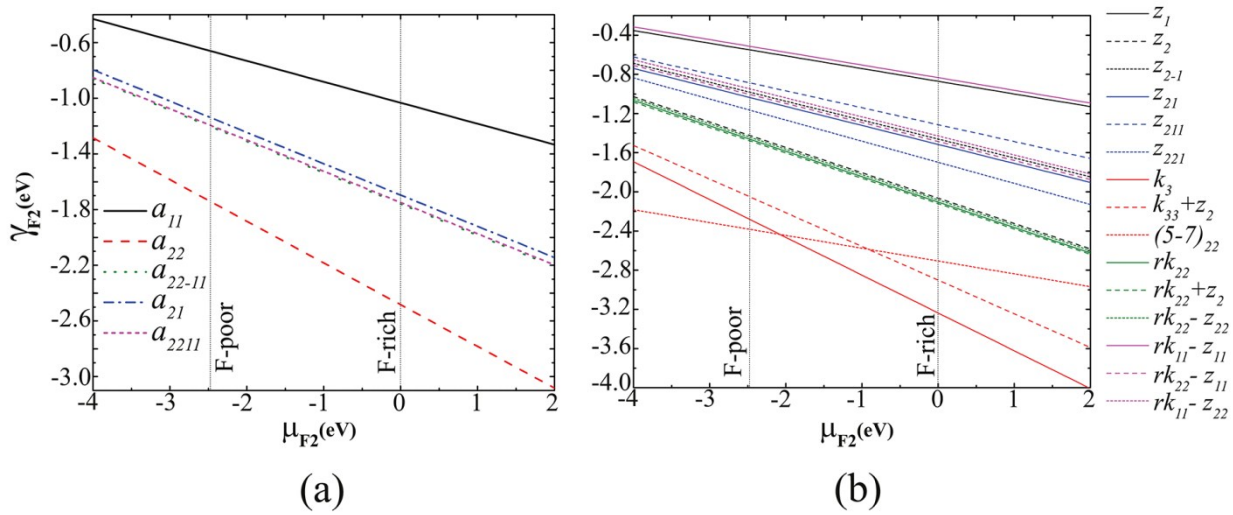


Fig. S1 (a) Edge free energy $\gamma_{F2}$ as a function of fluorine chemical potential $\mu_{F2}$, using $E_{F2}$ as the zero reference, for (a) different fluorinated edge ASiNRs (b) different edge structures of fluorinated SiNRs along $<2\bar{1}\bar{1}0>$. The allowed range for fluorine chemical potential is indicated by vertical dotted lines.

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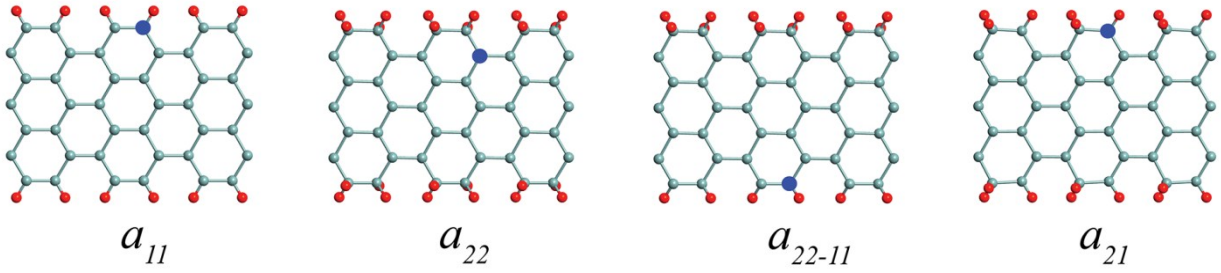


Fig. S2 Schematic structural models of the different edge functionalized ASiNRs doped with a N or B atom, in which the most stable substitution configurations are indicated. The cyan and red balls represent Si and functional addends (H, F, Cl, Br, and I), respectively, and the blue solid circle shows a N or B atom.

