Electronic supplementary information (ESI) available:

Water induced electrical hysteresis in germanium nanowire: a theoretical study

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Table S1 The optimized average bond lengths[a] (R) of ⟨100⟩ OH-GeNWs with different OH coverage percentage on the NW surface.

P_{SC}[b]	R_{Ge-Ge} (Surface)	R_{Ge-Ge} (Core)	R_{Ge-H}	R_{Ge-O}	R_{O-H}
0.00	2.47	2.49	1.57-1.58		
4.17	2.46-2.49	2.49-2.51	1.57-1.58	1.87-1.88	0.94
8.33	2.46-2.48	2.49-2.50	1.57-1.58	1.87	0.95
16.67	2.46-2.49	2.49-2.50	1.57-1.58	1.86-1.88	0.94
33.33	2.47	2.49	1.57	1.86	0.95
66.67	2.51-2.52	2.55	1.58	1.86	0.95
83.33	2.49-2.58	2.50-2.55	1.58	1.82-1.88	0.95-0.96
100.00	2.46	2.52		1.83-1.89	0.95-0.96

[a] The R values at Å, [b] P_{SC} is the surface OH coverage percentage.

Table S2 The optimized average bond length (R^a) of $\langle 110 \rangle$ OH-GeNWs with different OH coverage percentage on the NW surface.

$P_{SC}{}^b$	R_{Ge-Ge} (Surface)	R_{Ge-Ge} (Core)	R_{Ge-H}	R_{Ge-O}	R_{O-H}
0.00	2.47-2.50	2.50-2.52	1.58		
5.67	2.47-2.50	2.50-2.51	1.57-1.58	1.86-1.87	0.94
11.11	2.47-2.51	2.50-2.52	1.57-1.58	1.86-1.87	0.94
22.22	2.46-2.53	2.50-2.54	1.57-1.58	1.86-1.90	0.94-0.95
33.33	2.46-2.52	2.49-2.53	1.57-1.58	1.85-1.88	0.94-0.95
66.67	2.44-2.57	2.49-2.54	1.57-1.59	1.85-1.90	0.94-0.95
77.78	2.44-2.57	2.49-2.54	1.57-1.59	1.84-1.89	0.94-0.95
100.00	2.50-2.63	2.50-2.52		1.83-1.92	0.94-0.97

[a] The R values at Å, [b] P_{SC} is the surface OH coverage percentage.

Table S3 Positional effect of OH group on the stability and band gap of $\langle 100 \rangle$ GeNW

Systems	RE (eV)	E_{gap} (eV)
GeNW-1	0.00	2.02 i
GeNW-2	0.06	1.98 d
GeNW-3	0.14	2.01 i

Table S4 Positional effect of OH group on the stability and band gap of $\langle 110 \rangle$ GeNW

Systems	RE (eV)	E_{gap} (eV)
GeNW-1	0.14	1.17 d
GeNW-2	0.14	1.16 d
GeNW-3	0.02	1.11 d
GeNW-4	0.00	1.13 d
GeNW-5	0.03	1.13 d
GeNW-6	0.03	1.13 d
GeNW-7	0.02	1.13 d
GeNW-8	0.14	1.17 d
GeNW-9	0.13	1.16 d

Table S5 Results of regression analysis of E_{form} with OH coverage percentage

Systems	Equations	n	r^2	p
$\langle 100 \rangle$ OH-GeNW	$E_{form} = -0.024(\pm 0.000)\, P_{SC} + 0.203(\pm 0.025)$	8	0.998	<0.0001
$\langle 110 \rangle$ OH-GeNW	$E_{form} = -0.018(\pm 0.000)\, P_{SC} + 0.160\,(\pm 0.005)$	8	0.999	<0.0001

Table S6 Effective mass of electrons in $\langle 100 \rangle$ and $\langle 110 \rangle$ OH-GeNWs

$\langle 100 \rangle$ OH-GeNW		$\langle 110 \rangle$ OH-GeNW	
$P_{SC}{}^a$	m^*_e	$P_{SC}{}^a$	m^*_e
0.00	1.560	0.00	0.193
4.17	4.590	5.67	0.198
8.33	2.910	11.11	0.199
16.67	1.260	22.22	0.204
33.33	0.940	33.33	0.233
66.67	0.823	66.67	0.228
83.33	0.821	77.78	0.292
100.00	0.794	100.00	0.294

[a] P_{SC} is the surface OH coverage percentage.
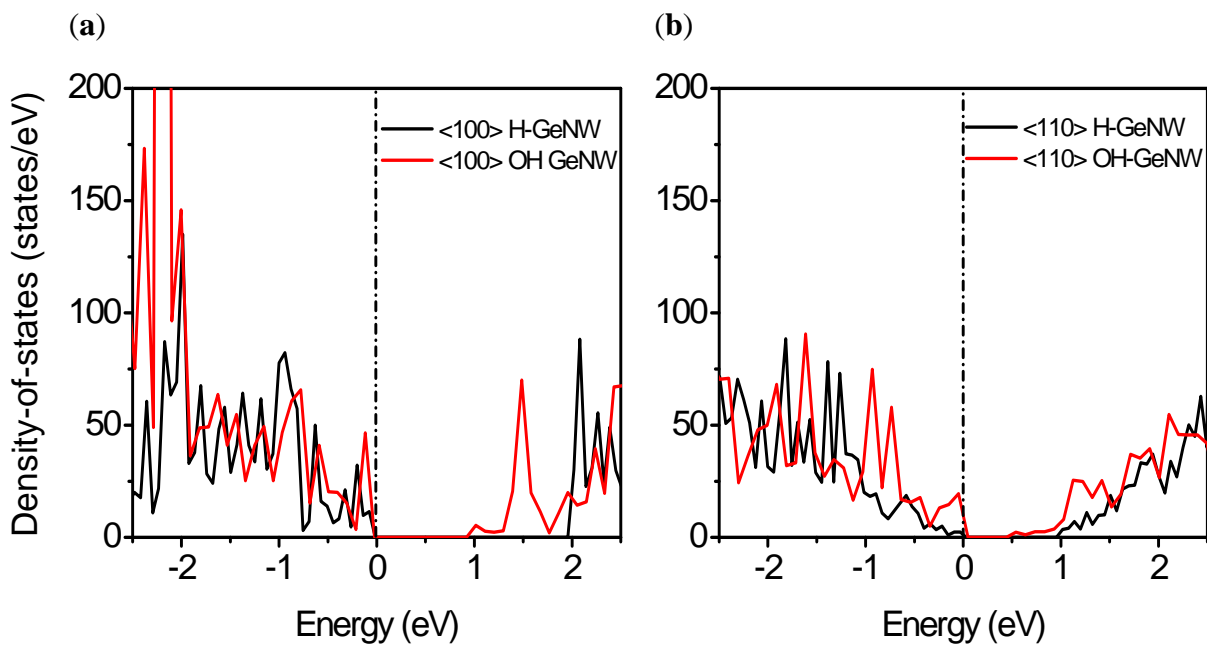
Fig. S1 Density of state (DOS) of (a) ⟨100⟩ GeNW and OH-GeNW and (b) ⟨110⟩ GeNW and OH-GeNW, red line is for 100.0% OH-GeNW, black is for GeNW, dash-dot line is the Fermi level. The Fermi level is set to zero.