Supporting Information

Phase transition and topological transistors based on monolayer Na_3Bi nanoribbons

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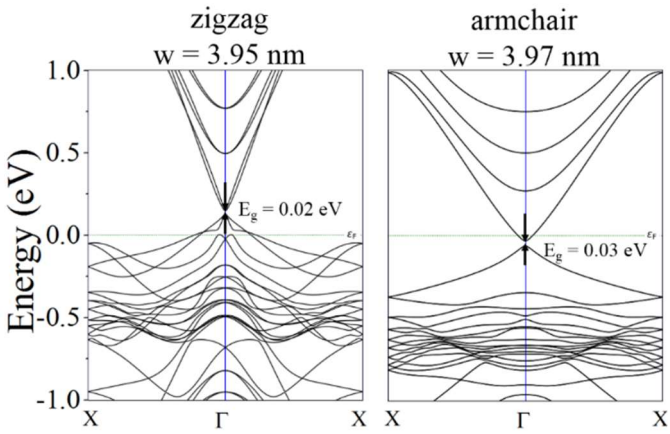

Fig. S1. Band structures of the (a) 3.95-nm width ML Na_3Bi ZNR and (b) 3.97-nm width ML Na_3Bi ANR with 0.02 and 0.03 eV whole bandgap, respectively. The Fermi level is set to 0.

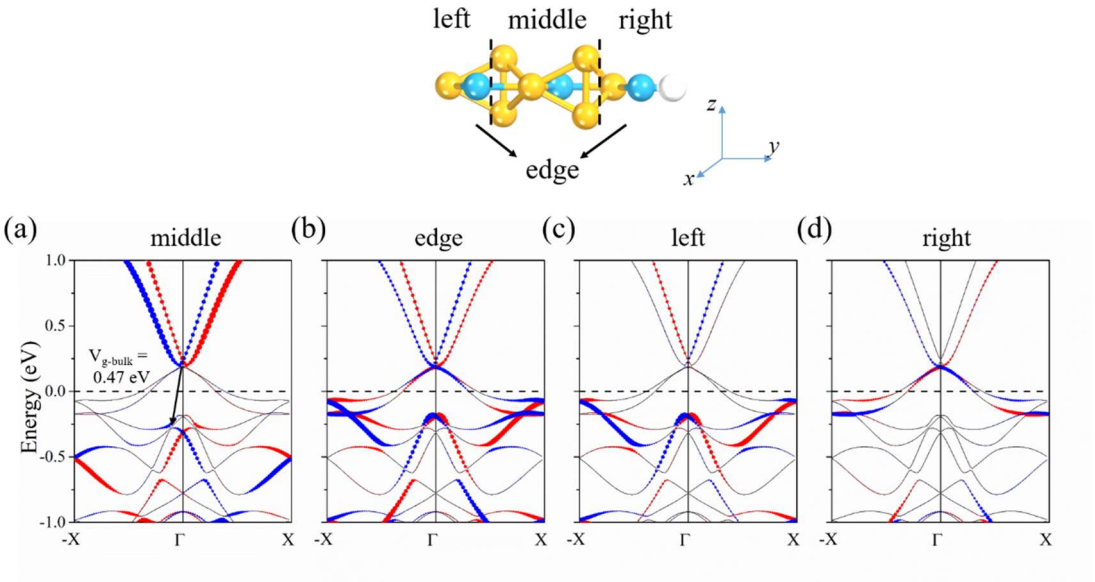

Fig. S2. Band structure projected on the (a) middle atoms, (b) edge atoms, (c) left atoms, and (d) right atoms of the 1.28-nm width ML Na_3Bi ZNR. The red/blue dots in the band structure represent the spin-up/spin-down states. The Fermi level is set to 0.