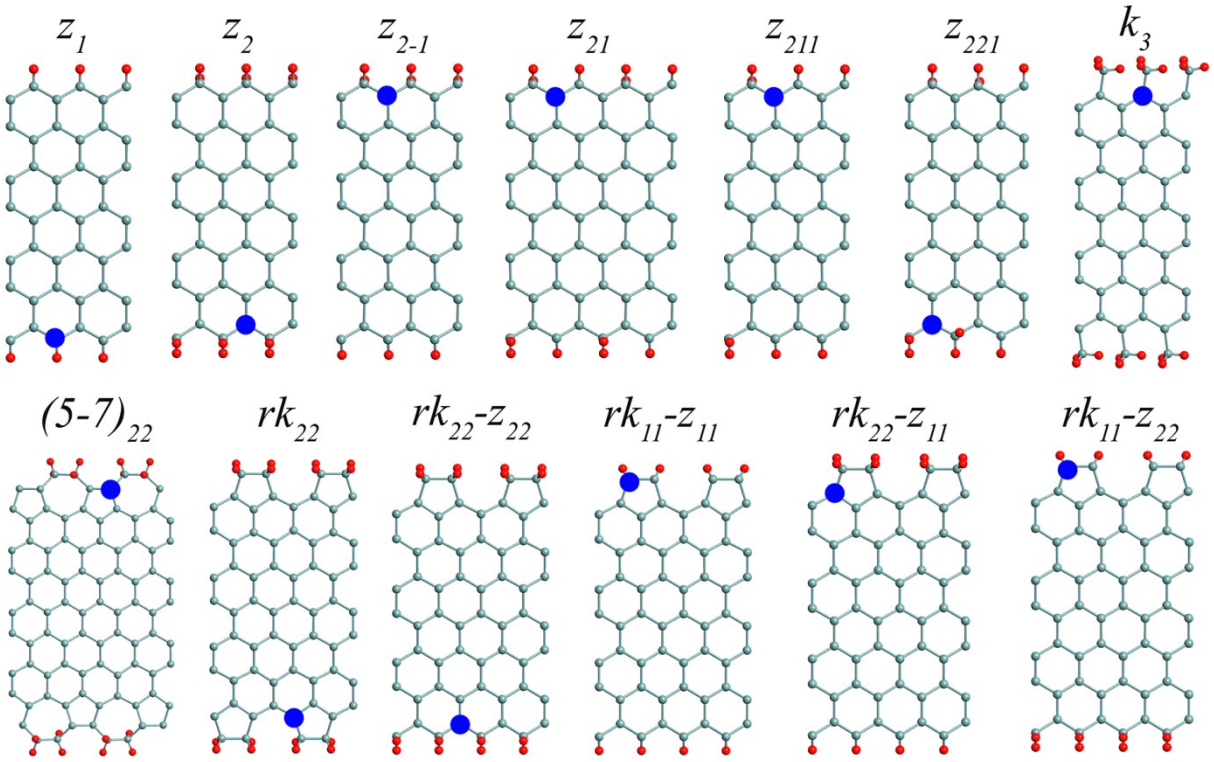


Fig. S3 Different edge structures of functionalized SiNRs along the $<2\bar{1}\bar{1}0>$ direction doped with a N or B atom, in which the most stable substitution configurations are indicated. The cyan and red balls represent Si and functional addends (H, F, Cl, Br, and I), respectively, and the blue solid circle shows a N or B atom.

Table S1 Edge formation energy $E_{edge}$ (eV), band gap $E_g$ (eV), magnetic state, the energy difference between the FM and AFM state $\Delta E_{FM\text{-}AFM}$ (eV), total magnetic moment $M_{total}$ ($\mu$B), and spin-polarized band gap (eV) for different armchair edge SiNRs functionalized with hydrogen and halogens.

