Supplementary Information

Electronic and optical properties of surface hydrogenated armchair graphene nanoribbons: A theoretical study

Xi Zhu*[a] and Min Wang*[b]

[a] Division of Materials Science, School of Materials Science and Engineering,

Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798,

Singapore. E-mail: zhuxi@ntu.edu.sg

[b] Institute for Clean Energy & Advanced Materials, Faculty of Materials and Energy,

Southwest University, Chongqing 400715, China. Email: minwang@swu.edu.cn

Table of Contents

S1. Comparison between W8:H2:H6 and W8:H2:H6-2

Table S 1. LDA band gaps, GW band gaps, BSE energies and bindind energies (E_b) in W8:H2:H6 and W8:H2:H6-2 cases.

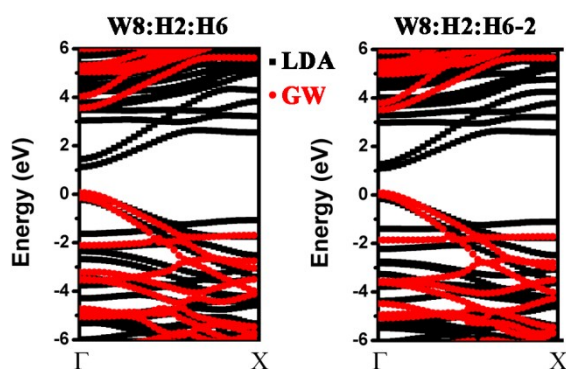|	LDA(eV)	GW(eV)	BSE(eV)	E_b(eV)
W8:H2:H6	1.12	3.49	1.74	1.75
W8:H2:H6-2	1.09	3.41	1.69	1.72

Fig. S1 LDA and GW band structures for W_8:H_2:H_6 and W_8:H_2:H_6-2 cases.
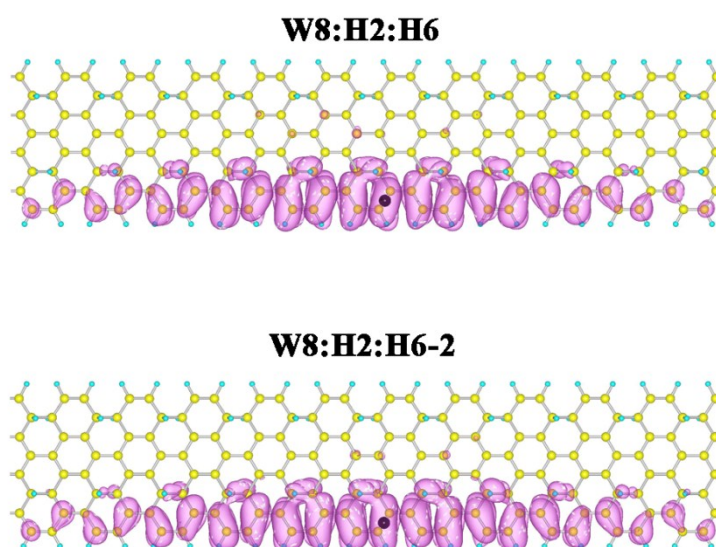

Fig. S2 Exciton wavecuntion plots for W8:H:2:H6 and W8:H:2:H6-2 cases.

S2. The effective width model in one-, two- and three-row H-AGNRs

The order of the band gaps in some pristine AGNRs is listed below:

$Gap_{W5} < Gap_{W6} < Gap_{W2} < Gap_{W3} < Gap_{W4} < Gap_{W1}$

2.1 One-row H-AGNRs

1. **For W8 serials:**

W8:H(n)	Segments	Effective width segment (EW-W(k))
W8:H2	W1,W6	EW-W6
W8:H4	W3,W4	EW-W3
W8:H6	W5,W2	EW-W5

The order of band gap is

$Gap_{W8} < Gap_{W8:H6} < Gap_{W8:H2} < Gap_{W8:H4}$

2. **For W9 serials:**

W9:H(n)	Segments	Effective width segment (EW-W(k))
W9:H3	W2,W6	EW-W6
W9:H5	W4,W4	EW-W4

The order of band gap is

$Gap_{W9} < Gap_{W9:H3} < Gap_{W9:H5}$

3. **For W10 serials:**

W10:H(n)	Segments	Effective width segment (EW-W(k))
W10:H2	W1,W8	EW-W8
W10:H4	W3,W6	EW-W6
W10:H6	W5,W4	EW-W5
W10:H8	W7,W2	EW-W2

