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SUPPLEMENTARY INFORMATION

Spin-Polarized Quantum Transport in Si Dangling Bond Wires

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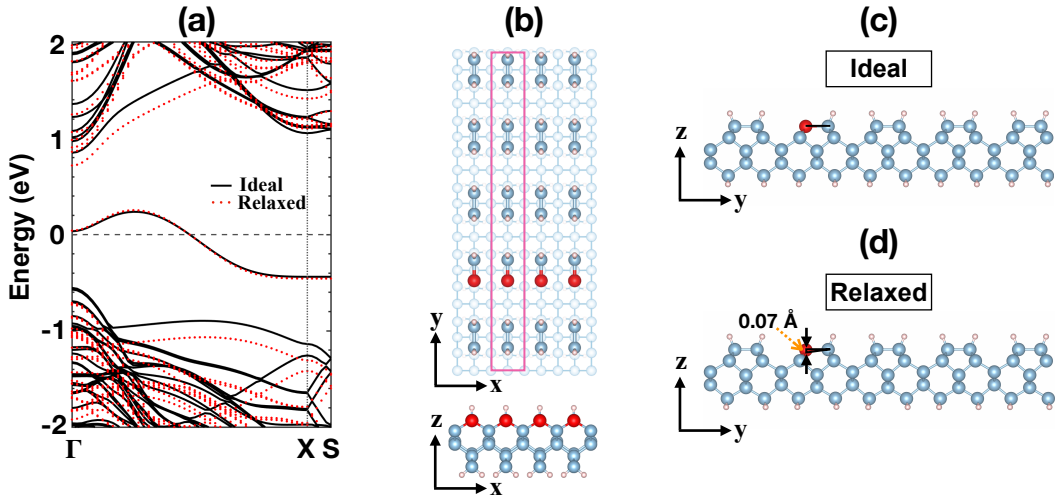

Fig. S1 (a) Comparison of electronic band structure near the Fermi level (set to zero) for an ideal DBW (black solid line) and a relaxed DBW (red dotted line). In the estimation of the influence of the Peierls distortion, the total energy and band structure are calculated by using a 1×5 supercell in both distorted and undistorted DBWs. (b) Top view of the 1×5 supercell (contains 79 atoms, 1DB). The supercell is marked by the solid pink line. The bottom panel shows the cross section side view of the vertical plane containing the Si atoms of the DBs. The red, blue and beige circles represent DB, Si and H atoms, respectively. For distinction, the surface DB, Si and H atoms are drawn with relatively larger circles and heavier color compared to the subsurface atoms. (c) Side view of the ideal 1×5 supercell. (d) Side view of the fully relaxed 1×5 supercell. Extraction of an H atom from a fully H-terminated Si dimer causes a height difference of $\sim$0.07 Å between the dimer atoms.

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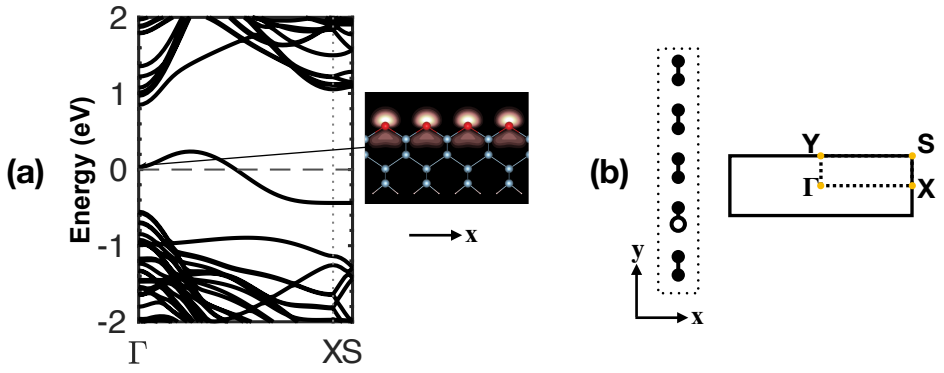

Fig. S2 (a) Calculated band structure of DB-∞ NM configuration using 1×5 supercell. The corresponding charge characters of the surface band at the Γ point is given in the right panel. (b) Ball and stick model of NM-1×5 supercell. The hollow circle represents the DB. The corresponding Brillouin zone is given in the right panel.