| Edge Type | Edge Atom | $E_{edge}$ (eV/A) | Band Gap (eV) | Magnetic State | Magnetic Edge State | | |
|---|---|---|---|---|---|---|---|
| | | | | | ΔE (meV) | Band Gap (eV) | Moment ($\mu$B) |
| $a_{11}$ | Bare | +0.330 | 0.357 (in) | NM | - | - | - |
| | H | −0.082 | 0.581 (d) | NM | - | - | - |
| | F | −1.032 | 0.514 (d) | NM | - | - | - |
| | Cl | −0.433 | 0.411 (d) | NM | - | - | - |
| | Br | −0.314 | 0.218 (d) | NM | - | - | - |
| | I | −0.183 | 0.201 (d) | NM | - | - | - |
| $a_{22}$ | Bare | +0.330 | 0.357 (in) | NM | - | - | - |
| | H | −0.129 | 0.096 (d) | NM | - | - | - |
| | F | −2.483 | 0.118 (d) | NM | - | - | - |
| | Cl | −1.219 | 0.026 (d) | NM | - | - | - |
| | Br | −0.985 | 0.034 (d) | NM | - | - | - |
| | I | −0.689 | 0.109 (d) | NM | - | - | - |
| $a_{22\text{-}11}$ | Bare | +0.330 | 0.357 (d) | NM | - | - | - |
| | H | −0.025 | 0.446 (d) | NM | - | - | - |
| | F | −1.759 | 0.452 (d) | NM | - | - | - |
| | Cl | −0.822 | 0.498 (d) | NM | - | - | - |
| | Br | −0.652 | 0.558 (d) | NM | - | - | - |
| | I | −0.439 | 0.584 (d) | NM | - | - | - |
| $a_{21}$ | Bare | +0.330 | 0.357 (in) | NM | - | - | - |
| | H | +0.058 | 0.00 | FM-S | −86.55 | Up (0.888) (d) – Down (0.697) (in) | 1.997 |
| | F | −1.695 | 0.00 | AFM-M | +6.38 | 0.00 | 0.00 |
| | Cl | −0.762 | 0.00 | FM-S | −18.12 | Up (0.650) (d) – Down (0.55) (in) | 1.960 |
| | Br | −0.603 | 0.00 | FM-S | −34.02 | Up (0.664) (d) – Down (0.584) (in) | 1.790 |
| | I | −0.394 | 0.00 | FM-S | −56.99 | Up (0.659) (d) – Down (0.551) (in) | 1.990 |
| $a_{2211}$ | Bare | +0.330 | 0.357 (in) | NM | - | - | - |
| | H | −0.021 | 0.334 (d) | NM | - | - | - |
| | F | −1.749 | 0.308 (d) | NM | - | - | - |
| | Cl | −0.761 | 0.378 (d) | NM | - | - | - |
| | Br | −0.659 | 0.397 (d) | NM | - | - | - |
| | I | −0.446 | 0.370 (d) | NM | - | - | - |

*a*: armchair, *z*: zigzag, *k*: Klein, *rk*: reconstructed Klein, subscripts: the number of fictional atoms attached to Si edge atom, NM: non-magnetic, FM: ferromagnetic, AFM: antiferromagnetic, S: semiconductor, M: metal, SGS: spin-gapless semiconductor, HF: half-metal, d: direct band gap, in: indirect band gap, ΔE: $E_{FM}$-$E_{AFM}$

Table S2 Edge formation energy $E_{edge}$ (eV), band gap $E_g$(eV), magnetic state, the energy difference between the FM and AFM state $\Delta E_{FM-AFM}$ (eV), total magnetic moment $M_{total}$ ($\mu$B), and spin-polarized band gap (eV) for different zigzag edge SiNRs functionalized with hydrogen and halogens.

