Supplementary Information

Influence of ab initio derived site-dependent hopping parameters on electronic transport in graphene nanoribbons

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Table S1 The values of bond lengths (Å) and hopping parameters (eV) of N_A-AGNRs.
(a) 4-AGNR

	Zigzag bond		Parallel bond	
	Bond length	Hopping parameter	Bond length	Hopping parameter
1	1.42	-2.82	1.44	-2.75
2	1.42	-2.84	1.43	-2.87
3	1.43	-2.84	1.43	-2.83
4	1.43	-2.85	1.37	-2.91
5	1.42	-2,84		
6	1.42	-2.84		
7	1.42	-2.82		

(b) 8-AGNR

	Zigzag bond		Parallel bond	
	Bond length	Hopping parameter	Bond length	Hopping parameter
1	1.42	-2.84	1.44	-2.74
2	1.42	-2.87	1.42	-2.88
3	1.43	-2.84	1.43	-2.86
4	1.43	-2.87	1.43	-2.86
5	1.42	-2.88	1.43	-2.88
6	1.43	-2.86	1.43	-2.87
7	1.43	-2.87	1.43	-2.83

8	1.42	-2.88	1.37	-2.92
9	1.43	-2.87		
10	1.43	-2.86		
11	1.42	-2.88		
12	1.43	-2.87		
13	1.43	-2.84		
14	1.42	-2.87		
15	1.42	-2.87		

12-AGNR

	Zigzag bond			Zigzag bond			Parallel bond	
	Bond length	Hopping parameter		Bond length	Hopping parameter		Bond length	Hopping parameter
1	1.41	-2.83	13	1.43	-2.87	1	1.44	-2.74
2	1.42	-2.87	14	1.43	-2.87	2	1.42	-2.88
3	1.43	-2.84	15	1.43	-2.86	3	1.43	-2.86
4	1.42	-2.87	16	1.42	-2.87	4	1.43	-2.85
5	1.42	-2.88	17	1.42	-2.87	5	1.43	-2.86
6	1.43	-2.86	18	1.43	-2.86	6	1.43	-2.86
7	1.43	-2.87	19	1.42	-2.88	7	1.43	-2.85
8	1.42	-2.87	20	1.42	-2.87	8	1.43	-2.86
9	1.43	-2.86	21	1.43	-2.84	9	1.43	-2.87
10	1.43	-2.87	22	1.42	-2.87	10	1.43	-2.84
11	1.43	-2.87	23	1.41	-2.83	11	1.43	-2.84
12	1.43	-2.86				12	1.37	-2.90

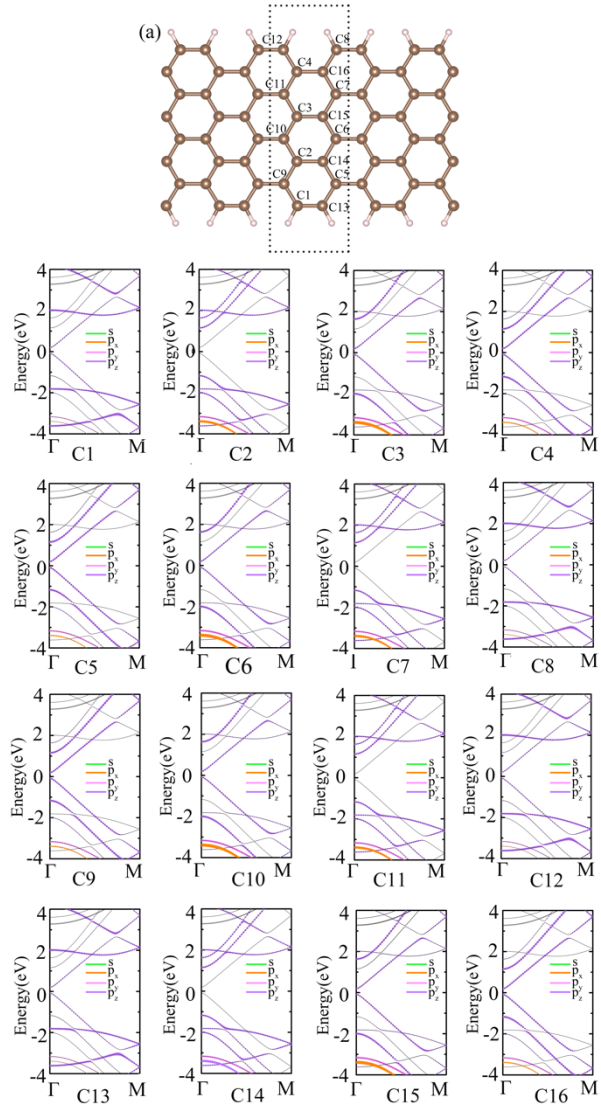
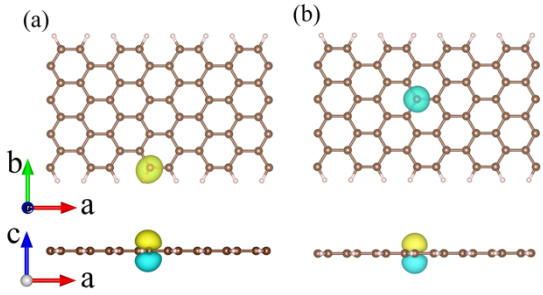


Fig. S1 The structures and fat bands of 4-AGNR. The Fermi level is set to zero.

Fig. S2 (a-b) The isosurface contours of MLWF of C1 and C3 from top and side view, respectively. It can be seen very clearly that the MLWFs is localized on a carbon atom.



The isosurface contours show the characteristics of p_z orbital.

Table S2 The values of bond lengths (Å) and hopping parameters (eV) of N_Z-ZGNRs.

(a) 4-ZGNR

	Bond length	Hopping parameter		Bond length	Hopping parameter
1	1.41	-2.85	5	1.42	-2.86
2	1.45	-2.70	6	1.45	-2.70
3	1.42	-2.86	7	1.41	-2.87
4	1.44	-2.76			

(b) 8-ZGNR

	Bond length	Hopping parameter		Bond length	Hopping parameter
1	1.41	-2.81	9	1.42	-2.87
2	1.46	-2.77	10	1.43	-2.85
3	1.42	-2.87	11	1.42	-2.87
4	1.43	-2.84	12	1.43	-2.84
5	1.42	-2.87	13	1.42	-2.87
6	1.43	-2.85	14	1.45	-2.77
7	1.42	-2.87	15	1.41	-2.80
8	1.43	-2.85			

(c) 12-ZGNR

	Bond length	Hopping parameter		Bond length	Hopping parameter
1	1.41	-2.79	13	1.42	-2.86
2	1.45	-2.77	14	1.43	-2.86
3	1.42	-2.86	15	1.42	-2.86
4	1.43	-2.84	16	1.43	-2.86
5	1.42	-2.86	17	1.42	-2.86
6	1.43	-2.85	18	1.43	-2.85
7	1.42	-2.86	19	1.42	-2.86
8	1.43	-2.86	20	1.43	-2.84

9	1.43	-2.86	21	1.42	-2.86
10	1.43	-2.86	22	1.45	-2.77
11	1.42	-2.86	23	1.41	-2.78
12	1.43	-2.86			