## Supplemental Material for "Evolution of Topological Properties of Two-Dimensional Group IVA Materials and Device Design"

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In Fig. 1 of the main text, the three nearest-neighbor (NN) and six next-nearest-neighbor (NNN) translation vectors are

$$\delta_{\mathbf{1}} = \frac{a}{\sqrt{3}} \left( \frac{\sqrt{3}}{2} \quad \frac{1}{2} \quad \cot \phi \right), \quad \delta_{\mathbf{2}} = \frac{a}{\sqrt{3}} \left( -\frac{\sqrt{3}}{2} \quad \frac{1}{2} \quad \cot \phi \right), \quad \delta_{\mathbf{3}} = \frac{a}{\sqrt{3}} \left( 0 \quad -1 \quad \cot \phi \right), \quad (1)$$

$$\mathbf{v_1} = a \left( \frac{1}{2} \ \frac{\sqrt{3}}{2} \ 0 \right), \ \mathbf{v_2} = a \left( 1 \ 0 \ 0 \right), \ \mathbf{v_3} = a \left( \frac{1}{2} \ -\frac{\sqrt{3}}{2} \ 0 \right), \mathbf{v_4} = a \left( -\frac{1}{2} \ -\frac{\sqrt{3}}{2} \ 0 \right), \ \mathbf{v_5} = a \left( -1 \ 0 \ 0 \right), \ \mathbf{v_6} = a \left( -\frac{1}{2} \ \frac{\sqrt{3}}{2} \ 0 \right).$$
(2)

The lattice constant a and the angle  $\phi$  are defined as the NNN distance and the angle between the NN bond and the z direction, respectively.

In Eq. (1) of the main text, the NN hopping integrals in the Slater-Koster frame along the  $\delta = 1, 2, 3$  directions (corresponding to  $\delta_1, \delta_2, \delta_3$ , respectively) from sublattice *B* to sublattice *A* read

