Electronic Supplementary Information

Robust spin-dependent Seebeck effect and remarkable spin thermoelectric performance in graphether nanoribbons

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A. Discussion on Magnetism Mechanism

To demonstrate the magnetism origination of asymmetrically passivated AGENRs, we take AGENR7 as an example and consider both I-type and II-type structures. Here, the I-type structures are fully passivated on the upper edge (denoted by the “2H@” prefix), while the II-type structures maintain their upper edge unpassivated (denoted by the “0H@” prefix). For both I-type and II-type structures, we calculate the band structures of three configurations with different passivation of the C dimer on the lower edge, i.e., unpassivated (denoted by the "@0H" suffix), fully passivated (denoted by the "@2H" suffix), and partially passivated (AGENR7-I/II in the main text), respectively, as shown in Fig. S1.

The four symmetrically passivated configurations [Fig. S1(a), (b), (d), and (e)] have completely degenerate band structures, showing the characteristics of a closed-shell system. However, in AGENR7-I [Fig. S1(c)] and AGENR7-II [Fig. S1(f)], the partial passivation of the lower edge changes the total number of electrons in the unit cell from even to odd, and the system turns to an open-shell one. The exchange coupling between open-shell electrons introduces the magnetism into the system, giving rise to the spin-splitting subbands, especially near the Fermi level.

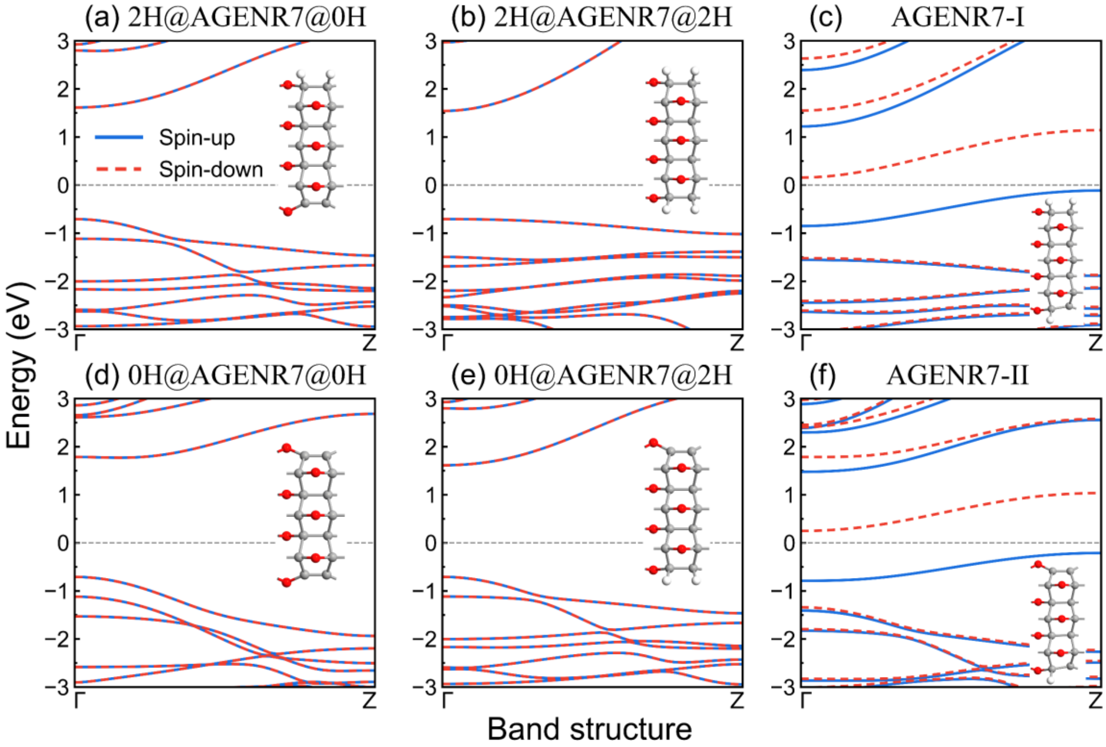

Fig. S1 Band structures of (a)-(c) I-type and (d)-(f) II-type AGENR7 with different passivated lower edges. The insets illustrate the unit cell of the configurations.

B. Transport Paths of the Spin-dependent Currents

We use the ATK package to calculate and depict the transmission pathways of the spin-up current at $E = -0.2$ eV (no spin-down current at this energy) and the spin-down current at $E = 0.2$ eV (no spin-up current) for AGENR7-I and AGENR7-II, as shown in Fig. S2. $E = -0.2$ and 0.2 eV are chosen because they are located within the broad peak of the spin-up and spin-down transmission spectra, respectively, for both configurations. The volume of each arrow indicates the magnitude of the local transmission between each pair of atoms, while the color indicates the transport direction, i.e., cyan for rightward and magenta for leftward. To show the main contributing paths clearly, we only display paths that contribute exceeding 30% of the total transmission.