The order of band gap is

$Gap_{W10:H2} < Gap_{W10:H6} < Gap_{W10:H4} < Gap_{W10:H8} < Gap_{W10}$,

2.2 Two-row H-AGNRs

1. For W8 seials:

W8:H(n):H(m)	Segments	Effective width segment (EW-W(k))
W8:H2:H4	W1,W1,W4	EW-W4
W8:H2:H6	W1,W2,W3	EW-W2
W8:H4:H6	W1,W2,W3	EW-W2

The order of band gap is

$Gap_{W8:H2:H6} \approx Gap_{W8:H4:H6} < Gap_{W8:H2:H4}$

2. For W9 serials:

(for symmetry, the structure of W9:H3:H5 is the same as W9:H5:H7)

W9:H(n):H(m)	Segments	Effective width segment (EW-W(k))
W9:H3:H5	W1,W2,W4	EW-W2
W9:H3:H7	W2,W2,W3	EW-W2

The order of band gap is

$Gap_{W9:H3:H7} \approx Gap_{W9:H3:H5}$

3. For W10 serials:

W9:H(n):H(m)	Segments	Effective width segment (EW-W(k))
W10:H2:H4	W1,W1,W6	EW-W6
W10:H2:H6	W1,W3,W4	EW-W3
W10:H2:H8	W1,W2,W5	EW-W5
W10:H4:H6	W1,W3,W4	EW-W3
W10:H4:H8	W2,W3,W3	EW-W2
W10:H6:H8	W1,W2,W5	EW-W5

The order of band gap is

$Gap_{W10:H6:H8} \approx Gap_{W10:H2:H8} < Gap_{W10:H2:H4} < Gap_{W10:H4:H8} < Gap_{W10:H2:H6} \approx Gap_{W10:H4:H6}$

2.3 Three-row H-AGNRs

There is only one case for the W8 and W9 serials when the adsorption row number is three.

For W10 serials

W10:H(n):H(m):H(l)	Segments	Effective width segment (EW-W(k))
W10:H2:H4:H6	W1,W1,W1,W4	EW-W4
W10:H2:H4:H8	W1,W1,W2,W3	EW-W2
W10:H2:H6:H8	W1,W1,W2,W3	EW-W2
W10:H4:H6:H8	W1,W1,W2,W3	EW-W2

The order of band gap is

$Gap_{W10:H2:H4:H8} \approx Gap_{W10:H2:H6:H8} \approx Gap_{W10:H4:H6:H8} < Gap_{W10:H2:H4:H6}$

S3. Electron wavefunction plot for all the cases

Fig. S3.VBM/CBM plot for the one-row H-AGNRs with an isovalue of 0.1 eV/Å³

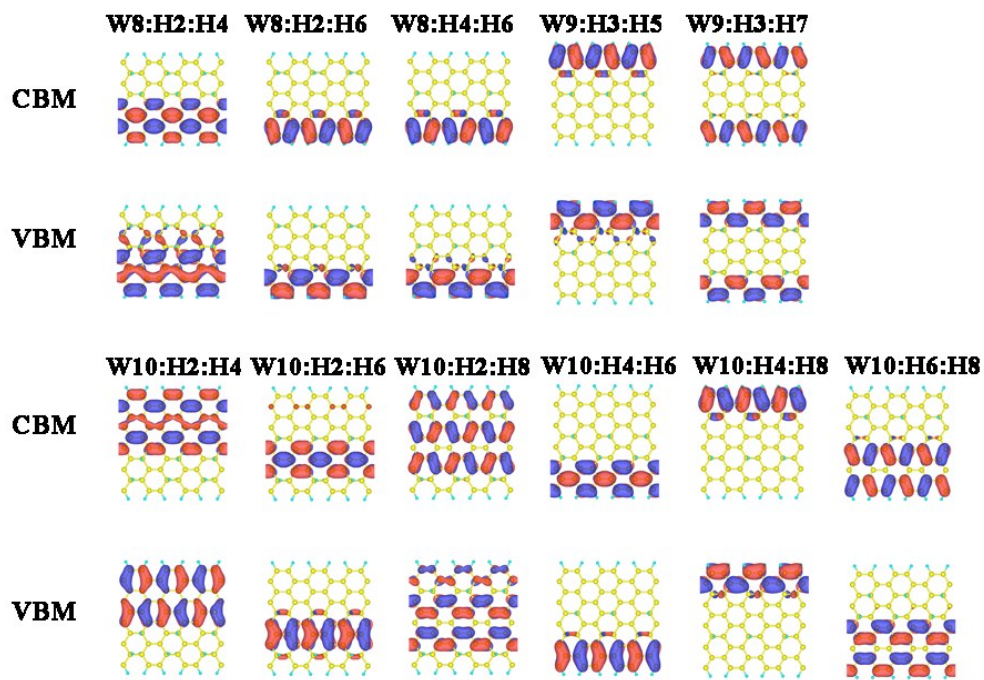Fig. S4.VBM/CBM plot for the two-row H-AGNRs with an isovalue of 0.1 eV/Å³