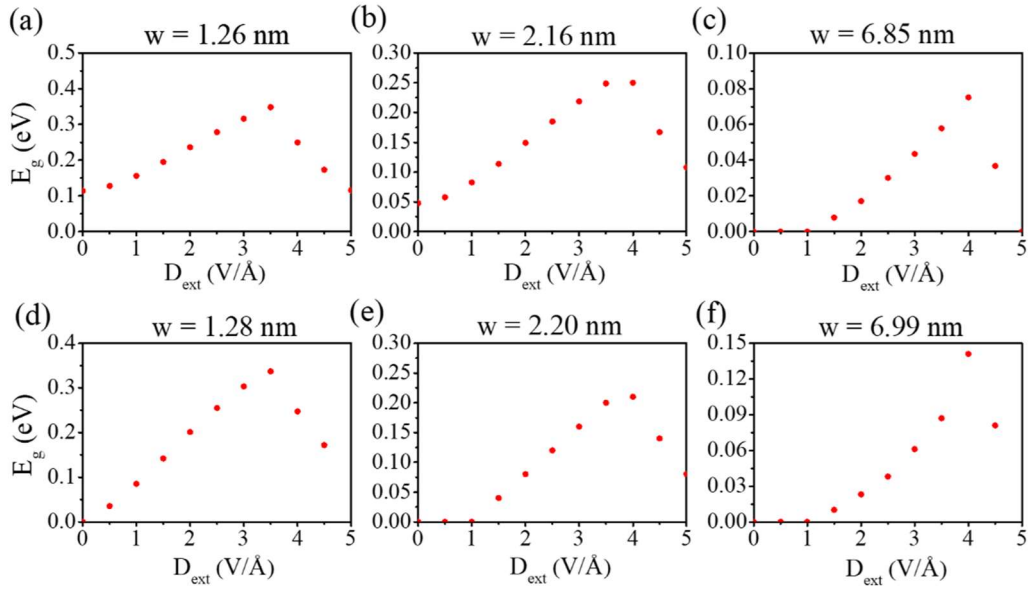

Fig. S3. Bulk bandgaps of the (a) 1.26, (b) 2.16, (c) 6.85, (d) 1.28, (e) 2.20, and (f) 6.99-nm width ML Na_3Bi ZNRs under different D_{ext}. (d), (e), and (f) have 2% strain applied in the width direction of (a), (b), and (c), respectively.

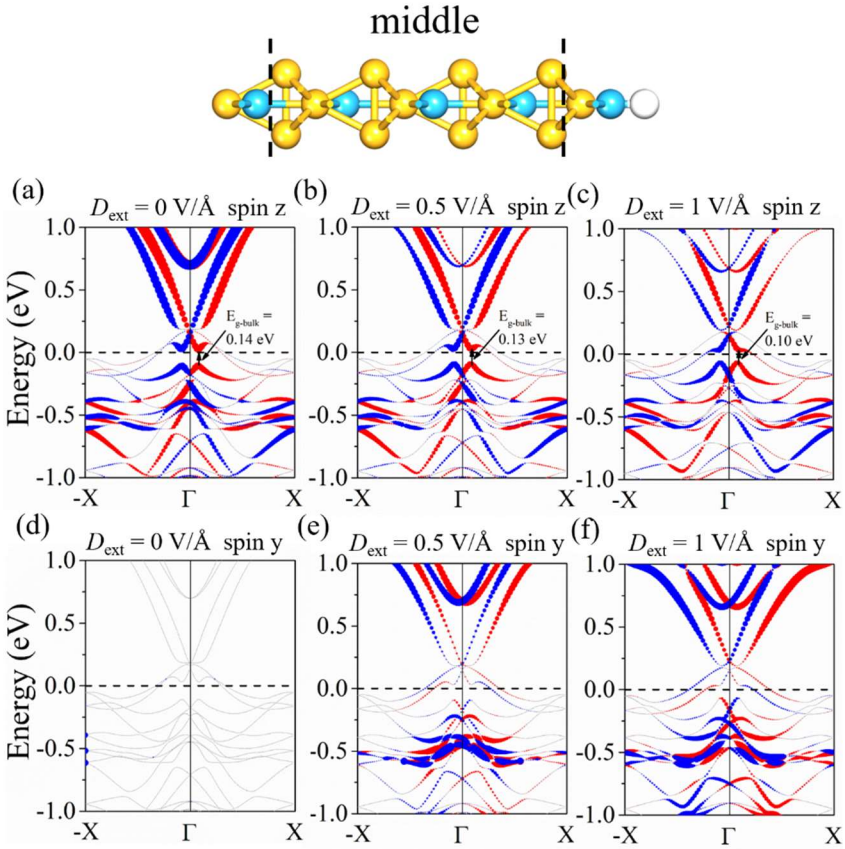

Fig. S4. Spin-resolved band structures projected on the middle atoms of the 2.20-nm width ML Na_3Bi ZNR under different D_{ext}. The blue dots represent the spin-up states and the red dots represent the spin-down states. The number of states is reflected in the size of the dots.

