

Electronic supplementary information to

**Modulating the Electronic Properties of Germanium Nanowires
via Applied Strain and Chemical Surface Passivation †**

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Table S1. Band gap of mono-substituted $\langle 110 \rangle$ F-GeNW with six different positions

$\langle 110 \rangle$ F-GeNW 1	E_{gap} (eV)
P1 ^a	1.39
P2 ^a	1.61
P3 ^a	1.39
P4 ^a	1.39
P5 ^a	1.40
P6 ^a	1.56

^a See Figure S1 for definition.

Table S2. Calculated band (E_{gap}) of 50.0% F- and Cl-GeNW **1** and **2** with applied strains

Applied	E_{gap} (eV)	
strain (%)	$\langle 100 \rangle$ 50% F-GeNW 1	$\langle 110 \rangle$ 50% F-GeNW 1
-10.0	2.29 <i>d</i>	0.51 <i>d</i>
0.0	2.23 <i>d</i>	0.83 <i>d</i>
10.0	2.08 <i>d</i>	0.42 <i>d</i>
	$\langle 100 \rangle$ 50% Cl-GeNW 1	$\langle 110 \rangle$ 50% Cl-GeNW 1
-10.0	1.75 <i>d</i>	0.58 <i>i</i>
0.0	1.75 <i>d</i>	0.82 <i>d</i>
10.0	1.39 <i>i</i>	0.41 <i>d</i>
	$\langle 100 \rangle$ 50% F-GeNW 2	$\langle 110 \rangle$ 50% F-GeNW 2
-10.0	1.49 <i>d</i>	0.25 <i>d</i>
0.0	1.61 <i>d</i>	0.60 <i>d</i>
10.0	1.20 <i>d</i>	0.18 <i>i</i>
	$\langle 100 \rangle$ 50% Cl-GeNW 2	$\langle 110 \rangle$ 50% Cl-GeNW 2
-10.0	1.12 <i>d</i>	0.18 <i>d</i>
0.0	1.37 <i>d</i>	0.56 <i>d</i>
10.0	0.92 <i>d</i>	0.17 <i>i</i>

Table S3. The calculated formation energy (E_{form}) of $\langle 100 \rangle$ and $\langle 110 \rangle$ F- and Cl-GeNW **2**.

$\langle 100 \rangle$ GeNW		$\langle 110 \rangle$ GeNW	
Surface coverage	E_{form} (eV per Ge atom)	Surface coverage	E_{form} (eV per Ge atom)
100.0% H	0.19	100.0% H	0.16
25.0% F	-0.38	22.2% F	-0.09
50.0% F	-0.93	50.0% F	-0.67
75.0% F	-1.46	72.2% F	-1.06
100.0% F	-2.00	100.0% F	-1.39
25.0% Cl	-0.08	22.2% Cl	-0.02
50.0% Cl	-0.32	50.0% Cl	-0.24
75.0% Cl	-0.54	72.2% Cl	-0.40
100.0% Cl	-0.74	100.0% Cl	-0.52