$$\begin{cases} t_{AB1ss} = V_{ss\sigma}, \\ t_{AB1sx} = l_1 V_{sp\sigma} = \frac{\sqrt{3} \sin \phi}{2} V_{sp\sigma}, \\ t_{AB1sy} = m_1 V_{sp\sigma} = \cos \phi V_{sp\sigma}, \\ t_{AB1sz} = n_1 V_{sp\sigma} = \cos \phi V_{sp\sigma}, \\ \\ t_{AB1xs} = -l_1 V_{sp\sigma} = -\frac{\sqrt{3} \sin \phi}{2} V_{sp\sigma}, \\ t_{AB1xx} = l_1^2 V_{pp\sigma} + (1 - l_1^2) V_{pp\pi} = \frac{3 \sin^2 \phi}{4} V_{pp\sigma} + \left(1 - \frac{3 \sin^2 \phi}{4}\right) V_{pp\pi}, \\ t_{AB1xy} = l_1 m_1 (V_{pp\sigma} - V_{pp\pi}) = \frac{\sqrt{3} \sin \phi \cos \phi}{2} (V_{pp\sigma} - V_{pp\pi}), \\ t_{AB1xz} = l_1 n_1 (V_{pp\sigma} - V_{pp\pi}) = \frac{\sqrt{3} \sin \phi \cos \phi}{2} (V_{pp\sigma} - V_{pp\pi}), \\ t_{AB1ys} = -m_1 V_{sp\sigma} = -\frac{\sin \phi}{2} V_{sp\sigma}, \\ t_{AB1yx} = l_1 m_1 (V_{pp\sigma} - V_{pp\pi}) = \frac{\sqrt{3} \sin^2 \phi}{4} (V_{pp\sigma} - V_{pp\pi}), \\ t_{AB1yz} = m_1 V_{sp\sigma} = -\frac{\sin \phi}{2} V_{sp\sigma}, \\ t_{AB1yz} = m_1 n_1 (V_{pp\sigma} - V_{pp\pi}) = \frac{\sin^2 \phi}{4} V_{pp\sigma} + \left(1 - \frac{\sin^2 \phi}{4}\right) V_{pp\pi}, \\ t_{AB1yz} = m_1 n_1 (V_{pp\sigma} - V_{pp\pi}) = \frac{\sin \phi \cos \phi}{2} (V_{pp\sigma} - V_{pp\pi}), \\ t_{AB1zz} = n_1 V_{sp\sigma} = -\cos \phi V_{sp\sigma}, \\ t_{AB1zz} = l_1 n_1 (V_{pp\sigma} - V_{pp\pi}) = \frac{\sqrt{3} \sin \phi \cos \phi}{2} (V_{pp\sigma} - V_{pp\pi}), \\ t_{AB1zz} = m_1 n_1 (V_{pp\sigma} - V_{pp\pi}) = \frac{\sqrt{3} \sin \phi \cos \phi}{2} (V_{pp\sigma} - V_{pp\pi}), \\ t_{AB1zz} = m_1 n_1 (V_{pp\sigma} - V_{pp\pi}) = \frac{\sin \phi \cos \phi}{2} (V_{pp\sigma} - V_{pp\pi}), \\ t_{AB1zz} = m_1 n_1 (V_{pp\sigma} - V_{pp\pi}) = \frac{\sin \phi \cos \phi}{2} (V_{pp\sigma} - V_{pp\pi}), \\ t_{AB1zz} = m_1 n_1 (V_{pp\sigma} - V_{pp\pi}) = \frac{\sin \phi \cos \phi}{2} (V_{pp\sigma} - V_{pp\pi}), \\ t_{AB1zz} = m_1 n_1 (V_{pp\sigma} - V_{pp\pi}) = \frac{\sin \phi \cos \phi}{2} (V_{pp\sigma} - V_{pp\pi}), \\ t_{AB1zz} = m_1 n_1 (V_{pp\sigma} - V_{pp\pi}) = \frac{\sin \phi \cos \phi}{2} (V_{pp\sigma} - V_{pp\pi}), \\ t_{AB1zz} = m_1 n_1 (V_{pp\sigma} - V_{pp\pi}) = \frac{\sin \phi \cos \phi}{2} V_{pp\sigma} + \sin^2 \phi V_{pp\pi}, \\ t_{AB2sx} = l_2 V_{sp\sigma} = -\frac{\sqrt{3} \sin \phi}{2} V_{sp\sigma}, \\ t_{AB2sy} = m_2 V_{sp\sigma} = \frac{\sin \phi}{2} V_{sp\sigma}, \\ t_{AB2sy} = m_2 V_{sp\sigma} = \cos \phi V_{sp\sigma}, \\ t_{AB2sz} = n_2 V_{sp\sigma} = \cos \phi V_{sp\sigma}, \\ t_{AB2sz} = n_2 V_{sp\sigma} = \cos \phi V_{sp\sigma}, \\ t_{AB2sz} = n_2 V_{sp\sigma} = \cos \phi V_{sp\sigma}, \\ t_{AB2sz} = n_2 V_{sp\sigma} = \cos \phi V_{sp\sigma}, \\ t_{AB2sz} = n_2 V_{sp\sigma} = \cos \phi V_{sp\sigma}, \\ t_{AB2sz} = n_2 V_{sp\sigma} = \cos \phi V_{sp\sigma}, \\ t_{AB2sz} = n_2 V_{sp\sigma} = \cos \phi V_{sp\sigma}, \\ t_{AB2sz} = n_2 V_{sp\sigma} = \cos \phi V_{sp\sigma}, \\ t_{AB2sz} = n_2 V_{sp\sigma} = \cos \phi V_{sp\sigma}, \\ t_{$$