| Edge Type | Edge Atom | $E_{edge}$ (eV/A) | Band Gap (eV) | Magnetic State | Magnetic Edge State | | |
|---|---|---|---|---|---|---|---|
| | | | | | ΔE (meV) | Band Gap (eV) | Moment (μB) |
| $z_1$ | Bare | +0.381 | 0.00 | NM | - | - | - |
| | H | +0.097 | 0.00 | AFM-S | +5.08 | 0.313 (d) | 0.00 |
| | F | −0.871 | 0.00 | AFM-S | +4.23 | 0.281 (d) | 0.00 |
| | Cl | −0.362 | 0.00 | AFM-S | +4.05 | 0.271 (d) | 0.00 |
| | Br | −0.282 | 0.00 | AFM-S | +4.01 | 0.269 (d) | 0.00 |
| | I | −0.165 | 0.00 | AFM-S | +3.71 | 0.253 (d) | 0.00 |
| $z_2$ | Bare | +0.381 | 0.00 | NM | - | - | - |
| | H | −0.101 | 0.036(in) | AFM-S | +34.46 | 0.414 (in) | 0.00 |
| | F | −2.064 | 0.00 | AFM-S | +25.44 | 0.312 (in) | 0.00 |
| | Cl | −0.951 | 0.00 | AFM-S | +14.29 | 0.174 (in) | 0.00 |
| | Br | −0.766 | 0.00 | AFM-S | +16.26 | 0.184 (in) | 0.00 |
| | I | −0.469 | 0.00 | AFM-S | +21.39 | 0.267 (in) | 0.00 |
| $z_{2\text{-}1}$ | Bare | +0.381 | 0.00 | NM | - | - | - |
| | H | +0.053 | 0.00 | FM-S | −12.14 | Up (0.540) (d) – Down (0.541) (d) | 1.00 |
| | F | −1.460 | 0.00 | FM-M | −8.12 | 0.00 | 0.981 |
| | Cl | −0.658 | 0.00 | FM-SGS | −6.17 | Up (0.505) (in) – Down (0.277) (in) | 0.909 |
| | Br | −0.529 | 0.00 | FM-SGS | −5.99 | Up (0.495) (in) – Down (0.273) (in) | 0.913 |
| | I | −0.346 | 0.00 | FM-M | −3.20 | 0.00 | 0.932 |
| $z_{21}$ | Bare | +0.372 | 0.00 | NM | - | - | - |
| | H | +0.002 | 0.175 (d) | NM | - | - | - |
| | F | −1.515 | 0.159 (d) | NM | - | - | - |
| | Cl | −0.699 | 0.162 (d) | NM | - | - | - |
| | Br | −568 | 0.156 (d) | NM | - | - | - |
| | I | −0.385 | 0.156 (d) | NM | - | - | - |
| $z_{211}$ | Bare | +0.350 | 0.00 | NM | - | - | - |
| | H | −0.003 | 0.160 (d) | NM | - | - | - |
| | F | −1.698 | 0.091 (d) | NM | - | - | - |
| | Cl | −0.786 | 0.110 (d) | NM | - | - | - |
| | Br | −0.637 | 0.109 (d) | NM | - | - | - |
| | I | −0.431 | 0.118 (d) | NM | - | - | - |
| $z_{221}$ | Bare | +0.383 | 0.00 | NM | - | - | - |
| | H | −0.402 | 0.140 (d) | AFM-S | +48.31 | 0.285 (in) | 0.00 |
| | F | −0.648 | 0.024 (in) | AFM-S | +10.56 | 0.078 (in) | 0.00 |
| | Cl | −0.199 | 0.025 (in) | AFM-S | +14.47 | 0.079 (in) | 0.00 |
| | Br | −0.152 | 0.040 (in) | AFM-S | +18.77 | 0.101 (in) | 0.00 |
| | I | −0.085 | 0.058 (in) | AFM-S | +22.01 | 0.133 (in) | 0.00 |

*a*: armchair, *z*: zigzag, *k*: Klein, *rk*: reconstructed Klein, subscripts: the number of fictional atoms attached to Si edge atom, NM: non-magnetic, FM: ferromagnetic, AFM: antiferromagnetic, S: semiconductor, M: metal, SGS: spin-gapless semiconductor, HF: half-metal, d: direct band gap, in: indirect band gap, ΔE: $E_{FM}$-$E_{AFM}$

Table S3 Edge formation energy $E_{edge}$ (eV), band gap $E_g$ (eV), magnetic state, the energy difference between the FM and AFM state $\Delta E_{FM-AFM}$ (eV), total magnetic moment $M_{total}$ ($\mu$B), and spin-polarized band gap (eV) for different Klein edge SiNRs functionalized with hydrogen and halogens.