It could be concluded that the spin-up and spin-down currents transport mainly on the partially passivated edge, and the fully passivated edge contributes little to the currents. We have checked AGENR spin caloritronic devices with other widths and the same conclusion can be drawn.

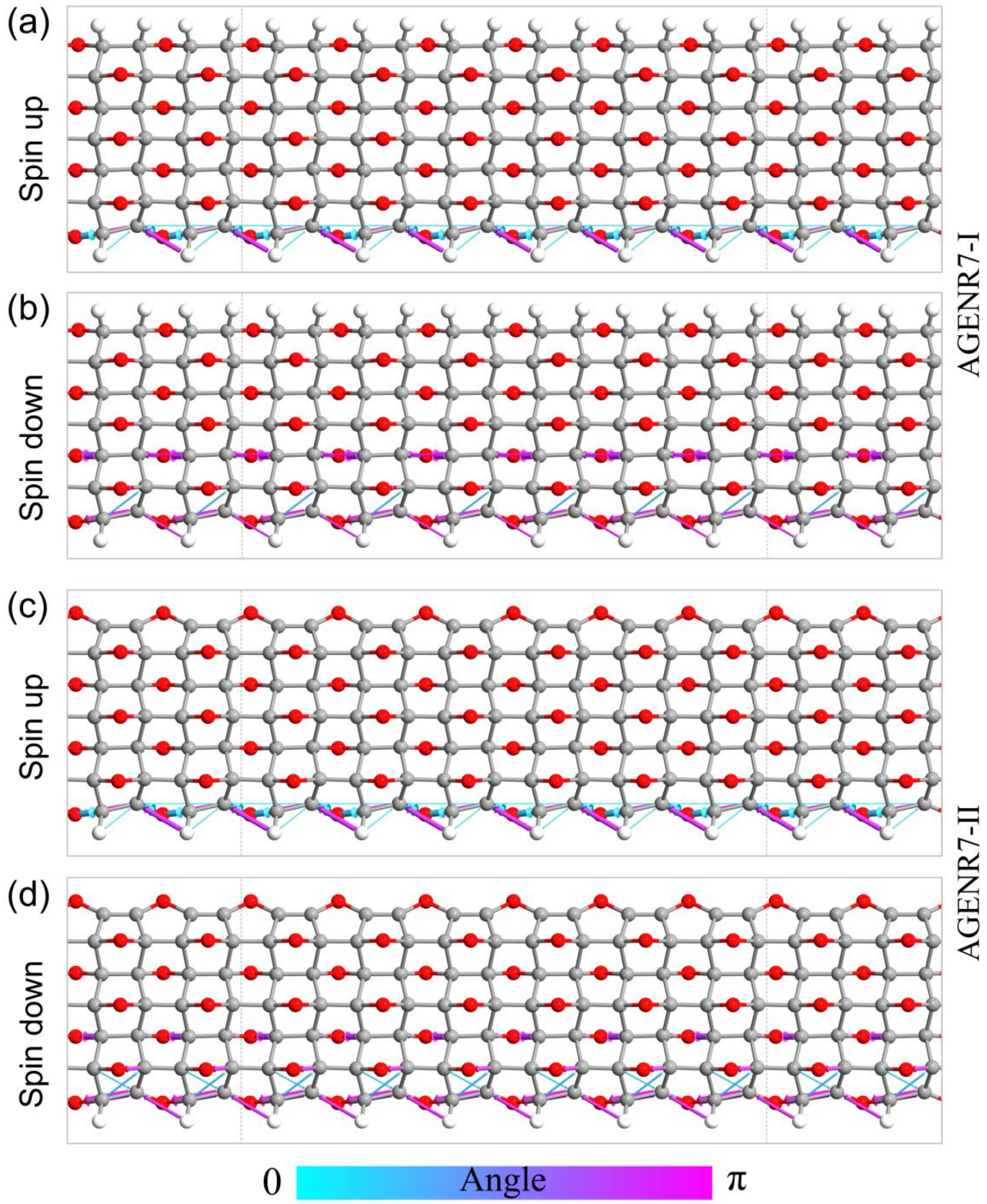

Fig. S2 Transmission pathways of (a) spin-up, (b) spin-down currents for AGENR7-I and (c) spin-up, (d) spin-down currents for AGENR7-II.