$$\begin{cases} t_{AB2xs} = -l_2 V_{sp\sigma} = \frac{\sqrt{3} \sin^2 \phi}{2} V_{sp\sigma}, \\ t_{AB2xx} = l_2^2 V_{pp\sigma} + (1 - l_2^2) V_{pp\pi} = \frac{\sqrt{3} \sin^2 \phi}{4} V_{pp\sigma} + \left(1 - \frac{3 \sin^2 \phi}{4}\right) V_{pp\pi}, \\ t_{AB2xy} = l_2 m_2 (V_{pp\sigma} - V_{pp\pi}) = -\frac{\sqrt{3} \sin^2 \phi}{2} (V_{pp\sigma} - V_{pp\pi}), \\ t_{AB2yx} = l_2 m_2 (V_{pp\sigma} - V_{pp\pi}) = -\frac{\sqrt{3} \sin^2 \phi}{2} (V_{pp\sigma} - V_{pp\pi}), \\ t_{AB2yy} = l_2 m_2 (V_{pp\sigma} - V_{pp\pi}) = -\frac{\sqrt{3} \sin^2 \phi}{4} (V_{pp\sigma} - V_{pp\pi}), \\ t_{AB2yy} = m_2^2 V_{pp\sigma} + (1 - m_2^2) V_{pn\pi} = \frac{\sin^2 \phi}{4} V_{pp\sigma} + \left(1 - \frac{\sin^2 \phi}{4}\right) V_{pp\pi}, \\ t_{AB2yy} = m_2^2 V_{pp\sigma} + (1 - m_2^2) V_{pn\pi} = \frac{\sin^2 \phi}{2} (V_{pp\sigma} - V_{pp\pi}), \\ t_{AB2yz} = m_2 n_2 (V_{pp\sigma} - V_{pp\pi}) = -\frac{\sqrt{3} \sin \phi \cos \phi}{4} (V_{pp\sigma} - V_{pp\pi}), \\ t_{AB2xz} = m_2 V_{sp\sigma} = -\cos \phi V_{sp\sigma}, \\ t_{AB2xz} = l_2 n_2 (V_{pp\sigma} - V_{pp\pi}) = -\frac{\sqrt{3} \sin \phi \cos \phi}{2} (V_{pp\sigma} - V_{pp\pi}), \\ t_{AB2xz} = l_2 n_2 (V_{pp\sigma} - V_{pp\pi}) = -\frac{\sqrt{3} \sin \phi \cos \phi}{2} (V_{pp\sigma} - V_{pp\pi}), \\ t_{AB2xz} = l_2 n_2 (V_{pp\sigma} - V_{pp\pi}) = -\frac{\sin \phi}{2} e^{2\phi \phi} (V_{pp\sigma} - V_{pp\pi}), \\ t_{AB2xz} = m_2 V_{sp\sigma} = -\cos \phi V_{sp\sigma}, \\ t_{AB3xz} = l_2 V_{pp\sigma} + (1 - n_2^2) V_{pp\pi} = \cos^2 \phi V_{pp\sigma} + \sin^2 \phi V_{pp\pi}, \\ t_{AB3xz} = l_3 V_{sp\sigma} = 0, \\ t_{AB3xz} = l_3 V_{sp\sigma} = \sin \phi V_{sp\sigma}, \\ t_{AB3xz} = l_3 N_{sp\sigma} = \sin \phi V_{sp\sigma}, \\ t_{AB3xz} = l_3 N_{sp\sigma} = \sin \phi V_{sp\sigma}, \\ t_{AB3xz} = l_3 N_{sp\sigma} = \sin \phi V_{sp\sigma}, \\ t_{AB3xz} = l_3 n_3 (V_{pp\sigma} - V_{pp\pi}) = 0, \\ t_{AB3yz} = m_3 n_3 (V_{pp\sigma} - V_{pp\pi}) = -\sin \phi \cos \phi (V_{pp\sigma} + \cos^2 \phi V_{pm}, \\ t_{AB3yz} = m_3 n_3 (V_{pp\sigma} - V_{pp\pi}) = -\sin \phi \cos \phi (V_{pp\sigma} - V_{pp\pi}), \\ t_{AB3yz} = m_3 n_3 (V_{pp\sigma} - V_{pp\pi}) = -\sin \phi \cos \phi (V_{pp\sigma} - V_{pp\pi}), \\ t_{AB3xz} = l_3 n_3 (V_{pp\sigma} - V_{pp\pi}) = -\sin \phi \cos \phi (V_{pp\sigma} - V_{pp\pi}), \\ t_{AB3xz} = n_3 V_{sp\sigma} = -\cos \phi V_{sp\sigma}, \\ t_{AB3xz} = n_3 V_{sp\sigma} = -\cos \phi V_{sp\sigma}, \\ t_{AB3xz} = n_3 V_{sp\sigma} = -\cos \phi V_{sp\sigma}, \\ t_{AB3xz} = n_3 V_{sp\sigma} + (1 - n_3^2) V_{pp\pi} = -\sin \phi \cos \phi (V_{pp\sigma} - V_{pp\pi}), \\ t_{AB3xz} = n_3 V_{sp\sigma} + (1 - n_3^2) V_{pp\pi} = -\sin^2 \phi V_{pp\pi} + \sin^2 \psi V_{pp\pi}. \\ The NNN hop$$