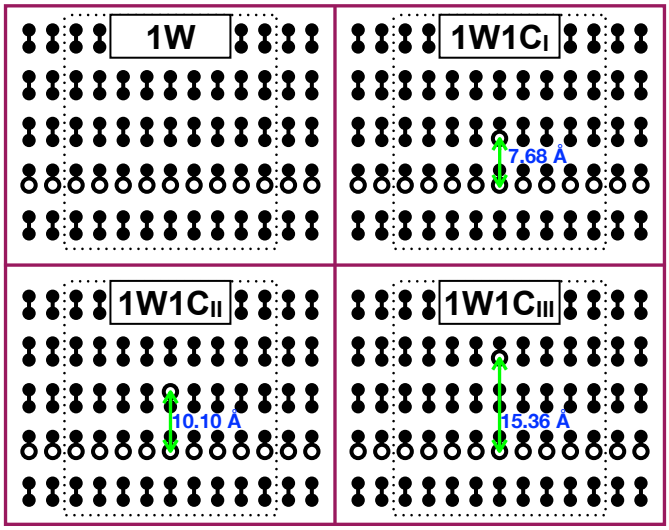

Fig. S3 Ball and stick model for NM-DBWs with DBCs at various distances.

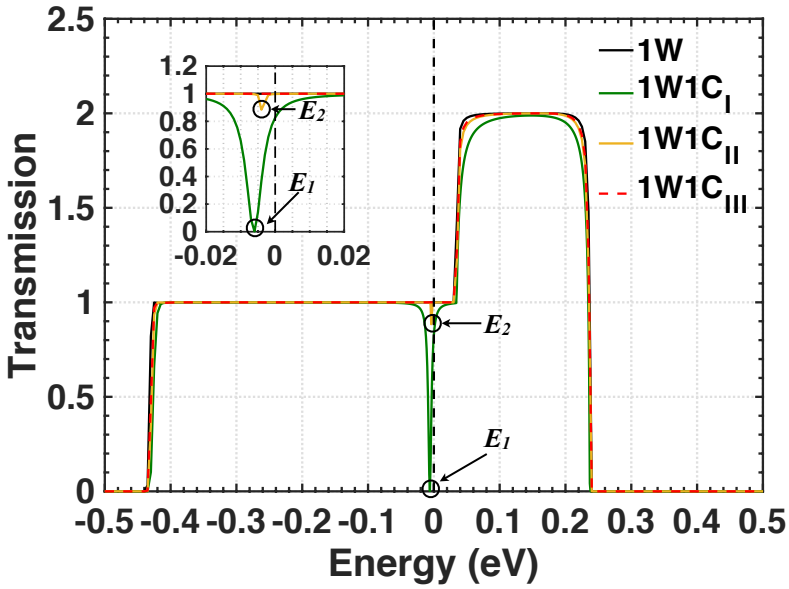

Fig. S4 Transmission spectra T(E) of the NM-DBWs gated by a single DBC located at 7.68 Å (green line, 1W1C$_I$), 10.10 Å (yellow line, 1W1C$_{II}$), and 15.36 Å (red dashed line, 1W1C$_{III}$). T(E) for the NM-DBW without a DBC nearby is shown by the black line, 1W. Inset: T(E) at energies between -0.02 eV and 0.02 eV.

