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 

\[ E_{\text{edge}} = \frac{(E_{\text{total}} - n_{\text{Si}}E_{\text{Si}} - n_{\text{H}}E_{\text{H}})}{(2L_{\text{edge}})} \]

\( E_{\text{total}} \) is the total energy of each system, \( n_{\text{Si}} \) and \( n_{\text{H}} \) are the number of Si and H atoms in nanoribbons, and \( E_{\text{Si}} \) and \( E_{\text{H}} \) are the energies of Si and H atoms in the silicene sheet and \( \text{H}_2 \) molecule, respectively. \( L_{\text{edge}} \) is the length of edge and the coefficient 2 accounts for the two edges of nanoribbons. For 558-defect and 57-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.

\textbf{Table S1} The edge energies of M2-M5 and M7-M10.

| Edge | M2  | M3  | M4  | M5  | M7  | M8  | M9  | M10 |
|------|-----|-----|-----|-----|-----|-----|-----|-----|
| E_{\text{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.