 $\mathbf{v_1}, \mathbf{v_2}, \mathbf{v_3}, \mathbf{v_4}, \mathbf{v_5}, \mathbf{v_6}$ , respectively) in sublattice A read

$$\begin{array}{l} t_{AA1ss} = t_{AA2ss} = t_{AA3ss} = V_{ss\sigma}^{\prime}, \\ t_{AA4ss} = t_{AA3ss} = t_{AA5ss} = t_{AA5ss} = V_{ss\sigma}^{\prime}, \\ t_{AA1sx} = t_{1}^{\prime}V_{sp\sigma}^{\prime} = \frac{V_{ss\sigma}^{\prime}}{2}, \\ t_{AA4sx} = -\frac{V_{ss\sigma}^{\prime}}{2}, \\ t_{AA4sx} = t_{AA3sz} = 0, \\ t_{AA4sz} = t_{AA5sz} = t_{AA6sz} = 0, \\ t_{AA4sz} = t_{AA5sz} = t_{AA6sz} = 0, \\ t_{AA4sx} = t_{AA5sx}^{\prime} = V_{sp\sigma}^{\prime}, \\ t_{AA4sx} = \frac{V_{ss\sigma}^{\prime}}{2}, \\ t_{AA4sx} = \frac{V_{ss\sigma}^{\prime}}{2}, \\ t_{AA4sx} = \frac{V_{ss\sigma}^{\prime}}{2}, \\ t_{AA4sx} = \frac{V_{ss\sigma}^{\prime}}{4}, \\ t_{AA5sx} = V_{sp\sigma}^{\prime}, \\ t_{AA4sx} = \frac{V_{ss\sigma}^{\prime}}{4}, \\ t_{AA5sx} = V_{sp\sigma}^{\prime}, \\ t_{AA4sx} = \frac{V_{ss\sigma}^{\prime}}{4}, \\ t_{AA5sx} = V_{sp\sigma}^{\prime}, \\ t_{AA4sx} = V_{ss\sigma}^{\prime}, \\ t_{AA4sx} = V_{AA5sx}^{\prime}, \\ t_{AA4sx} = V_{AA5sx}^{\prime}, \\ t_{AA4sx} = V_{ss\sigma}^{\prime}, \\ t_{AA4sx} = V_{ss\sigma}^{\prime}, \\ t_{AA4sx} = V_{AA5sx}^{\prime}, \\ t_{AA4sx} = V_{AA5s$$



Fig. S 1: (Color online) Band structures of **graphene** (a) without spin–orbit coupling (SOC) and (b) with SOC. The blue and red curves correspond to the first-principles and tight-binding calculations, respectively.

 $\begin{cases} t_{AA1zz} = n_1'^2 V'_{pp\sigma} + (1 - n_1'^2) V'_{pp\pi} = V'_{pp\pi}, t_{AA2zz} = V'_{pp\pi}, t_{AA3zz} = V'_{pp\pi}, \\ t_{AA4zz} = V'_{pp\pi}, t_{AA5zz} = V'_{pp\pi}, t_{AA6zz} = V'_{pp\pi}. \\ \text{The NNN hopping integrals in sublattice } B \text{ can be obtained by replacing the index } A \text{ with } B \text{ in the above equations.} \end{cases}$ 



Fig. S 2: (Color online) Band structures of **silicene** (a) without SOC and (b) with SOC. The blue and red curves correspond to the first-principles and tight-binding calculations, respectively.



Fig. S 3: (Color online) Band structures of **germanene** (a) without SOC and (b) with SOC. The blue and red curves correspond to the first-principles and tight-binding calculations, respectively.



Fig. S 4: (Color online) Band structures of **stanene** (a) without SOC and (b) with SOC. The blue and red curves correspond to the first-principles and tight-binding calculations, respectively.



Fig. S 5: (Color online) Band structures of **plumbene** (a) without SOC and (b) with SOC [1]. The blue and red curves correspond to the first-principles and tight-binding calculations, respectively.



Fig. S 6: (Color online) Band structures of **stanene** with SOC strength  $\xi_0 =$  (a) 0.28, (b) 0.67, and (c) 1.0 eV. With increasing SOC strength, the gap at the  $\Gamma$  point closes and then reopens.  $\xi_0 = 0.67$  eV is the critical point between topologically nontrivial and trivial phases.