| Edge Type | Edge Atom | $E_{edge}$ (eV/A) | Band Gap (eV) | Magnetic State | Magnetic Edge State | | |
|---|---|---|---|---|---|---|---|
| | | | | | ΔE (meV) | Band Gap (eV) | Moment ($\mu$B) |
| $k_2$ | Bare | +0.383 | 0.00 | NM | - | - | - |
| | H | +0.255 | 0.00 | NM | - | - | - |
| | F | −1.837 | 0.00 | NM | - | - | - |
| | Cl | −0.812 | 0.00 | NM | - | - | - |
| | Br | −0.628 | 0.00 | NM | - | - | - |
| | I | −0.426 | 0.00 | NM | - | - | - |
| $k_3$ | Bare | +0.383 | 0.00 | NM | - | - | - |
| | H | −0.072 | 0.00 | AFM-S | +4.60 | 0.290 (d) | 0.00 |
| | F | −3.237 | 0.00 | AFM-S | +4.55 | 0.273 (in) | 0.00 |
| | Cl | −1.477 | 0.00 | AFM-S | +5.10 | 0.278 (in) | 0.00 |
| | Br | −1.154 | 0.00 | AFM-S | +4.53 | 0.200 (in) | 0.00 |
| | I | −0.763 | 0.00 | AFM-S | +1.01 | 0.101 (in) | 0.00 |
| $k_{33}$+$z_2$ | Bare | +0.334 | 0.00 | NM | - | - | - |
| | H | −0.103 | 0.161 (d) | NM | - | - | - |
| | F | −2.901 | 0.157 (d) | NM | - | - | - |
| | Cl | −1.390 | 0.156 (d) | NM | - | - | - |
| | Br | −1.103 | 0.159 (d) | NM | - | - | - |
| | I | −0.797 | 0.112 (d) | NM | - | - | - |
| $(5\text{-}7)_{22}$ | Bare | +0.354 | 0.00 | NM | - | - | - |
| | H | −0.020 | 0.00 | NM | - | - | - |
| | F | −2.076 | 0.00 | NM | - | - | - |
| | Cl | −0.970 | 0.00 | NM | - | - | - |
| | Br | −0.372 | 0.00 | NM | - | - | - |
| | I | −0.288 | 0.00 | NM | - | - | - |
| $rk_{22}$ | Bare | +0.338 | 0.00 | NM | - | - | - |
| | H | −0.069 | 0.00 | AFM-S | +8.80 | 0.281 (d) | 0.00 |
| | F | −2.104 | 0.00 | AFM-S | +8.64 | 0.284 (d) | 0.00 |
| | Cl | −1.011 | 0.00 | AFM-S | +8.44 | 0.275 (d) | 0.00 |
| | Br | −0.827 | 0.00 | AFM-S | +8.49 | 0.276 (d) | 0.00 |
| | I | −0.584 | 0.00 | AFM-S | +8.14 | 0.289 (in) | 0.00 |
| $rk_{22}$+$z_2$ | Bare | +0.333 | 0.00 | NM | - | - | - |
| | H | −0.083 | 0.160 (d) | NM | - | - | - |
| | F | −2.120 | 0.150 (d) | NM | - | - | - |
| | Cl | −1.014 | 0.151 (d) | NM | - | - | - |
| | Br | −0.835 | 0.141 (d) | NM | - | - | - |
| | I | −0.588 | 0.144 (d) | NM | - | - | - |

*a*: armchair, *z*: zigzag, *k*: Klein, *rk*: reconstructed Klein, subscripts: the number of fictional atoms attached to Si edge atom, NM: non-magnetic, FM: ferromagnetic, AFM: antiferromagnetic, S: semiconductor, M: metal, SGS: spin-gapless semiconductor, HF: half-metal, d: direct band gap, in: indirect band gap, ΔE: $E_{FM}$-$E_{AFM}$

Table S4 Edge formation energy $E_{edge}$ (eV), band gap $E_g$ (eV), magnetic state, the energy difference between the FM and AFM state $\Delta E_{FM-AFM}$ (eV), total magnetic moment $M_{total}$ ($\mu$B), and spin-polarized band gap (eV) for reconstructed Klein edge and zigzag edge SiNRs combinations functionalized with hydrogen and halogens.

