

Supporting Information

Catching the electron in action in real space inside a Ge-Si core-shell nanowire transistor

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Figure S3. Gate bias dependent transmission at a fixed source-drain bias of $V_{ds} \sim (0.27 \text{ V})$ in Ge-Si core-shell nanowire FETs; channel length ~ 2 nm. (a) Ge-core diameter is 11.7 Å, (b) Ge-core diameter is 4.7 Å; dotted lines represent the chemical potential window.

Table S1. Optimized atomic coordinates in the unit cell of Ge-Si core-shell nanowire; Ge-core diameter is 4.7 Å; lattice parameter is 3.91 Å.

Serial Number	Atom	x-axis	y-axis	z-axis
1	Ge	13.40939	13.19978	0.343533
2	Ge	15.41443	14.6291	0.344314
3	Ge	17.42524	13.20633	0.343256
4	Ge	17.42851	11.73809	2.297581
5	Ge	15.42357	10.30864	2.297846
6	Ge	13.41284	11.7314	2.298
7	Si	13.45014	7.605664	0.342602
8	Si	15.42644	8.906776	0.342842
9	Si	17.40756	7.612876	0.340909
10	Si	21.27749	11.79481	2.295661
11	Si	21.27478	13.16284	0.34135
12	Si	17.38901	17.33058	2.300016
13	Si	15.41155	16.03094	2.299463
14	Si	13.43066	17.32602	2.301072
15	Si	9.560493	13.14257	0.342611
16	Si	9.563571	11.77403	2.297065
17	Si	5.716806	13.11722	0.339229
18	Si	25.11934	13.15295	0.337419
19	Si	25.12154	11.81878	2.292
20	Si	5.720001	11.78279	2.294034
21	Si	23.17207	9.079847	0.335673
22	Si	7.679529	9.0507	0.337488
23	Si	19.39577	10.35182	2.295081
24	Si	23.21028	10.42775	2.291092
25	Si	11.45071	10.33749	2.296799
26	Si	7.636336	10.39883	2.292792
27	Si	7.665144	15.85873	2.299941
28	Si	23.16017	15.88468	2.299247
29	Si	19.388	14.59959	0.343571
30	Si	23.20304	14.53642	0.343327
31	Si	11.442	14.58687	0.34468
32	Si	7.62732	14.50992	0.34422
33	Si	11.4878	15.94099	2.30028
34	Si	9.550457	17.29796	2.305634
35	Si	19.3367	15.95312	2.299244
36	Si	21.26991	17.31555	2.304434
37	Si	19.35028	8.998013	0.339489
38	Si	21.28725	7.641165	0.332927
39	Si	11.50221	8.983601	0.341376

40	Si	9.570169	7.619544	0.33591
41	Si	21.2358	18.6568	0.35107
42	Si	17.3791	18.68575	0.344556
43	Si	13.43705	18.68161	0.345457
44	Si	9.581287	18.64018	0.352026
45	Si	21.25736	6.299181	2.286691
46	Si	17.40166	6.257301	2.296813
47	Si	13.46091	6.250301	2.298395
48	Si	9.605137	6.277435	2.289822
49	Si	19.3463	4.89959	2.309652
50	Si	15.43392	4.919628	2.336795
51	Si	11.52147	4.885299	2.313056
52	Si	19.3203	20.04873	0.332036
53	Si	15.40683	20.01725	0.307924
54	Si	11.49265	20.03994	0.331909
55	Si	19.2952	21.38916	2.285868
56	Si	15.40588	21.37308	2.25839
57	Si	11.51584	21.38099	2.285405
58	Si	19.32519	3.558583	0.356326
59	Si	15.43711	3.564036	0.386968
60	Si	11.54882	3.544487	0.359638
61	Si	17.34342	22.6691	2.611173
62	Si	13.46682	22.66503	2.612065
63	Si	13.50182	2.26427	0.036755
64	Si	17.37635	2.271493	0.035766
65	H	4.483465	13.98582	0.338636
66	H	26.34777	14.02826	0.336219
67	H	26.35332	10.94826	2.293286
68	H	4.490911	10.90854	2.294685
69	H	24.41427	8.223427	0.337124
70	H	6.440373	8.190032	0.339011
71	H	6.422316	16.7147	2.300359
72	H	24.39907	16.74626	2.300504
73	H	22.45632	19.54382	0.350633
74	H	8.357311	19.52264	0.350502
75	H	22.48219	5.417975	2.288908
76	H	8.383883	5.391972	2.292173
77	H	20.51161	22.28047	2.301186
78	H	10.29834	22.27109	2.300461
79	H	20.54495	2.672271	0.342343
80	H	10.33331	2.652602	0.345849
81	H	17.31873	22.88799	0.190512
82	H	17.33588	24.0482	2.022505
83	H	13.49149	22.88427	0.191526
84	H	13.47568	24.04376	2.022829