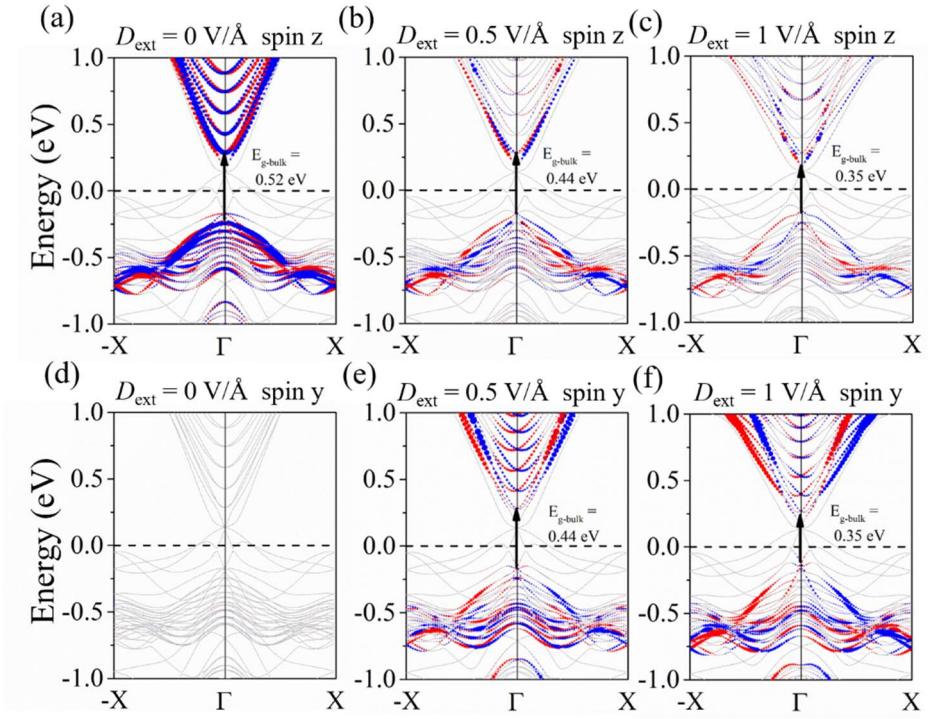

Fig. S5. Spin-resolved band structures projected on the middle atoms of the 6.85-nm width

ML Na_3Bi ZNR under different displacement electric fields. The middle atoms are shown in Fig. 3. The blue dots represent the spin-up states and the red dots represent the spin-down states. The number of states is reflected in the size of the dots.