| Edge Type | Edge Atom | $E_{edge}$ (eV/A) | Band Gap (eV) | Magnetic State | Magnetic Edge State | | |
|---|---|---|---|---|---|---|---|
| | | | | | ΔE (meV) | Band Gap (eV) | Moment ($\mu$B) |
| $rk_{22}$-$z_{22}$ | Bare | +0.355 | 0.00 | NM | - | - | - |
| | H | −0.036 | 0.00 | FM-S | −22.46 | Up (0.524) (in) – Down (0.473) (in) | 2.003 |
| | F | −2.082 | 0.00 | FM-M | −14.71 | 0.00 | 1.607 |
| | Cl | −0.982 | 0.00 | FM-S | −13.26 | Up (0.528) (in) – Down (0.270) (in) | 1.660 |
| | Br | −0.799 | 0.00 | FM-S | −13.96 | Up (0.520) (in) – Down (0.276) (in) | 1.875 |
| | I | −0.557 | 0.00 | FM-M | −4.66 | 0.00 | 0.492 |
| $rk_{11}$-$z_{11}$ | Bare | +0.355 | 0.00 | NM | - | - | - |
| | H | +0.127 | 0.00 | FM-M | −6.94 | 0.00 | 0.921 |
| | F | −0.834 | 0.00 | FM-M | −4.04 | 0.00 | 1.037 |
| | Cl | −0.329 | 0.00 | FM-M | −4.43 | 0.00 | 1.016 |
| | Br | −0.248 | 0.00 | FM-M | −3.67 | 0.00 | 1.031 |
| | I | −0.158 | 0.00 | FM-M | −1.21 | 0.00 | 1.012 |
| $rk_{22}$-$z_{11}$ | Bare | +0.355 | 0.00 | NM | - | - | - |
| | H | +0.015 | 0.00 | AFM-S | +9.5 | Up (0.297) (d) – Down (0.301) (d) | 0.00 |
| | F | −1.486 | 0.00 | AFM-S | +8.04 | Up (0.343) (d) – Down (0.198) (d) | 0.00 |
| | Cl | −0.685 | 0.00 | AFM-S | +8.02 | Up (0.328) (d) – Down (0.200) (d) | 0.00 |
| | Br | −0.554 | 0.00 | AFM-S | +7.94 | Up (0.326) (d) – Down (0.201) (d) | 0.00 |
| | I | −0.365 | 0.00 | AFM-S | +7.52 | Up (0.310) (d) – Down (0.188) (d) | 0.00 |
| $rk_{11}$-$z_{22}$ | Bare | +0.355 | 0.00 | NM | - | - | - |
| | H | +0.009 | 0.00 | AFM-M | +8.2 | 0.00 | 0.00 |
| | F | −1.429 | 0.00 | AFM-M | +6.69 | 0.00 | 0.00 |
| | Cl | −0.627 | 0.00 | AFM-M | +2.12 | 0.00 | 0.00 |
| | Br | −0.496 | 0.00 | AFM-M | +1.23 | 0.00 | 0.00 |
| | I | −0.341 | 0.00 | AFM-M | +0.091 | 0.00 | 0.00 |

*a*: armchair, *z*: zigzag, *k*: Klein, *rk*: reconstructed Klein, subscripts: the number of fictional atoms attached to Si edge atom, NM: non-magnetic, FM: ferromagnetic, AFM: antiferromagnetic, S: semiconductor, M: metal, SGS: spin-gapless semiconductor, HF: half-metal, d: direct band gap, in: indirect band gap, ΔE: $E_{FM}$-$E_{AFM}$

Table S5 Edge formation energy $E_{edge}$ (eV), band gap $E_g$ (eV), magnetic state, the energy difference between the FM and AFM state $\Delta E_{FM-AFM}$ (eV), and spin-polarized band gap (eV) for different N- and B-doped armchair edge SiNRs functionalized with hydrogen and fluorine.

| Edge Type | Edge Atom | Dopant | $E_{edge}$ (eV/A) | Band gap (eV) | Magnetic State | Magnetic Edge State | |
|---|---|---|---|---|---|---|---|
| | | | | | | ΔE (meV) | Band gap (eV) |
| $a_{11}$ | H | N | −1.005 | 0.00 | FM-S | −0.31 | Up (0.137) (in) – Down (0.540) (d) |
| | H | B | −4.401 | 0.00 | NM | - | - |
| | F | N | −2.301 | 0.00 | FM-SGS | −0.10 | Up (0.092) (in) – Down (0.463) (d) |
| | F | B | −4.662 | 0.00 | FM-SGS | −0.09 | Up (0.481) (in) – Down (0.259) (in) |
| $a_{22}$ | H | N | −0.683 | 0.00 | NM | - | - |
| | H | B | −4.412 | 0.00 | NM | - | - |
| | F | N | −1.170 | 0.00 | NM | - | - |
| | F | B | −4.662 | 0.00 | NM | - | - |
| $a_{22\text{-}11}$ | H | N | −1.026 | 0.00 | NM | - | - |
| | H | B | −4.403 | 0.00 | NM | - | - |
| | F | N | −1.344 | 0.00 | NM | - | - |
| | F | B | −4.584 | 0.00 | NM | - | - |
| $a_{21}$ | H | N | −2.067 | 0.00 | FM-S | −170.91 | Up (0.310) (d) – Down (0.188) (d) |
| | H | B | −4.864 | 0.00 | FM-S | −180.46 | Up (0.44) (d) – Down (0.630) (in) |
| | F | N | −1.87 | 0.00 | AFM-S | +43.59 | Up (0.248) (in) – Down (0.241) (d) |
| | F | B | −5.123 | 0.00 | AFM-S | +4.57 | Up (0.103) (in) – Down (0.221) (in) |