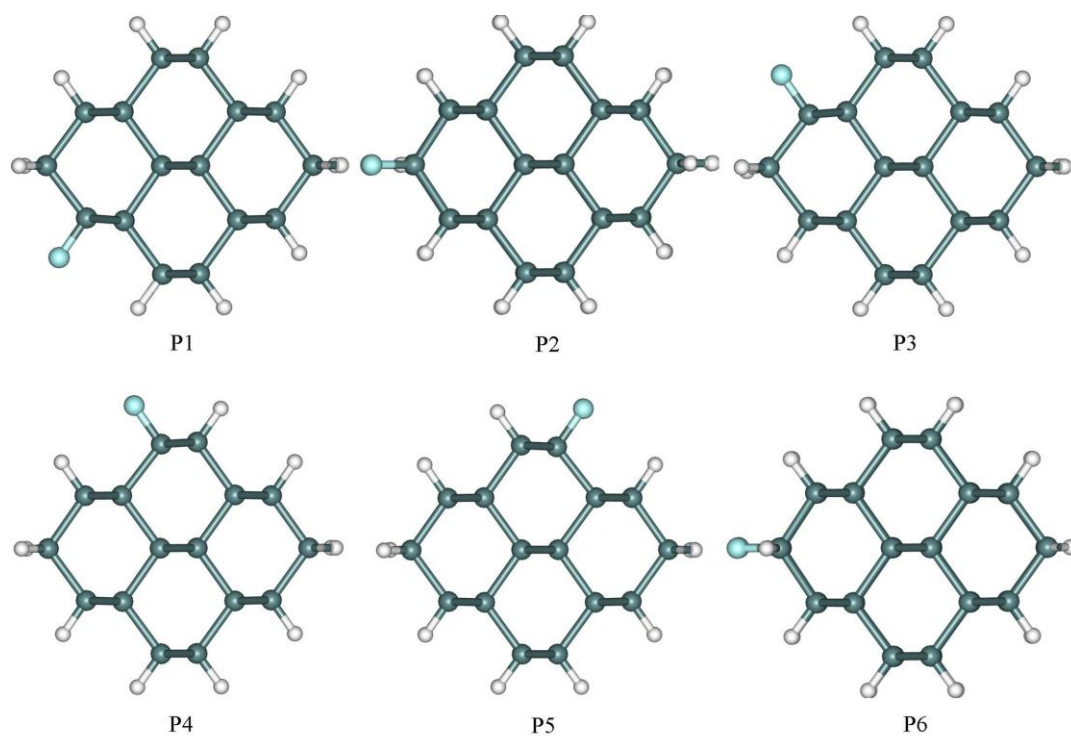


Figure S1. The optimized structures of mono-substituted $\langle 110 \rangle$ F-GeNW **1** with six different positions. Dark green, light blue and white spheres are Ge, F and H atoms, respectively.

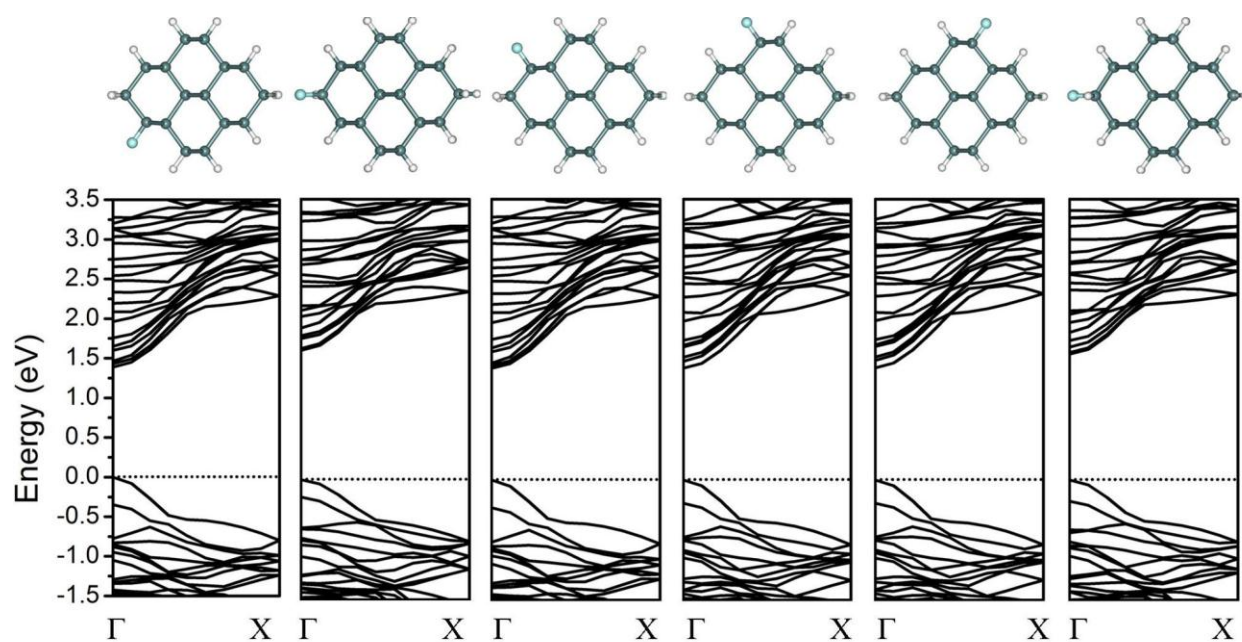


Figure S2. The band structures of mono-substituted $\langle 110 \rangle$ F-GeNW **1** with six different positions. The energy zero is taken arbitrarily to be the VBM.