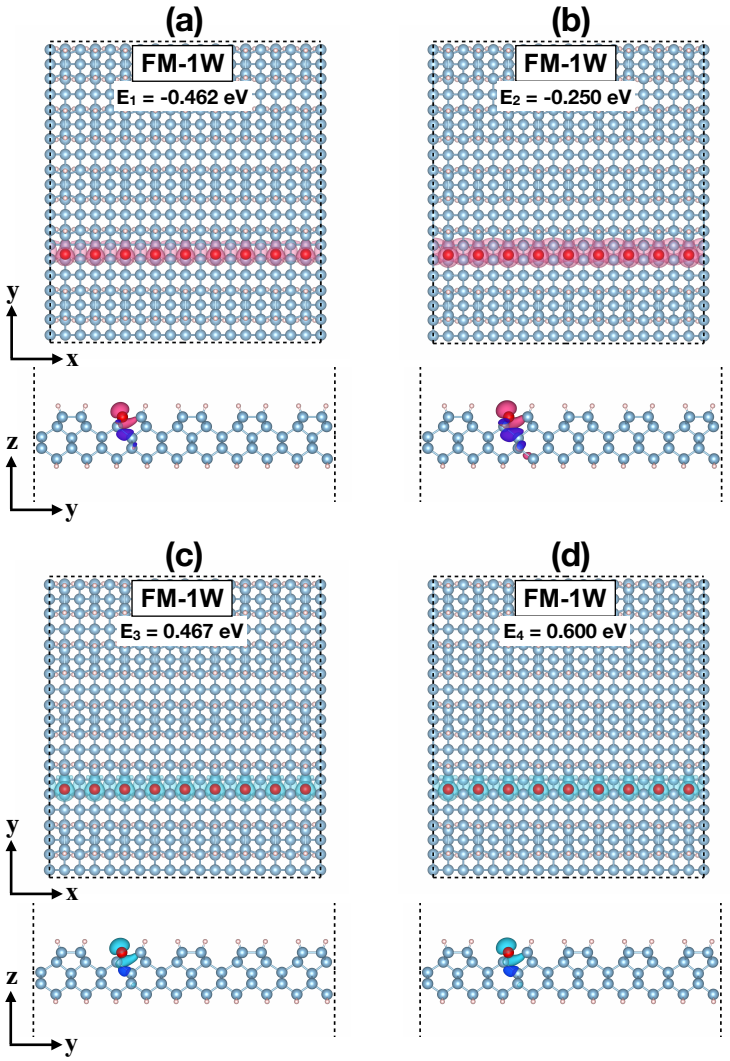

Fig. S5 (a) Top view and side view of the calculated scattering states for the transmission of FM-1W at 1-channel energy E_1=-0.462 eV. (b) Top view and side view of the calculated scattering states for the transmission of FM-1W at 2-channel energy E_2=-0.250 eV. (c) Top view and side view of the calculated scattering states for the transmission of FM-1W at 1-channel energy E_3=0.467 eV. (d) Top view and side view of the calculated scattering states for the transmission of FM-1W at 2-channel energy E_4=0.600 eV. The pink isosurface represents the spin-up states while the blue isosurface represents the spin-down states. A uniform increment is used.

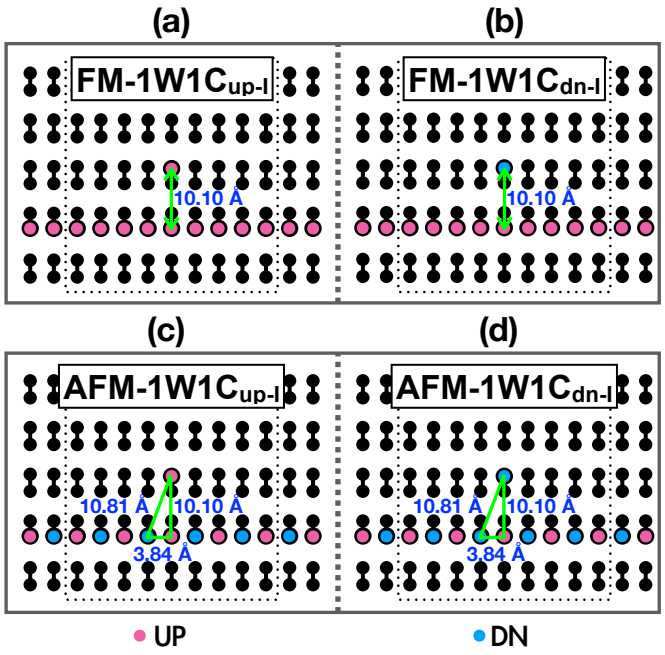

Fig. S6 Ball and stick model for (a) FM-1W1Cup-I, (b) FM-1W1Cdn-I, (c) AFM-1W1Cup-I, and (d) AFM-1W1Cdn-I structures, in which the DBCs are placed at 10.10 Å from the DBWs. The pink and blue dots represent spin-up and spin-down states, respectively. The distance between the DBC and its nearby DBs in the DBW and the distance between the neighboring DBs in the DBW are marked.