*a*: armchair, *z*: zigzag, *k*: Klein, *rk*: reconstructed Klein, subscripts: the number of fictional atoms attached to Si edge atom, NM: non-magnetic, FM: ferromagnetic, AFM: antiferromagnetic, S: semiconductor, M: metal, SGS: spin-gapless semiconductor, HF: half-metal, d: direct band gap, in: indirect band gap, ΔE: $E_{FM}$-$E_{AFM}$

 

Table S6 Edge formation energy $E_{edge}$ (eV), band gap $E_g$ (eV), magnetic state, the energy difference between the FM and AFM state $\Delta E_{FM-AFM}$ (eV), and spin-polarized band gap (eV) for different N- and B-doped zigzag edge SiNRs and Klein edge SiNRs functionalized with hydrogen and fluorine.

| Edge Type | Edge Atom | Dopant | $E_{edge}$ (eV/A) | Band gap (eV) | Magnetic State | Magnetic Edge State | |
|---|---|---|---|---|---|---|---|
| | | | | | | ΔE (meV) | Band gap (eV) |
| $z_1$ | H | N | −1.251 | 0.00 | AFM-S | +0.001 | Up (0.161) (d) – Down (0.191) (d) |
| | H | B | −4.765 | 0.00 | AFM-S | +0.001 | Up (0.219) (d) – Down (0.106) (d) |
| | F | N | −2.699 | 0.00 | AFM-S | +0.009 | Up (0.159) (d) – Down (0.155) (d) |
| | F | B | −5.050 | 0.00 | AFM-S | +0.002 | Up (0.198) (d) – Down (0.840) (d) |
| $z_2$ | H | N | −1.452 | 0.00 | AFM-S | +99.79 | Up (0.365) (d) – Down (0.352) (in) |
| | H | B | −4.598 | 0.00 | AFM-S | +93.55 | Up (0.444) (in) – Down (0.243) (in) |
| | F | N | −2.386 | 0.00 | AFM-S | +5.94 | Up (0.131) (in) – Down (0.035) (in) |
| | F | B | −4.700 | 0.00 | AFM-S | +7.62 | Up (0.184) (in) – Down (0.031) (d) |
| $z_{2\text{-}1}$ | H | N | −1.725 | 0.00 | FM-S | −28.43 | Up (0.486) (in) – Down (0.200) (in) |
| | H | B | −4.849 | 0.00 | FM-S | −20.96 | Up (0.238) (in) – Down (0.373) (in) |
| | F | N | −2.416 | 0.00 | FM-HM | −8.42 | Up (0.00) – Down (0.174) (d) |
| | F | B | −4.709 | 0.00 | FM-M | −7.59 | 0.00 |
| $z_{221}$ | H | N | −2.187 | 0.00 | AFM-SGS | +0.008 | Up (0.163) (d) – Down (0.252) (in) |
| | H | B | −5.508 | 0.00 | AFM-S | +0.007 | Up (0.372) (d) – Down (0.111) (d) |
| | F | N | −2.069 | 0.00 | AFM-M | +0.003 | 0.00 |
| | F | B | −4.637 | 0.00 | AFM-HM | +0.002 | Up (0.238) (in) – Down (0.00) |
| $k_3$ | H | N | −1.904 | 0.00 | FM-S | −0.010 | Up (0.158) (d) – Down (0.170) (d) |
| | H | B | −5.310 | 0.00 | FM-S | −0.011 | Up (0.202) (d) – Down (0.0.089) (d) |
| | F | N | −2.682 | 0.00 | FM-S | −0.020 | Up (0.149) (d) – Down (0.134) (in) |
| | F | B | −6.066 | 0.00 | FM-HM | −0.015 | Up (0.221) (d) – Down (0.00) |
| $rk_{22}$ | H | N | −1.171 | 0.00 | FM-S | −0.011 | Up (0.129) (d) – Down (0.186) (d) |
| | H | B | −4.590 | 0.00 | FM-S | −0.020 | Up (0.198) (d) – Down (0.072) (d) |
| | F | N | −1.893 | 0.00 | FM-S | −0.013 | Up (0.123) (d) – Down (0.183) (d) |
| | F | B | −4.648 | 0.00 | FM-S | −0.022 | Up (0.203) (d) – Down (0.073) (d) |