Fig. S 7: (Color online) The evolution lines of Wannier function centers for **stanene** with SOC strength  $\xi_0 = 1.0$  eV. The green dashed line is the reference line. As the reference line is moved up or down, it always crosses the evolution lines zero or two (even) times, indicating that stanene with this SOC strength is a normal insulator.



Fig. S 8: (Color online) Band structures of **graphene** without SOC. The line thickness represents the weight of (a) s, (b)  $p_x + p_y$ , and (c)  $p_z$  character.



Fig. S 9: (Color online) Band structures of **graphene** with SOC. The line thickness represents the weight of (a) s, (b)  $p_x + p_y$ , and (c)  $p_z$  character.



Fig. S 10: (Color online) Band structures of **silicene** without SOC. The line thickness represents the weight of (a) s, (b)  $p_x + p_y$ , and (c)  $p_z$  character.

![](_page_9_Figure_2.jpeg)

Fig. S 11: (Color online) Band structures of **silicene** with SOC. The line thickness represents the weight of (a) s, (b)  $p_x + p_y$ , and (c)  $p_z$  character.

![](_page_10_Figure_0.jpeg)

Fig. S 12: (Color online) Band structures of **germanene** without SOC. The line thickness represents the weight of (a) s, (b)  $p_x + p_y$ , and (c)  $p_z$  character.

![](_page_10_Figure_2.jpeg)

Fig. S 13: (Color online) Band structures of **germanene** with SOC. The line thickness represents the weight of (a) s, (b)  $p_x + p_y$ , and (c)  $p_z$  character.

![](_page_11_Figure_0.jpeg)

Fig. S 14: (Color online) Band structures of **stanene** without SOC. The line thickness represents the weight of (a) s, (b)  $p_x + p_y$ , and (c)  $p_z$  character.

![](_page_11_Figure_2.jpeg)

Fig. S 15: (Color online) Band structures of **stanene** with SOC. The line thickness represents the weight of (a) s, (b)  $p_x + p_y$ , and (c)  $p_z$  character.

![](_page_12_Figure_0.jpeg)

Fig. S 16: (Color online) Band structures of **plumbene** without SOC. The line thickness represents the weight of (a) s, (b)  $p_x + p_y$ , and (c)  $p_z$  character.

![](_page_12_Figure_2.jpeg)

Fig. S 17: (Color online) Band structures of **plumbene** with SOC. The line thickness represents the weight of (a) s, (b)  $p_x + p_y$ , and (c)  $p_z$  character.

![](_page_13_Figure_0.jpeg)

Fig. S 18: (Color online) Band structures of **stanene** with hydrostatic strains  $\Delta_{hs} = 5\%$  (a–c), 10% (d–f), and 15% (g–i).  $\Delta_{hs}$  is defined as  $\Delta_{hs} = (a-a_0)/a_0 \times 100\%$ . The line thickness represents the weight of s,  $p_x + p_y$ , and  $p_z$  character, and SOC is considered.

We have studied the electronic structures of stanene and plumbene under hydrostatic strain. When stanene is stretched under large enough strain, the  $s^-$  state at the  $\Gamma$  point drops below the p states owing to the larger bond length. For example, in Figs. S 15 and S 18, when the hydrostatic strain is increased to 15% from 0%, the  $s^-$  state drops below -4.0 eV from 0.3 eV at the  $\Gamma$  point. However, from the topological state, the system does not become a normal insulator, but instead becomes a metal. This is because several bands cross the Fermi level. Similarly, for plumbene, a band inversion between the  $s^-$  and p states can appear at the  $\Gamma$  point under large enough compressive strain (Figs. S 17 and S 19), but it will also enter a metallic phase.

## Band structures and edge states obtained from an effective four-band model

An effective tight-binding model is employed to study the global properties of graphene, silicene, germanene, and stanene, which are all topological insulators (plumbene is a normal band insulator[1–3]). By diagonalizing the model Hamiltonian (Eq. (12) of the main text), we can obtain the band structure, as shown in Fig. S 22 (a). With increasing effective SOC strength  $\lambda_{\text{eff}}$ , the gap widens in a linear manner. The effective model captures the key features of these 2D group IVA materials near the Fermi level[4–7]. For example, there is a Dirac cone at the K point without SOC; when SOC is considered, an energy gap is opened, leading to a conduction-band valley at the K point[8].