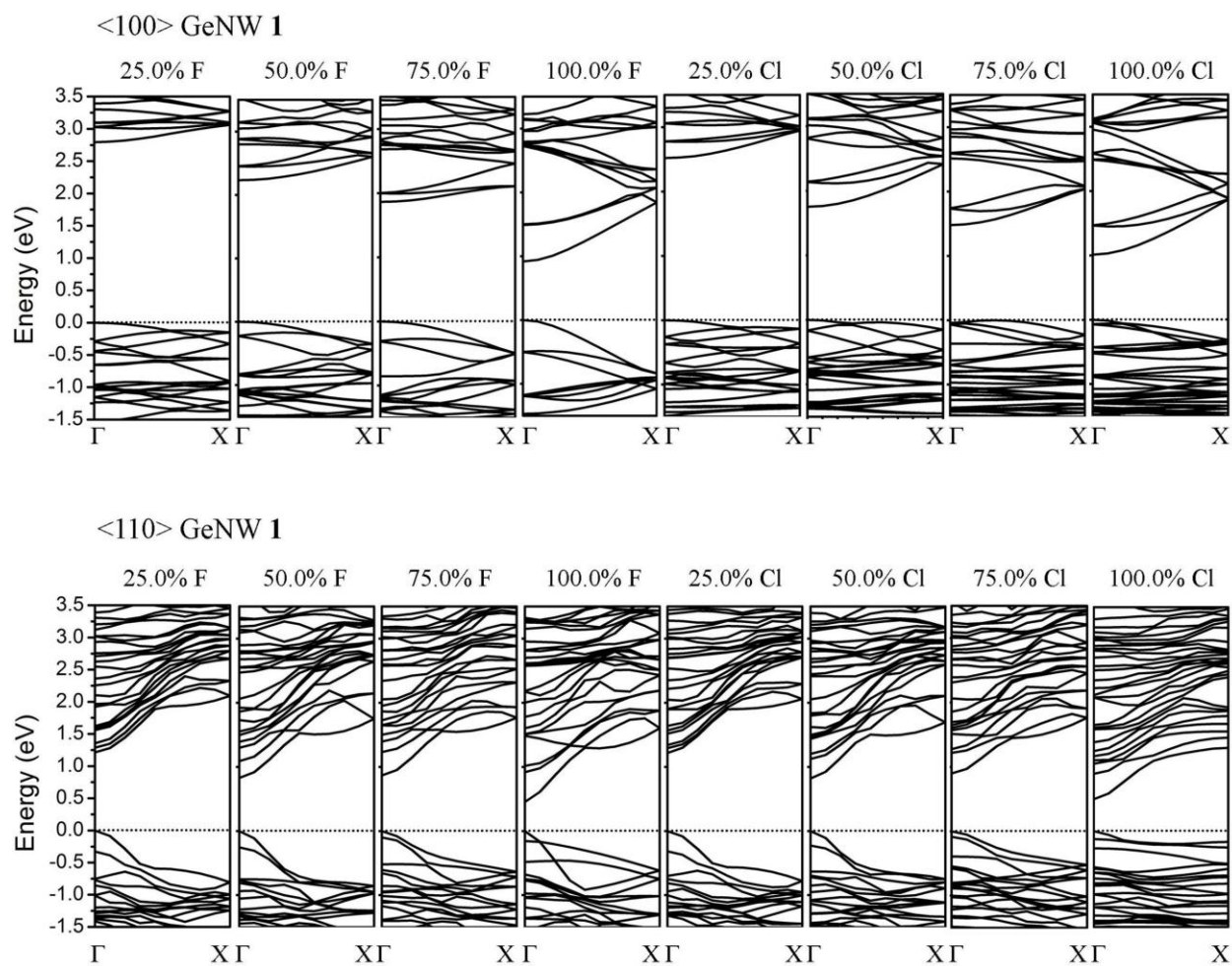
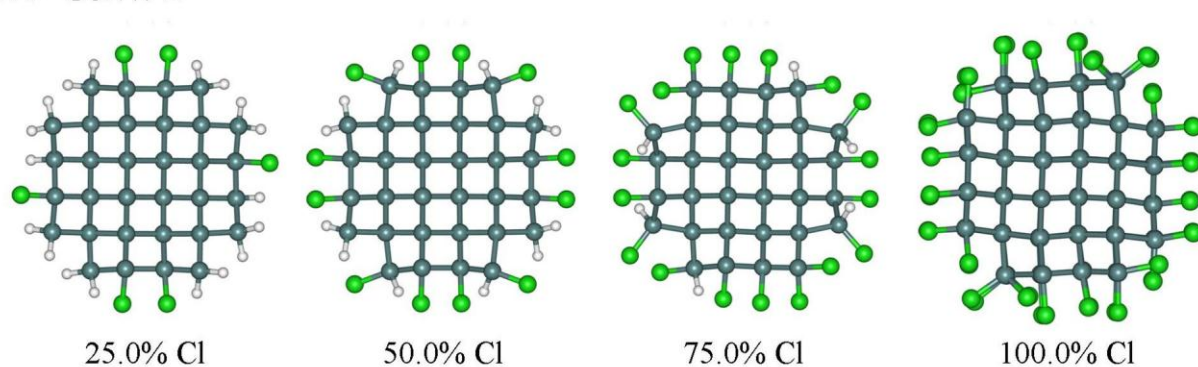


