Supplementary Data

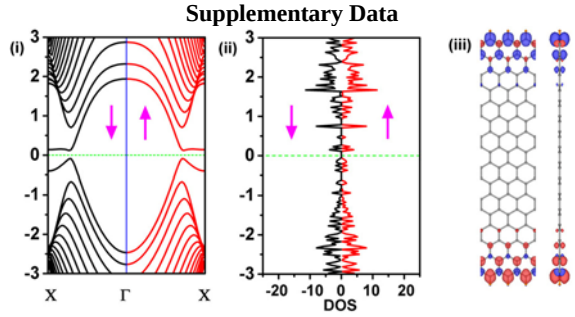

Fig. S 1 (i) Electronic spin-polarized band structures, (ii) projected density of states (DOS) and (iii) top- and side-view spin density plots of 16-ZGNR. The majority- (up-) spin bands are plotted at right parts with red color, while the minority- (down-) spin bands are plotted at left parts with black color. The up (or down) pink arrows denotes for up- (or down-) spin bands. Each band line is from Γ (0.0000, 0.0000, 0.0000) to X (0.5000, 0.0000, 0.0000). In projected DOS structures, the red (black) lines and blue (cyan) lines denote as the majority- (minority-) spin projected DOS of whole devices and oxygen atoms, respectively. The Fermi energy is set to zero. Isosurfaces of spin density (± 0.01 e /Å^3) are denoted by blue (positive) and red (negative) lobes.

Table S 1 Energy data of a set of n-ZGOs and n-ZGNR structures containing NM, FM and AFM states. Each total energy result is listed inside parentheses. The total energy differences of NM and AFM states are compared with corresponding FM ones. Each total magnetic moment is listed the value of corresponding favorable ground state.

Structure	NM (meV/unit cell)	FM (meV/unit cell)	AFM (meV/ unit cell)
8-ZGO-0	53.9 (-3378074.9)	0.0 (-3378128.8)	15.7 (-3378113.1)
12-ZGO-0	51.8 (-4620068.2)	0.0 (-4620120.0)	7.0 (-4620113.0)
16-ZGO-0	57.7 (-5862022.3)	0.0 (-5862080.0)	6.6 (-5862073.4)
16-ZGO-2	56.3 (-5862002.9)	0.0 (-5862059.2)	1.7 (-5862057.5)
20-ZGO-0	60.1 (-7103982.8)	0.0 (-7104042.9)	5.9 (-7104037.0)
12-ZGNR	47.4 (-3755969.3)	0.0 (-3756016.7)	-3.2 (-3756019.9)
16-ZGNR	52.2 (-4997919.4)	0.0 (-4997971.6)	-4.0 (-4997975.6)

Optimized Atomic Coordinates (unit: Angstrom)

Coordinates for 16-ZGO-0 per unit cell

C	1	-0.00000036	9.84894580	5.00000119
C	2	-0.00000011	14.10671419	4.99999906
C	3	-0.00000026	18.35610828	5.00000041
C	4	-0.00000570	22.58248991	4.99999726
C	5	0.00000069	27.59604006	5.00000047
C	6	-0.00000020	31.84965757	4.99999945
C	7	0.00000015	36.10549486	4.99999994
C	8	0.00000025	40.37959514	4.99999919
C	9	-0.00000017	8.41277871	5.00000141
C	10	-0.00000013	12.68679024	4.99999853
C	11	-0.00000011	16.94264793	5.00000087
C	12	-0.00000157	21.19664007	4.99999778
C	13	-0.00000178	26.21034544	5.00000210
C	14	0.00000038	30.43625093	5.00000177
C	15	-0.00000018	34.68556154	5.00000103
C	16	0.00000043	38.94338622	4.99999863
C	17	1.22999988	7.73015894	4.99999859
C	18	1.22999990	11.97851962	4.99999980
C	19	1.23000007	16.23275396	5.00000042
C	20	1.22999876	20.47505250	5.00000127
C	21	1.22999717	25.41123972	5.00000063
C	22	1.23000064	29.72372957	5.00000061
C	23	1.22999978	33.97660750	5.00000028
C	24	1.23000052	38.23758384	5.00000099
H	25	1.23000011	42.16823906	4.99999928
H	26	1.22999997	6.62413720	4.99999892
C	27	1.22999962	10.55476000	4.99999897
C	28	1.22999987	14.81565657	5.00000149
C	29	1.22999965	19.06871163	5.00000268
C	30	1.22998259	23.38161821	4.99999969
C	31	1.23000113	28.31747594	4.99999823
C	32	1.22999984	32.55951345	5.00000086
C	33	1.23000024	36.81376358	5.00000188
C	34	1.23000028	41.06221765	4.99999811
O	35	1.22998787	24.39665813	6.04026312
O	36	1.22998779	24.39665815	3.95973701

Coordinates for 16-ZGO-2 per unit cell

C	1	1.23000039	8.35604679	5.00000044
C	2	0.00000048	10.47617407	4.99999996
H	3	1.22999994	7.24976548	5.00000033
C	4	0.00000034	9.03912020	4.99999797
C	5	1.23000062	11.18275504	5.00000175
C	6	0.00000026	13.31727418	4.99999719
C	7	1.23000034	12.60819534	5.00000004
C	8	-0.00000070	14.73960350	4.99999720
C	9	1.22999960	16.86928537	5.00000129
C	10	-0.00000005	18.99681931	5.00000180
C	11	1.22999334	21.12194629	4.99999929
C	12	-0.00000114	23.24498648	4.99999673
C	13	1.22999911	15.44897711	4.99999961
C	14	-0.00000100	17.57811648	5.00000318
C	15	1.22999520	19.70489765	5.00000221
C	16	-0.00001569	21.82956920	4.99999625
C	17	1.22999494	23.95266163	5.00000048
C	18	-0.00000127	26.07512591	5.00000120
C	19	1.22999969	25.36651987	5.00000251
C	20	-0.00000083	27.48648652	5.00000105
C	21	1.22999701	29.60344954	4.99999758
C	22	-0.00000907	31.70992476	5.00000269
C	23	1.22998674	34.53908412	5.00000630
C	24	-0.00000515	36.72642255	5.00000120
C	25	1.22999842	28.19822656	4.99999843
C	26	-0.00000395	30.32459464	4.99999843
C	27	1.22998826	32.50869163	5.00000595
C	28	-0.00001147	35.33828508	5.00000532
C	29	1.22999525	37.44738409	4.99999686
C	30	-0.00000086	39.56980268	4.99999836
C	31	1.22999870	38.86005914	4.99999574
C	32	0.00000028	41.00218072	5.00000164
H	33	1.23000027	42.79247921	5.00000232
C	34	1.23000038	41.68644052	5.00000387
O	35	1.22997672	33.52393647	6.04075955
O	36	1.22998264	33.52393943	3.95925416