*a*: armchair, *z*: zigzag, *k*: Klein, *rk*: reconstructed Klein, subscripts: the number of fictional atoms attached to Si edge atom, NM: non-magnetic, FM: ferromagnetic, AFM: antiferromagnetic, S: semiconductor, M: metal, SGS: spin-gapless semiconductor, HF: half-metal, d: direct band gap, in: indirect band gap, ΔE: $E_{FM}$-$E_{AFM}$

Table S7 Edge formation energy $E_{edge}$ (eV), band gap $E_g$ (eV), magnetic state, the energy difference between the FM and AFM state $\Delta E_{FM\text{-}AFM}$ (eV), and spin-polarized band gap (eV) for N- and B-doped reconstructed Klein edge and zigzag edge SiNRs combinations functionalized with hydrogen and fluorine.

| Edge Type | Edge Atom | Dopant | $E_{edge}$ (eV/A) | Band gap (eV) | Magnetic State | Magnetic Edge State | |
|---|---|---|---|---|---|---|---|
| | | | | | | ΔE (meV) | Band gap (eV) |
| $rk_{22}$-$z_{22}$ | H | N | −1.710 | 0.00 | FM-S | −13.660 | Up (0.424) (in) – Down (0.383) (in) |
| | H | B | −4.590 | 0.00 | FM-S | −12.530 | Up (0.186) (in) – Down (0.483) (d) |
| | F | N | −1.893 | 0.00 | FM-S | −13.360 | Up (0.479) (d) – Down (0.395) (in) |
| | F | B | −4.648 | 0.00 | FM-HM | −1.810 | Up (0.00) – Down (0.353) (d) |
| $rk_{11}$-$z_{11}$ | H | N | −1.543 | 0.00 | FM-S | −10.150 | Up (0.423) (in) – Down (0.416) (in) |
| | H | B | −4.522 | 0.00 | FM-M | −0.110 | 0.00 |
| | F | N | −1.915 | 0.00 | FM-S | −8.230 | Up (0.384) (in) – Down (0.423) (d) |
| | F | B | −5.154 | 0.00 | FM-M | −0.080 | 0.00 |
| $rk_{22}$-$z_{11}$ | H | N | −0.517 | 0.00 | AFM-M | +0.007 | 0.00 |
| | H | B | −4.397 | 0.00 | AFM-M | +0.005 | 0.00 |
| | F | N | −0.999 | 0.00 | AFM-M | +0.002 | 0.00 |
| | F | B | −4.569 | 0.00 | AFM-M | +0.001 | 0.00 |
| $rk_{11}$-$z_{22}$ | H | N | −0.556 | 0.00 | FM-S | −12.41 | Up (0.320) (d) – Down (0.178) (in) |
| | H | B | −3.504 | 0.00 | FM-SGS | −6.070 | Up (0.082) (in) – Down (0.124) (in) |
| | F | N | −0.940 | 0.00 | FM-HM | −11.03 | Up (0.178) (d) – Down (0.00) |
| | F | B | −5.199 | 0.00 | FM-HM | −5.84 | Up (0.00) – Down (0.307) (d) |

*a*: armchair, *z*: zigzag, *k*: Klein, *rk*: reconstructed Klein, subscripts: the number of fictional atoms attached to Si edge atom, NM: non-magnetic, FM: ferromagnetic, AFM: antiferromagnetic, S: semiconductor, M: metal, SGS: spin-gapless semiconductor, HF: half-metal, d: direct band gap, in: indirect band gap, ΔE: $E_{FM}$-$E_{AFM}$