Electronic Supplementary Information

Edge Hydrogenation-Induced Spin-Filtering and Negative Differential Resistance Effects in Zigzag Silicene Nanoribbons with Line Defects

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The edge energy is defined as $E_{edge} = (E_{total} - n_{Si}E_{Si} - n_{H}E_{H})/(2L_{edge})$, E_{total} is the total energy of each system, n_{Si} and n_{H} are the number of Si and H atoms in nanoribbons, and E_{Si} and E_{H} are the energies of Si and H atoms in the silicene sheet and H_2 molecule, respectively. L_{edge} is the length of edge and the coefficient 2 accounts for the two edges of nanoribbons.[1] For 558-defect and57-defect ZSiNRs, the edge energy decreases with increasing the number of H atoms. Their most stable edge types are M5 and M10 that the two edges are terminated by two H atoms.

Table S1 The edge energies of M2-M5 and M7-M10.

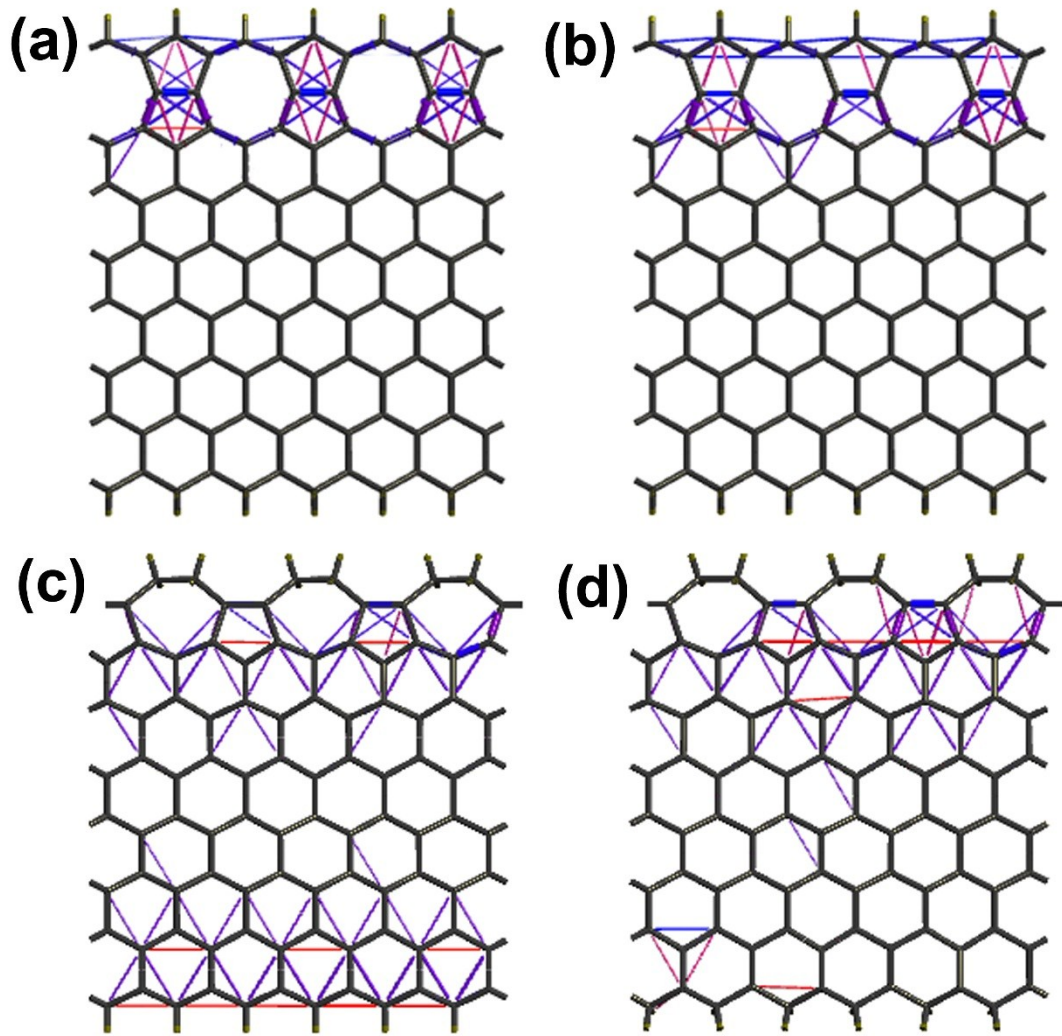|	M2	M3	M4	M5	M7	M8	M9	M10
E_{edge} (eV/A)	0.021	-0.091	-0.121	-0.232	0.050	-0.066	-0.098	-0.213

Fig. S1 Transmission pathways for (a) and (b) spin-up and spin-down of M3 at 0 eV energy with 0.2 V, (c) spin-up of M9 at 0 eV energy with 0.3 V, (d) spin-down of M10 at 0.1 eV energy with 0.3 V.

References

1.   Y. Ding and Y. Wang, *Applied Physics Letters*, 2014, **104**, 083111.