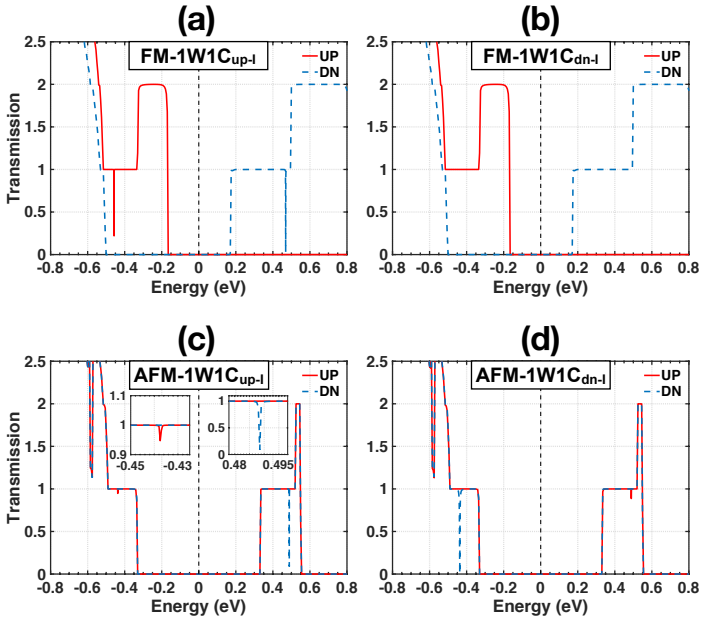

Fig. S7 (a) The spin-dependent electron transmission T(E) of a spin-up FM-DBW gated by a spin-up DBC as shown in Fig.S6(a) FM-1W1Cup-I. This system has a transmission dip in both occupied and unoccupied energy range for the transmission of the majority spin and for the transmission of the minority spin respectively. (b) T(E) of a spin-up FM-DBW gated by a spin-down DBC as shown in Fig.S6(b) FM 1W1Cdn-I. This configuration exhibits no dips in the transmission spectra. (c) T(E) of the AFM-DBW gated by a spin-up DBC as shown in Fig.S6(c) AFM-1W1Cup-I. This system has a transmission dip in both occupied and unoccupied energy range for the transmission of the majority spin and for the transmission of the minority spin respectively. (d) T(E) of the AFM-DBW gated by a spin-down DBC as shown in Fig.S6(d) AFM-1W1Cdn-I. This system has a transmission dip in both the occupied and unoccupied energy range for the transmission of the minority spin and for the transmission of the majority spin respectively.