85	H	13.52879	2.036616	2.459404
86	H	13.51125	0.8894	0.63372
87	H	17.34876	2.041989	2.458127
88	H	17.37282	0.896354	0.633548

Table S2. Optimized atomic coordinates in the unit cell of Ge-Si core-shell nanowire; Ge-core diameter is 11.7 Å; lattice parameter is 3.96 Å.

Serial Number	Atom	x-axis	y-axis	z-axis
1	Ge	13.41796	7.43168	3.265047
2	Ge	15.42623	8.874996	3.266321
3	Ge	17.43972	7.438885	3.263995
4	Ge	21.48012	11.7411	1.282765
5	Ge	21.47743	13.21566	3.263426
6	Ge	17.4222	17.5059	1.289895
7	Ge	15.41336	16.06344	1.288673
8	Ge	13.39951	17.499	1.289365
9	Ge	9.35808	13.1958	3.265823
10	Ge	9.361645	11.72068	1.285247
11	Ge	13.39783	13.19282	3.267877
12	Ge	15.41567	14.61379	3.268619
13	Ge	17.43804	13.19942	3.266333
14	Ge	17.44049	11.74614	1.285964
15	Ge	15.42319	10.32479	1.286333
16	Ge	13.40093	11.73932	1.287528
17	Ge	19.45496	10.32253	1.283503
18	Ge	11.39172	10.30851	1.285474
19	Ge	19.44816	14.62885	3.266896
20	Ge	11.38266	14.61584	3.268358
21	Ge	11.36116	16.07803	1.288823
22	Ge	19.46482	16.09093	1.287477
23	Ge	19.47707	8.86065	3.263145
24	Ge	11.37517	8.84622	3.265095
25	Si	5.60446	13.11989	3.26221
26	Si	25.23259	13.15342	3.258715
27	Si	25.23522	11.81526	1.277888
28	Si	5.607594	11.7814	1.281391
29	Si	23.36241	8.947122	3.255456
30	Si	7.489799	8.9189	3.258739
31	Si	23.41883	10.2902	1.276233
32	Si	7.428697	10.26204	1.279528
33	Si	7.475896	15.99072	1.2896
34	Si	23.35037	16.0157	1.286891
35	Si	23.41125	14.67275	3.265551
36	Si	7.41921	14.64702	3.268363
37	Si	9.367335	17.4519	1.29615
38	Si	21.45451	17.47072	1.294118
39	Si	21.47079	7.486862	3.253768
40	Si	9.386508	7.465036	3.256393
41	Si	21.33001	18.80349	3.275827

