Supplementary Material (ESI) for Nanoscale

Supplementary Information

Excitonic properties of hydrogen saturation-edged armchair graphene nanoribbons

Min Wang[1,2], *Chang Ming Li*[1,2*]

[1]School of Chemical and Biomedical Engineering, Nanyang Technological University, 70 Nanyang Drive, Singapore 637457

[2]Center for Advanced Bionanosystems, Nanyang Technological University, 70 Nanyang Drive, Singapore 637457

[*]Corresponding author. Tel: +65 67904485; Fax: +65 67911761. E-mail: ecmli@ntu.edu.sg.

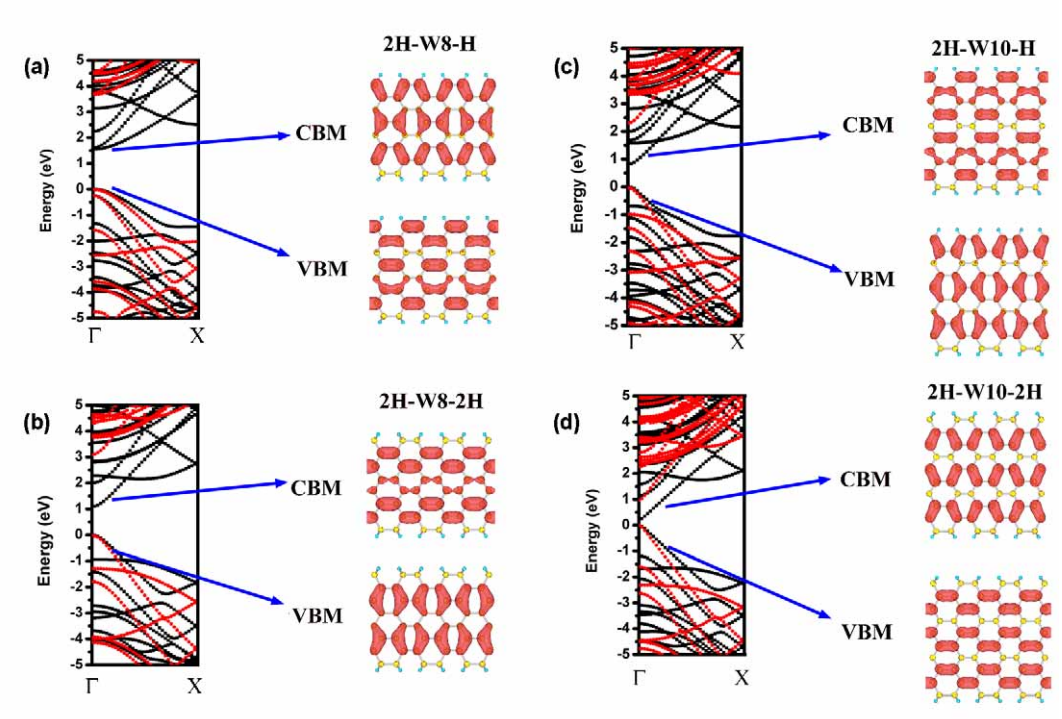

Fig. S1 Band structures and VBM/CBM plot for the (a) 2H-W8-H, (b) 2H-W8-H, (c) 2H-W10-H, and (d) 2H-2W-2H structures. The black and red lines representative the LDA and GW parts respectively, the Fermi lever is set to zero. The isosurfaces (0.002 e/Bohr^3) for the VBM and CBM are denoted as red lobes.

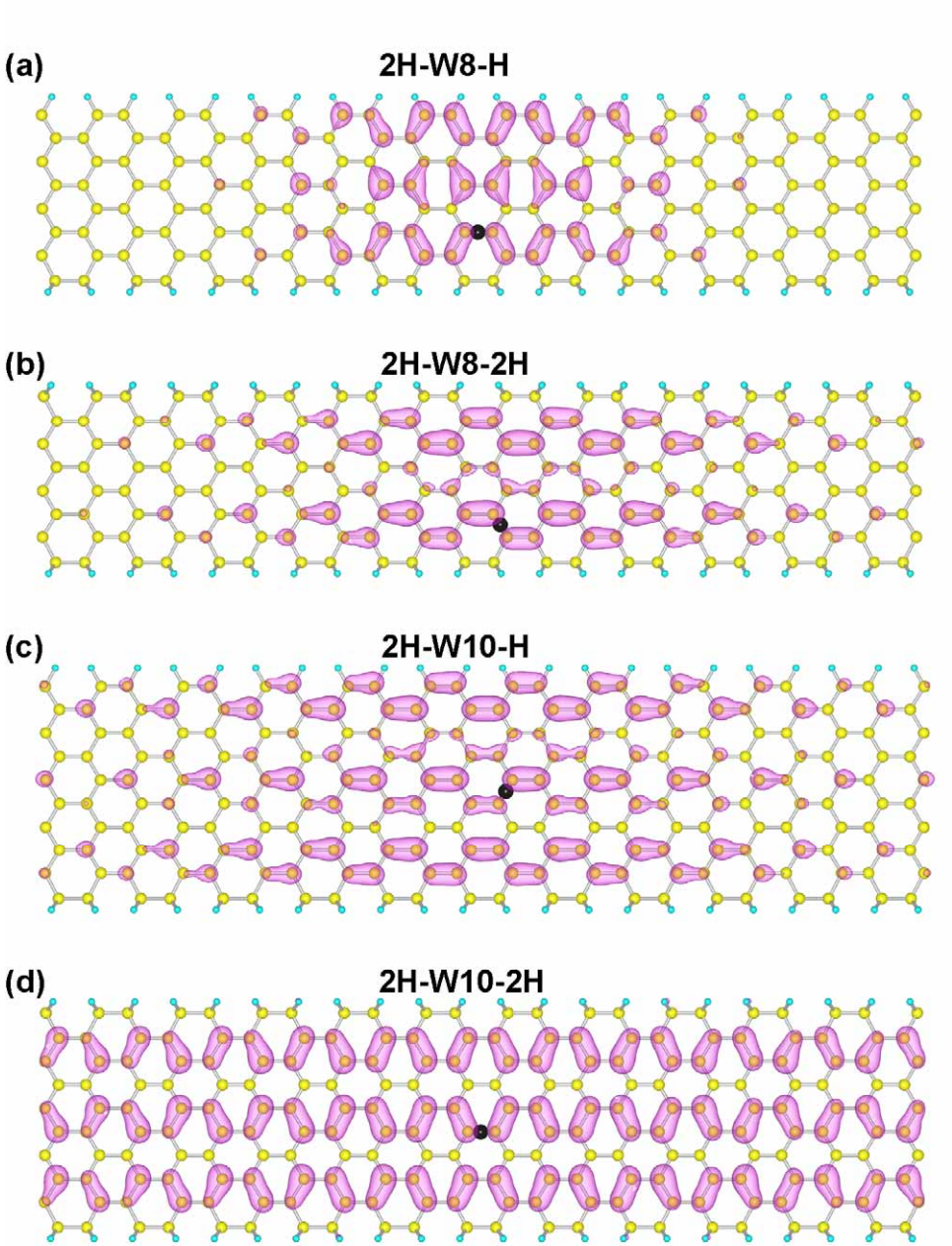

Fig. S2 Isosurfaces of exciton wavefunctions (0.01 e/Bohr^3) for (a) 2H-W8-H, (b) 2H-W8-H, (c) 2H-W10-H, and (d) 2H-2W-2H structures are denoted as pink lobes. The hole is fixed in the middle of one bone and marked as black spot.