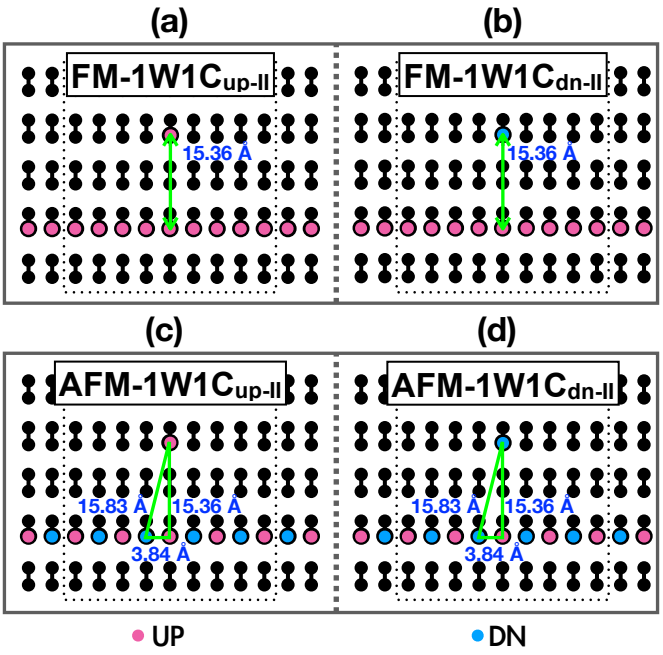

Fig. S8 Ball and stick model for (a) FM-1W1Cup-II, (b) FM-1W1Cdn-II, (c) AFM-1W1Cup-II, and (d) AFM-1W1Cdn-II structures, in which the DBCs are placed at 15.36 Å from the DBWs. The pink and blue dots represent spin-up and spin-down states, respectively. The distance between the DBC and its nearby DBs in the DBW and the distance between the neighboring DBs in the DBW are marked.

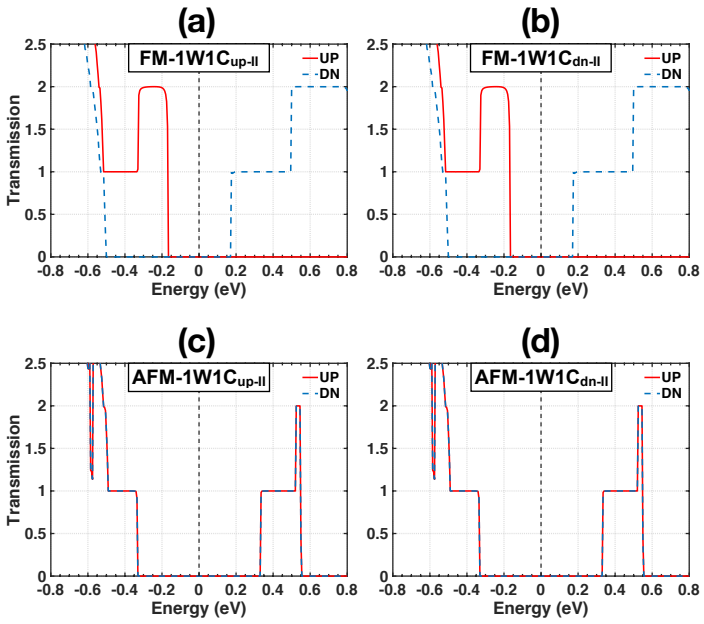

Fig. S9 (a) The spin-dependent electron transmission spectra T(E) of a spin-up FM-DBW gated by a spin-up DBC as shown in Fig.S8(a) FM-1W1Cup-II. (b) T(E) of a spin-up FM-DBW gated by a spin-down DBC as shown in Fig.S8(b) FM 1W1Cdn-II. (c) T(E) of the AFM-DBW gated by a spin-up DBC as shown in Fig.S8(c) AFM-1W1Cup-II. (d) T(E) of AFM-DBW gated by a spin-down DBC as shown in Fig.S8(d) AFM-1W1Cdn-II. All the configurations exhibit no dips in the transmission spectra.

