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Investigations of the band structures of edge-defect zigzag graphene nanoribbons using density functional theory

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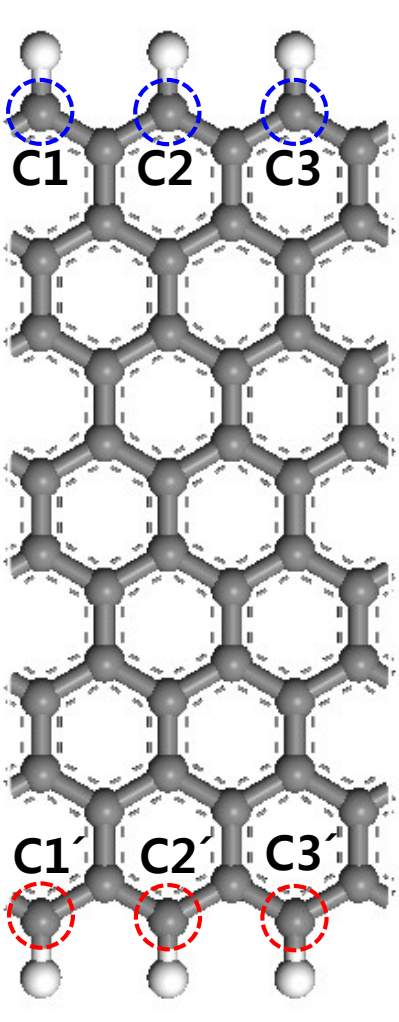

Fig. S1. Naming of edge carbon atoms for Tables S1 and S2.

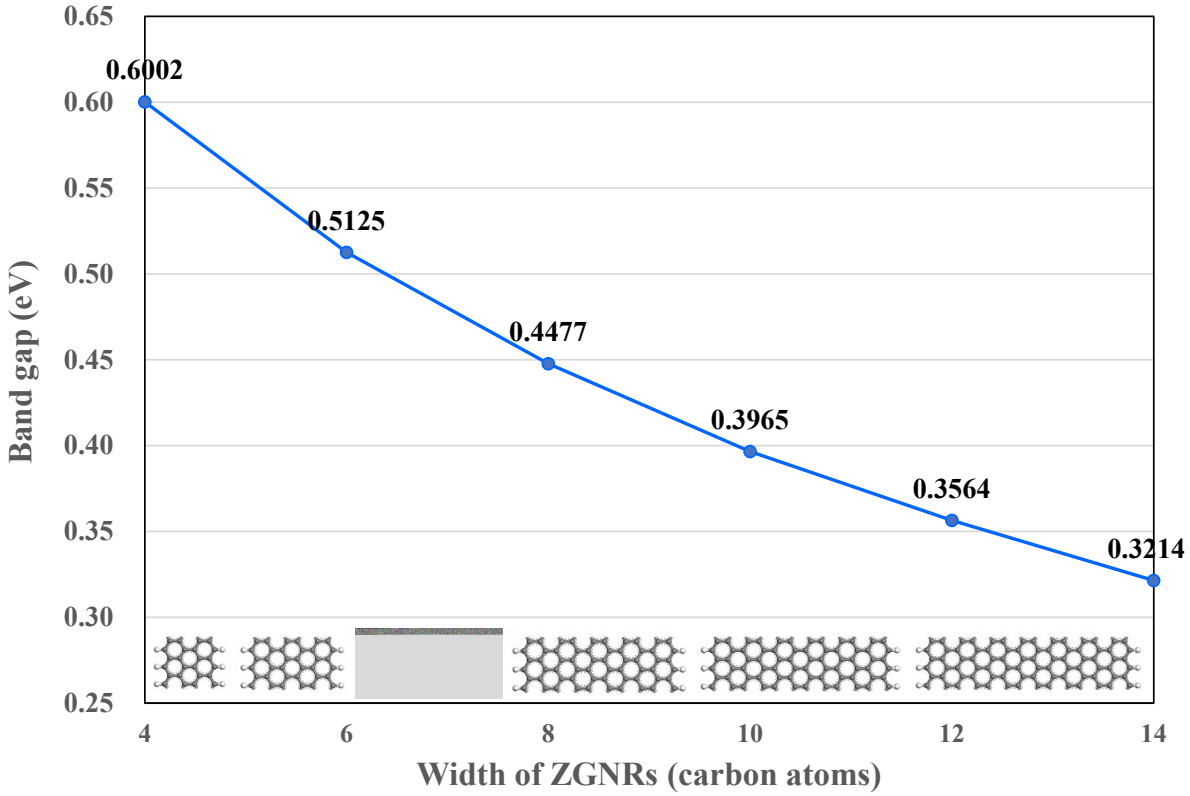

Fig. S2. Band gap magnitude as a function of ZGNR width. Wider ZGNRs were observed to yield narrower band gaps.

Table S1. The magnetizations of edge atoms of ZGNRs with oxygen-containing functional groups. C1, C2, C3 represent magnetizations at the edge containing the oxygen group. C1′, C2′, C3′ represent magnetizations of carbon atoms at the opposite edge. A star (*) indicates a carbon atom bonded to an oxygen group. In the case of the ether, C2 denotes an oxygen atom.

	Magnetization (μ_B) of edges carbon atoms						
Oxygen groups	C1	C2	C3	C1′	C2′	C3′	Total
Carboxyl	-0.139	-0.145*	-0.138	0.145	0.145	0.145	-0.010
Carboxyl (both edges)	-0.139	-0.145*	-0.139	0.139	0.145*	0.139	0.000
Hydroxyl	-0.131	-0.135*	-0.132	0.145	0.145	0.145	-0.015
Hydroxyl (both edges)	-0.131	-0.135*	-0.132	0.131	0.135*	0.132	0.000
Ketone	-0.001	0.000*	-0.001	0.150	0.154	0.150	0.511
Ketone (both edges)	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ether	-0.002	0.003	-0.002	0.150	0.154	0.150	0.513
Ether (both edges)	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Table S2. The magnetizations of edge atoms of ZGNRs with nitrogen-containing functional groups. C1, C2, C3 represent magnetizations of carbon atoms at the edge containing the nitrogen group. C1′, C2′, C3′ represent magnetizations of carbon atoms at the opposite edge. A star (*) indicates a carbon atom bonded to a nitrogen group. In the case of pyridinic and graphitic N-substitution, C3 denotes a nitrogen atom.

	Magnetization (μ_B) of edges carbon atoms						
Nitrogen groups	C1	C2	C3	C1′	C2′	C3′	Total
Pyridinic	-0.150	-0.150	-0.149	0.145	0.145	0.145	-0.026
Pyridinic (both edges)	-0.153	-0.153	-0.151	0.153	0.153	0.151	0.000
Pyrrolic	-0.112	-0.099*	-0.107	0.142	0.141	0.142	-0.016
Pyrrolic (both edges)	-0.114	-0.101*	-0.109	0.114	0.100	0.109	0.000
Graphitic	0.000	0.000	0.004	0.149	0.149	0.152	0.508
Graphitic (both edges)	0.000	0.000	0.000	0.000	0.000	0.000	0.000