42	Si	17.38635	18.89856	3.269141
43	Si	13.43049	18.89176	3.268616
44	Si	9.487955	18.78548	3.277831
45	Si	21.35079	6.153448	1.272599
46	Si	17.40889	6.045923	1.284891
47	Si	13.4536	6.038655	1.285965
48	Si	9.511399	6.131873	1.275184
49	Si	19.40412	4.76385	1.29369
50	Si	15.43379	4.716309	1.327077
51	Si	11.4632	4.749073	1.295981
52	Si	19.37812	20.18595	3.257675
53	Si	15.40608	20.22117	3.229049
54	Si	11.43558	20.17421	3.259191
55	Si	19.33797	21.51572	1.276751
56	Si	15.40483	21.55816	1.243103
57	Si	11.47325	21.50447	1.278367
58	Si	19.36816	3.433633	3.274915
59	Si	15.43674	3.379242	3.313535
60	Si	11.50494	3.419135	3.277307
61	Si	17.37834	22.80732	1.592667
62	Si	13.42848	22.80286	1.593999
63	Si	13.4649	2.12696	2.965656
64	Si	17.41285	2.134083	2.964797
65	H	4.303361	13.88501	3.260802
66	H	26.52973	13.92502	3.257209
67	H	26.53488	11.04791	1.276663
68	H	4.310495	11.00968	1.280036
69	H	24.60484	8.089003	3.254612
70	H	6.250462	8.056266	3.257949
71	H	6.233953	16.8498	1.289127
72	H	24.59004	16.87788	1.286709
73	H	22.50201	19.75579	3.272856
74	H	8.312959	19.73421	3.275176
75	H	22.52646	5.205878	1.274374
76	H	8.339404	5.179732	1.276591
77	H	20.53552	22.43286	1.289447
78	H	10.27438	22.41976	1.289876
79	H	20.56784	2.519477	3.262566
80	H	10.30908	2.499517	3.264598
81	H	17.3626	23.04672	3.079274
82	H	17.41146	24.17567	0.979171
83	H	13.44387	23.04163	3.080615
84	H	13.38951	24.17102	0.981004
85	H	13.48113	1.883454	1.480264
86	H	13.43197	0.76136	3.584024

87	H	17.39523	1.889539	1.479473
88	H	17.45198	0.768292	3.583394

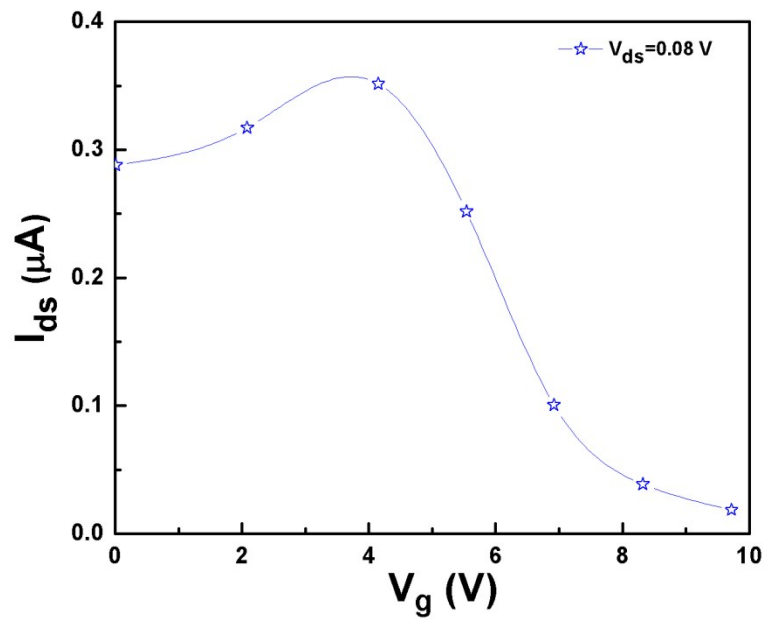


Figure S1. Drain Current vs. gate voltage plot at a fixed source-drain bias in a Ge-Si core-shell nanowire FET for longer channel length of ~ 2.4 nm; Ge-core diameter is 4.7 Å.