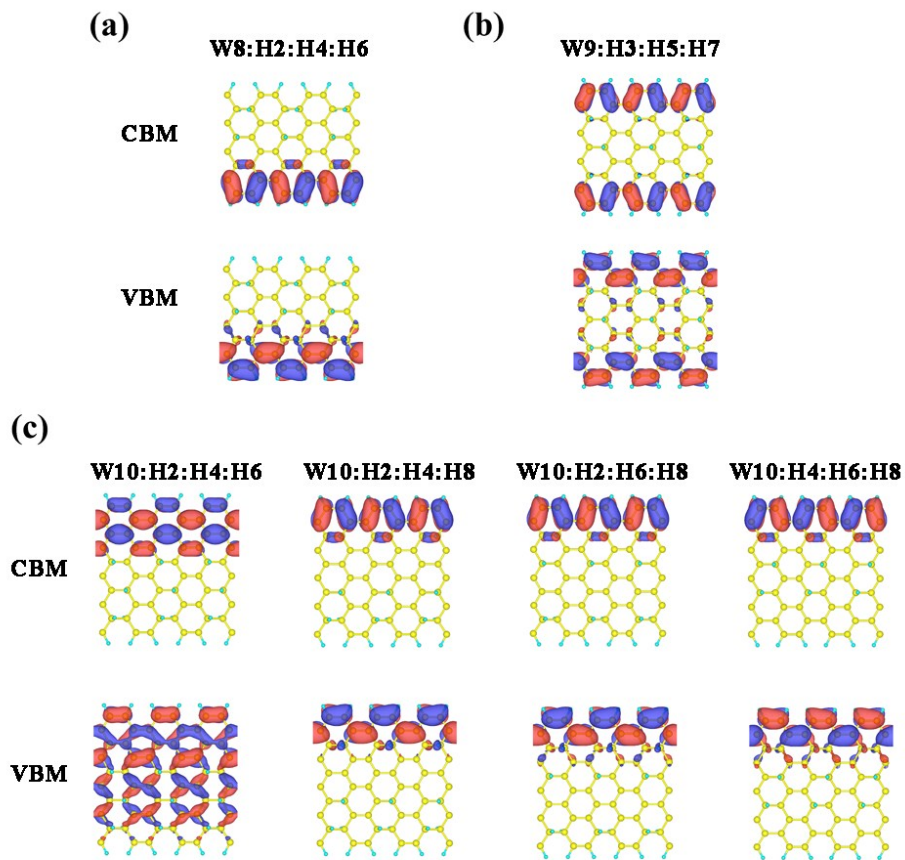Fig. S5.VBM/CBM plot for the three-row H-AGNRs with an isovalue of 0.1 eV/Å³
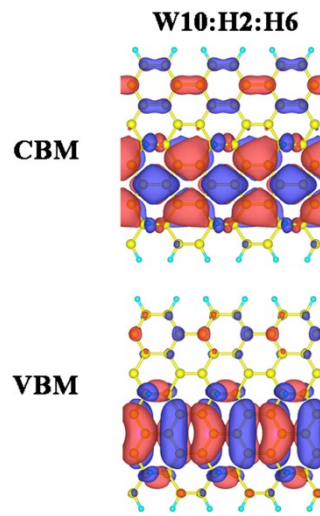
S4. Soft wall in the H-AGNRS

Fig. S6. VBM/CBM plot for W10:H2:H6 case with an isovalue of 0.05 eV/Å^3