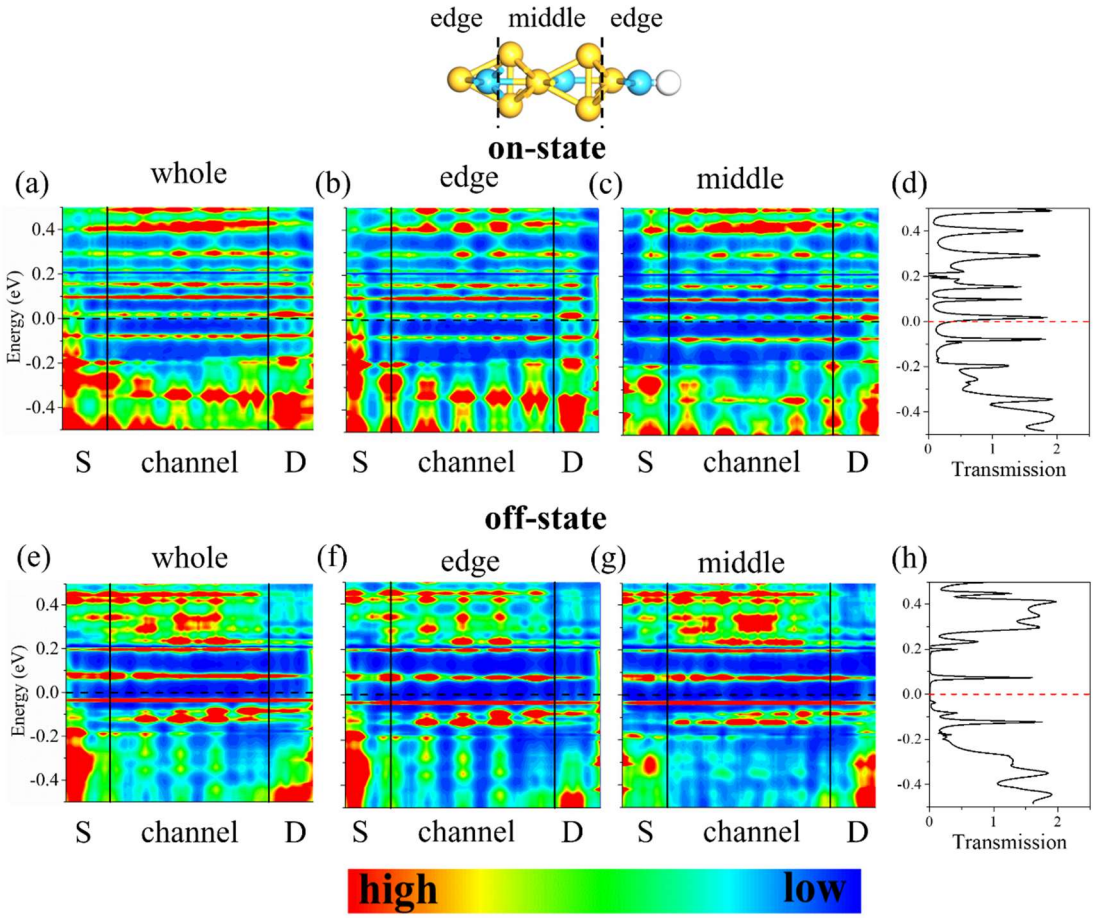

Fig. S6. Local device density of states (LDOS) of the ML Na_3Bi NR topological transistor at V_{bias} = 0 V. (a) ~ (c) and (e) ~ (g) are the LDOS of the on-state (V_{diff} = 11 V), and off-state (V_{diff} = 24 V). (a, e), (b, f), and (c, g) represent the states contributed by all the atoms, the middle atoms, and the edge atoms (as shown on the top), respectively. The solid vertical black lines divide the device into three parts: source, channel, and drain. (d) and (h) is the transmission spectrum of V_g = 11 V and V_g = 24 V, respectively. The dash horizontal black/red lines represent the bias window in the LDOS/ transmission spectrum. The yellow, blue, and white atoms represent the Na, Bi, and H, respectively.

In the simplest model, the transmission probability of a free electron (hole) going through a limited height barrier is[1]:

$$T = \frac{4k^2k'^2}{(k^2-k'^2)^2\sinh^2(k'a)+(k^2-k'^2)^2\cosh^2(k'a)}$$

$$\approx \frac{16E(V-E)}{V^2}\exp\left(-2\sqrt{\frac{2m^*(V-E)}{\hbar^2}}a\right)$$

where $k=\frac{\sqrt{2m^*E}}{\hbar^2}$, $k'=\frac{\sqrt{2m^*(V-E)}}{\hbar^2}$, $\sinh(k'a)=\frac{e^{k'a}-e^{-k'a}}{2}$, $\cosh(k'a)=\frac{e^{k'a}+e^{-k'a}}{2}$. a is the length of the barrier. For electrons, m^* is the electron effective mass, *E* is the Fermi energy of the source, and *V* is the energy of the conduction band minimum (CBM). For holes, m^* is the hole effective mass, *E* is the Fermi energy of the drain, and *V* is the energy of the valance band maximum (VBM).

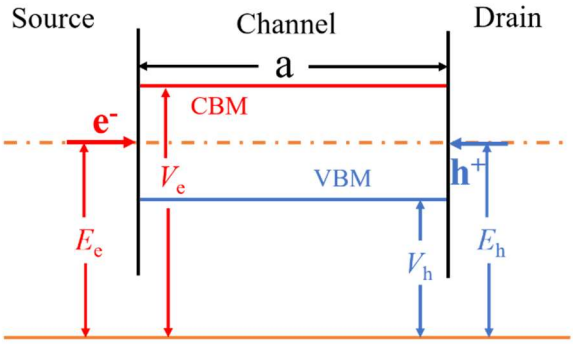

Fig. S7. Schematic diagram of a free electron/hole tunneling through a finite height barrier under an infinitesimal bias voltage. The voltage of the source $V_{source} < 0$ and the voltage of the drain $V_{drain} > 0$. The dash-dot line is the Fermi level.

Reference

1. SZE, S. M., *Physics of Semiconductor Devices*. John Wiley & Sons, Inc.: Hoboken, NJ 07030, USA, 2021.