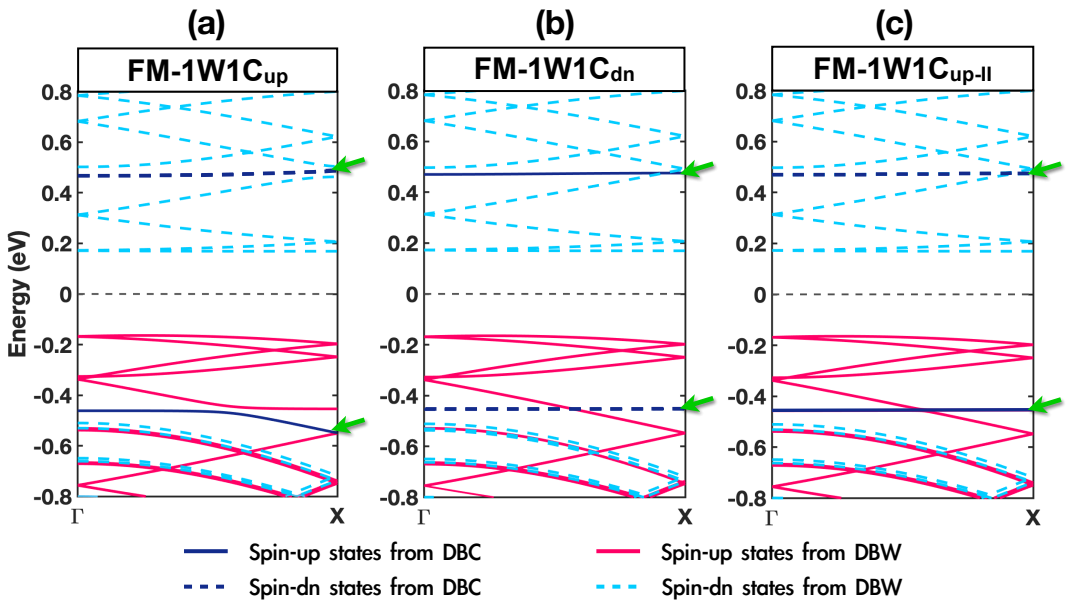

Fig. S10 (a) Calculated band structure of the scattering region of a spin-up FM-DBW gated by a spin-up DBC, named FM-1W1Cup in Fig.3(b). (b) Calculated band structure of the scattering region of a spin-up FM-DBW gated by a spin-dn DBC, named FM-1W1Cdn in Fig.3(c). (c) Calculated band structure of the scattering region of a spin-up FM-DBW gated by a spin-up DBC placed at a distance of 15.36 Å, named FM-1W1Cup-II in Fig.S8(a). The solid navy lines (marked by green arrows) are corresponding to spin-up states from the DBC; the dashed navy lines (marked by green arrows) are corresponding to spin-dn states from the DBC. The solid pink lines represent spin-up states from the DBW; the dashed blue lines represent spin-dn states from the DBW.

