

Supporting information for
Scaling of Excitons in Graphene Nanoribbons with Armchair Shaped Edges

Xi Zhu¹ and Haibin Su^{*, 1, 2, 3}

¹Division of Materials Science, Nanyang Technological University,

50 Nanyang Avenue, Singapore 639798, Singapore

²Institute of Advanced Studies, Nanyang Technological University, 60 Nanyang

View, Singapore 639673, Singapore

³Institute of High Performance Computing, 1 Fusionopolis Way, Connexis 138632,

Singapore

* Email: hbsu@ntu.edu.sg

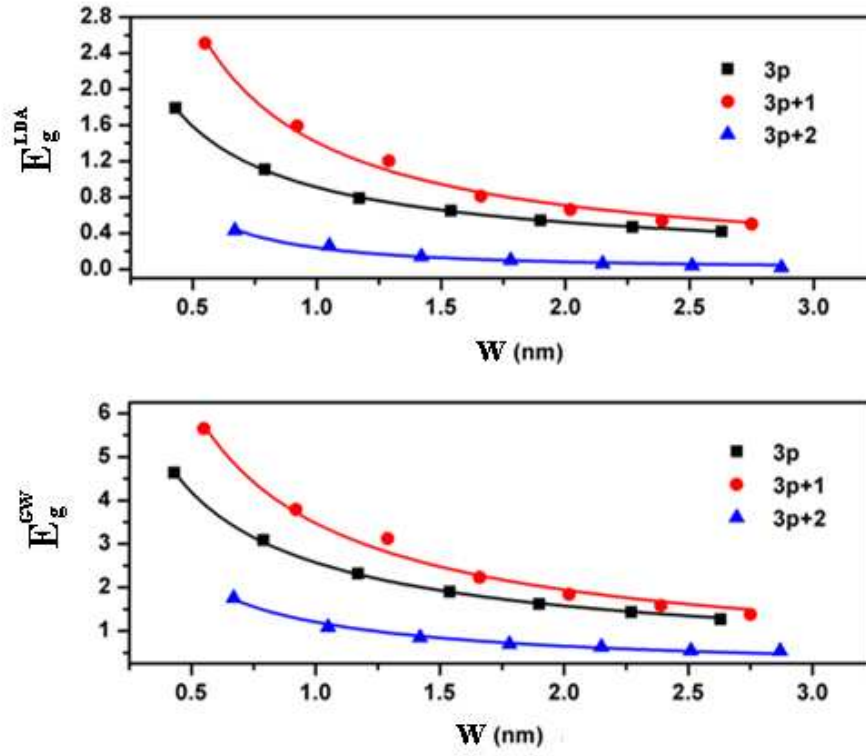


Figure S1. The scaling behavior of LDA and GW band gaps with the width of the AGNRs. The points are the raw data, and the lines are fitted to the formula: $E_g = A * W^\lambda$

	A_{LDA}	λ_{LDA}	A_{GW}	λ_{GW}
3p	0.91	-0.80	2.57	-0.70
3p+1	1.40	-0.99	3.48	-0.84
3p+2	0.23	-1.54	1.20	-0.88

Table SI. LDA band gap (E_g^{LDA}), GW band gap (E_g^{GW}) transition energy(E_t) and exciton binding energy (E_b) for all the AGNRs studied in this work into 3 families. The unit of energy is eV, the width of the 3p, 3p+1 and 3p+2 can refer to Table SII

3p	E_g^{LDA}	E_g^{GW}	E_t	3p+1	E_g^{LDA}	E_g^{GW}	E_t	E_b	3p+2	E_g^{LDA}	E_g^{GW}	E_t	E_b
W3	1.79	4.64	2.56	W4	2.51	5.65 (5.64) ¹	3.25	2.40	W5	0.43	1.76 (1.75)	0.63	1.13
W6	1.11	3.09 (2.90) ¹	1.53	W7	1.59	3.79 (3.80) ¹	2.03	1.76	W8	0.26	1.09 (1.19) ¹ (1.00) ²	0.29 (0.40) ²	0.80 (0.60) ²
W9	0.79	2.29 (2.16) ¹ (2.00) ² (2.27) ⁴	1.12 (1.12) ¹ (1.00) ² (0.99) ⁴			3.11 (3.01) ¹ (2.80) ² (3.00) ³	1.70 (1.51) ² (1.51) ³	1.42 (1.39) ² (1.40) ³	W11	0.20	0.85 (0.89) ¹	0.17	0.68 (0.70) ³
W12	0.65	1.90 (1.80) ¹ (1.80) ³	0.89 (1.10) ³	W13	0.89	2.25 (2.47) ¹	1.14	1.09	W14	0.16	0.71 (0.75) ¹	0.08	0.65
W15	0.54	1.62	0.74	W16	0.72	1.84	0.92	0.94	W17	0.12	0.63	0.04	0.59
W18	0.47	1.43	0.65	W19	0.54	1.58	0.78	0.80	W20	0.09	0.55	0.01	0.54
W21	0.44	1.27	0.55	W22	0.52	1.38	0.65	0.73	W23	0.02	0.54	0.01	0.53

Table SII. AGNRs width (w) and reduced mass of all the AGNRs in this work. The unit of w is angstrom, The definition of reduced mass is $m=m_e^*m_h/(m_e+m_h)$ in the unit of the mass of free electron (m_0 .)

3p	w	m	3p+1	w	m	3p+2	w	m
W3	4.3	1.16	W4	5.5	1.53	W5	6.7	0.27
W6	7.9	0.43	W7	9.2	0.68	W8	10.5	0.10
W9	11.7	0.24	W10	12.9	0.47	W11	14.2	0.05
W12	15.4	0.15	W13	16.6	0.28	W14	17.8	0.039
W15	19.0	0.10	W16	20.2	0.21	W17	21.5	0.034
W18	22.7	0.07	W19	23.9	0.17	W20	25.1	0.029
W21	26.3	0.06	W22	27.5	0.12	W23	28.7	0.026

- [1] Yang, L.; Park, C. H.; Son, Y. W.; Cohen, M. L.; Louie, S. G. *Phys. Rev. Lett.* **2007**, *99*, 186801
- [2] Prezzi, D.; Varsano, D.; Ruini, A.; Marini, A.; Molinari, E. *Phys. Rev. B* **2008**, *77*, 041404.
- [3] Yang, L.; Cohen, M. L.; Louie, S. G. *Nano Lett.* **2007**, *7*, 3112.
- [4] Zhu, X.; Su, H. B. *J. Phys. Chem. C* **2010**, *114*, 17257