Figure S3. The band structures of $\langle 100 \rangle$ and $\langle 110 \rangle$ F- and Cl-GeNWs **1** with different surface coverage. The energy zero is taken arbitrarily to be the VBM.

<100> GeNW 2



<110> GeNW 2

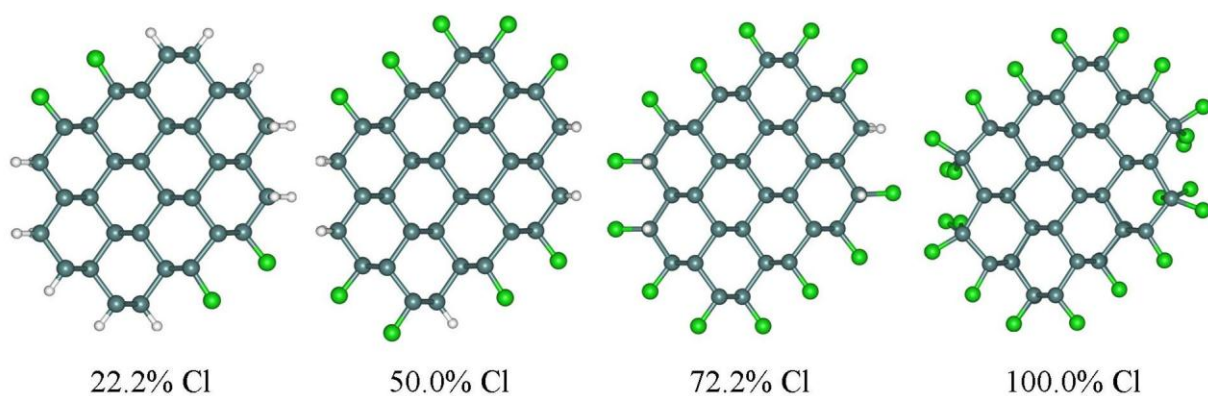


Figure S4. The optimized structures of $\langle 100 \rangle$ and $\langle 110 \rangle$ Cl-GeNWs **2** with different surface coverage of Cl. Dark green, green and white spheres are Ge, Cl and H atoms, respectively.