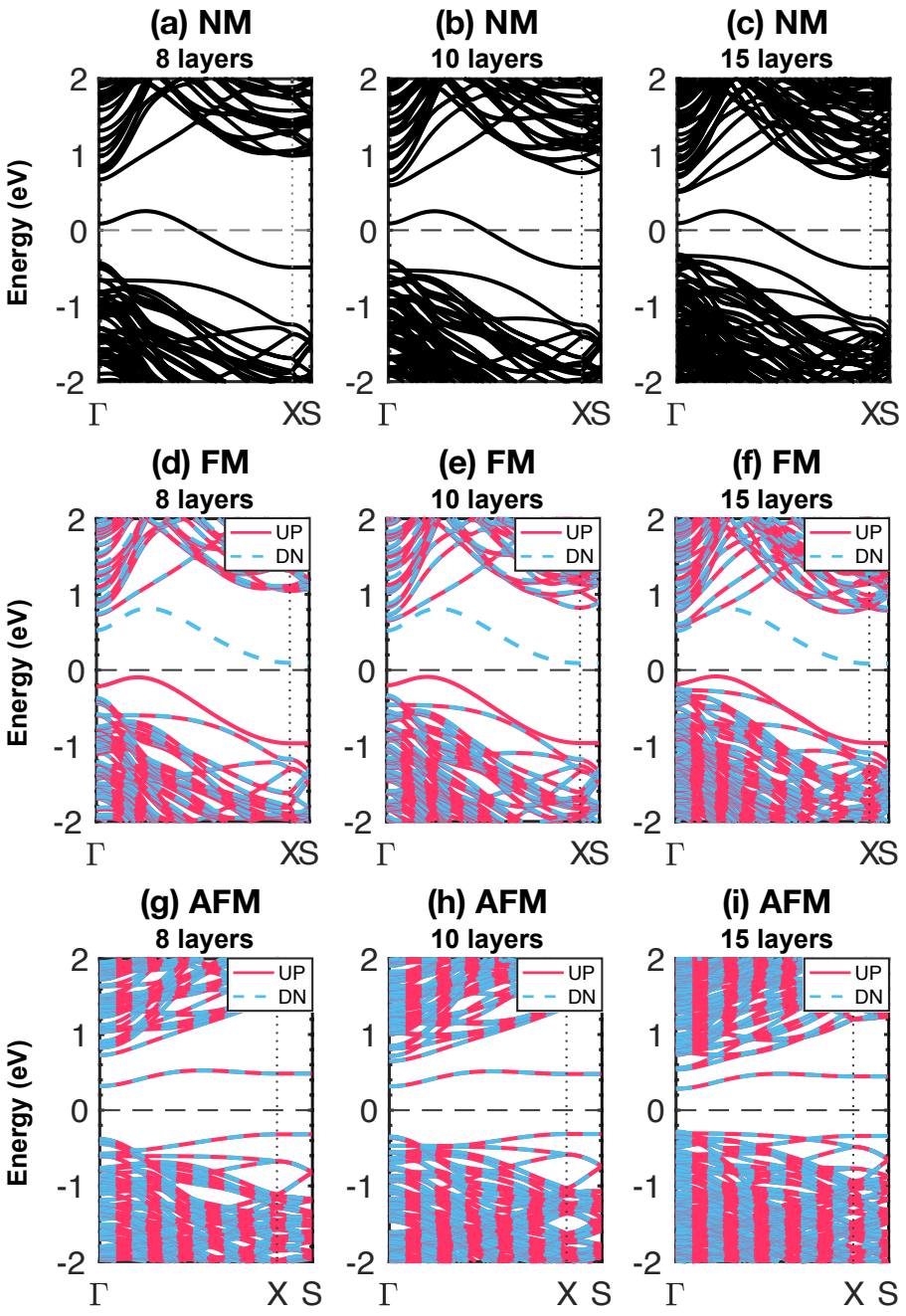

Fig. S11 Calculated band structure of DB-∞ NM configuration using 1×5 supercell with (a). 5-layer slabs, (b) 8-layer slabs, (c). 10-layer slabs, (d) 15-layer slabs. Calculated band structure of DB-∞ FM configuration using 1×5 supercell with (e). 5-layer slabs, (f) 8-layer slabs, (g). 10-layer slabs, (h) 15-layer slabs. Calculated band structure of DB-∞ AFM configuration using 1×5 supercell with (i). 5-layer slabs, (j) 8-layer slabs, (k). 10-layer slabs, (l) 15-layer slabs.

The electronic properties of the DB states of Si samples with different thickness

It has been reported that the thickness of the Si slab used in the DFT simulation will affect the position of DB states[1]. In our calculations, to isolate the DBW in our simulation super-cell with its neighboring images (due to periodic boundary condition), a large lateral cross-section of the Si surface is required. In the Ref.[1], they used a 6-layer Si slab in their non-spin-polarized transport simulation. In our case, with spin, the complexity of computation is significantly increased which limits the total number atoms in the transport system and with 5-layers, there are already more than 700 atoms.

We performed calculations with 5-, 8-, 10- and 15-layers of Si as the slab to check the DBW energy dispersion inside the Si gap. The results are shown in Fig.S11.

Without spin, the DBW energy dispersion is clearly located inside the Si gap, very similar to the 5-layer case. With spin, due to the lifting of spin degeneracy, the DBW energy dispersion - both occupied and unoccupied, are isolated inside the Si gap up to 10-layer Si slab. For 15-layer slab, the occupied state of DBW starts to merge with the bulk valence states and the unoccupied state of the DBW remains isolated inside the Si gap.

In addition, the fabrication of Si films as thin as 3 nm has been reported[2]. There are also theoretical studies[1,3] showing that stain tensile can effectively remove the overlap between the DB states and the bulk states. And the fabrication of 9 nm thick stained Si layer on insulator has been achieved[4]. So experimental realization of such thin Si slabs with well-isolated DB states should be possible in the near future.

References

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