2D topological insulators are characterized by topologically protected metallic edge states with helical spin polarization residing inside the bulk gap. In order to confirm this point in the effective model, we have investigated a zigzag nanoribbon. Figure S 22 (b) shows the band structure of the nanoribbon with a width  $N_y = 50$  and  $\lambda_{\text{eff}} = 0.01$ . From a comparison with the bulk band structure, one can see that two bands cross the bulk gap. We further choose two points on the two bands to perform a spatial and spin weight analysis  $(k_x = 2.806, E = -0.02 \text{ and } k_x = 3.477, E = -0.02)$ . From Fig. S 22 (c), we can see that the two bands are completely contributed by the edge states. The band with a positive slope is contributed mainly by the spin-up states at the  $n_y = 1$  edge and the spin-down states at the  $n_y = 50$  edge; the band with a negative slope is contributed mainly by the spin-down states at the  $n_y = 1$  edge and the spin-up states at the  $n_y = 50$  edge (the spin direction is perpendicular to the plane of the 2D material). Therefore, this effective model can be used to describe the topological characteristics of the 2D group IVA materials.

![](_page_15_Figure_0.jpeg)

Fig. S 19: (Color online) Band structures of **plumbene** with hydrostatic strains  $\Delta_{hs} = -5\%$  (a-c), -10% (d-f) and -15% (g-i). The line thickness represents the weights of s,  $p_x + p_y$ , and  $p_z$  character and SOC is considered.

![](_page_16_Figure_0.jpeg)

Fig. S 20: (Color online) Band structures and spin polarizations of (a, b) silicene with  $E_z = 0.002$  eV/Å and  $B_z = 0.00035$  eV, (c, d) germanene with  $E_z = 0.02$  eV/Å and  $B_z = 0.0065$  eV, and (e, f) stanene with  $E_z = 0.5$  eV/Å and  $B_z = 0.053$  eV.  $P_{\uparrow/\downarrow}^0$  and  $R_p$  are defined as the spin polarizations on the sides of the Fermi level and the energy range of spin polarization, respectively. To facilitate comparison with Fig. 6 of the main text, the first two cases and the last one are chosen to be in the critical phases C1 and C2, respectively. These results are based on the 16-band tight-binding model.

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![](_page_17_Figure_0.jpeg)

Fig. S 21: (Color online)  $B_z$ ,  $R_p$ ,  $P^0_{\uparrow}$ , and  $P^0_{\downarrow}$  as functions of  $E_z$  in the critical phases C1 (pink) and C2 (yellow) for (a) silicene, (b) germanene, and (c) stanene.  $R_p$  and  $P^0_{\uparrow/\downarrow}$  are defined in Fig. S 20. C1 and C2 are illustrated in the phase diagram (Fig. 5 of the main text). Both  $B_z$  and  $R_p$  exhibit nearly linear behavior in the two phases.  $P^0_{\uparrow}$  is smaller in the C2 phase than in the C1 phase. In particular, for stanene, when  $E_z = 0.5 \text{ eV}/\text{Å}$ ,  $P^0_{\uparrow}$  falls to 91.3%. Conversely,  $|P^0_{\downarrow}|$  is larger in the C2 phase than in the C1 phase. At the critical point between the two phases, the system is not spin-polarized with  $B_z = 0$ , leading to  $P^0_{\uparrow} = P^0_{\downarrow} = 0$ , which is not marked in the figures. These results are based on the 16-band tight-binding model.

![](_page_17_Figure_2.jpeg)

Fig. S 22: (Color online) Electronic structures obtained from the four-band tight-binding model. (a) The bulk band structure with  $\lambda_{eff} = 0.01$ . The inset shows the energy gap as a function of  $\lambda_{eff}$ . (b) The band structure of the zigzag nanoribbon with a width  $N_y = 50$  and  $\lambda_{eff} = 0.01$ . (c) Spin-resolved spatial weight distributions along the y direction of the zigzag nanoribbon at  $(k_x = 2.806, E = -0.02)$  and  $(k_x = 3.477, E = -0.02)$ . The two points are marked in (b).

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