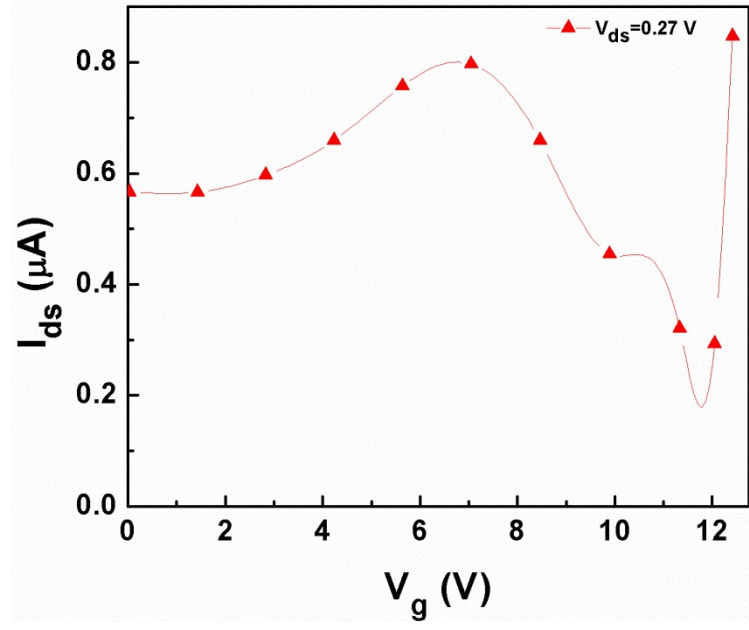


Figure S2. Drain current vs. gate voltage plot at a fixed source-drain bias in a Ge-Si core-shell nanowire FET; Ge-core diameter is 11.7 Å; channel length $\sim$ 2 nm.

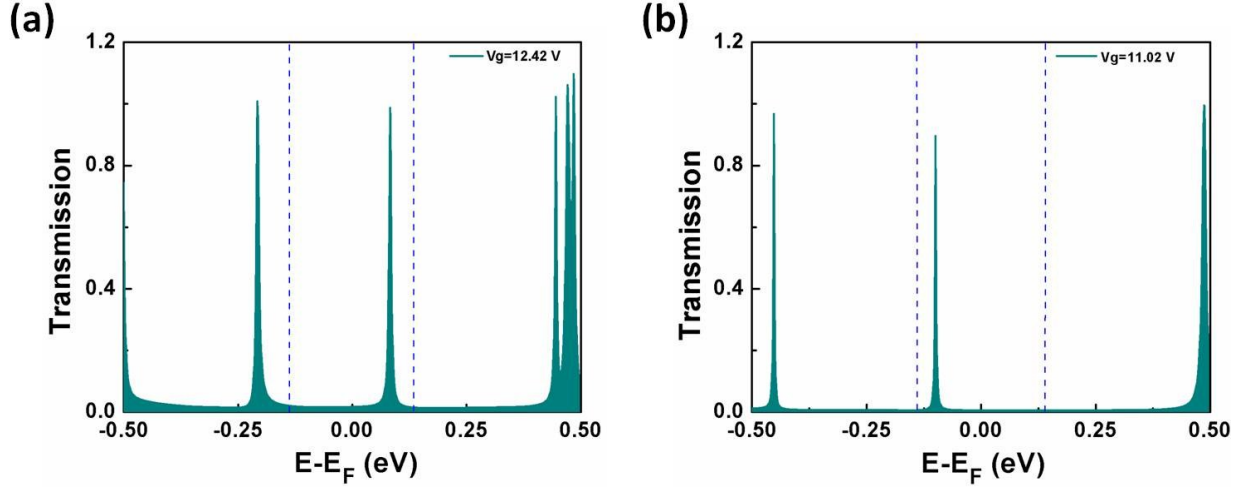


Figure S3. Gate bias dependent transmission at a fixed source-drain bias of $V_{ds} \sim 0.27$ V in Ge-Si core-shell nanowire FETs; channel length ~ 2 nm. (a) Ge-core diameter is 11.7 Å, (b) Ge-core diameter is 4.7 Å; dotted lines represent the chemical potential window.