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Supplementary Materials for

Quantum spin Hall insulator with a large bandgap, Dirac fermions, and bilayer graphene analog

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This PDF file includes:

- Supplementary Text
- fig. S1. Comparison between calculations within the eight-band Kane model and by using the effective Hamiltonians for three-layer InAs/GaSb QWs.
- fig. S2. Bandgap in QSHI state in asymmetrical three-layer InAs/GaInSb QWs.
- table S1. Parameters involved in the effective Hamiltonian $H_{\mathrm{InAs}}(k_x, k_y)$ for three-layer InAs/GaSb QWs with InAs geometry grown on GaSb buffer.
- table S2. Parameters of the effective 2D Hamiltonian $H_{\mathrm{GaSb}}(k_x, k_y)$ for three-layer InAs/GaSb QWs with GaSb geometry grown on GaSb buffer.

Supplementary Text

Figures S1A and S1B provide a comparison of the bulk electronic subbands, calculated within the 8-band Kane model and 2D effective Hamiltonians $H_{InAs}(k_x, k_y)$ and $H_{GaSb}(k_x, k_y)$ with the parameters, corresponding to the crossing of $E1$ and $H1$ subbands, shown in Fig. 1B and 3B in the main text. The parameters for $H_{InAs}(k_x, k_y)$ and $H_{GaSb}(k_x, k_y)$ at different thicknesses of InAs d_1 and GaSb d_2 layers are given in tables S1 and S2 respectively. One can see good agreement between results from both models at small quasimomentum values. Comparisons of the calculation within two approaches for trivial band insulator, quantum spin Hall insulator and “bilayer graphene” phases look qualitatively the same.

In the main text, we consider the evolution of the inverted bandgap in the symmetrical the three-layer QWs with two InAs layers of the same width. Figure S2 shows the bandgap in QSHI state in asymmetrical InAs/$Ga_{0.6}In_{0.4}Sb$ QW grown on $Ga_{0.68}In_{0.32}Sb$ buffer as a function of the thicknesses difference δ between two the InAs layers with d_2 = 11 ML at different d_1 values. By comparing the calculated dependences with the blue curve in Fig. 6A in the main text, which describes the bandgap evolution with changing of d_1 for $\delta = 0$, one can see that the maximum values of the inverted bandgap in three-layer InAs/GaInSb QWs can be achieved in symmetrical geometry only.

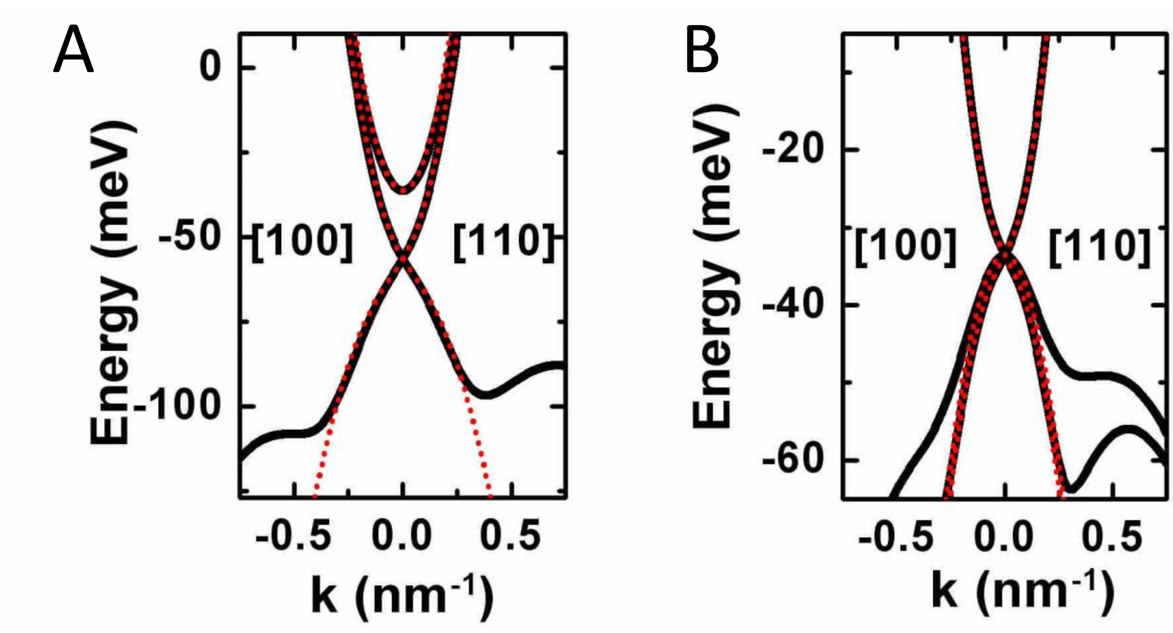

fig. S1. Comparison between calculations within the eight-band Kane model and by using the effective Hamiltonians for three-layer InAs/GaSb QWs. (**A**,**B**) Comparison between calculations within the 8-band Kane model (black solid curves) and by using the effective Hamiltonians (red dotted curves) for three-layer InAs/GaSb QWs with (A) InAs-geometry and (B) GaSb-geometry at the layer thicknesses, corresponding to the crossing of *E*1 and *H*1 subbands shown in Fig. 1B and 3B in the main text. The band parameters, used in the calculations, are given in tables S1 and S2.

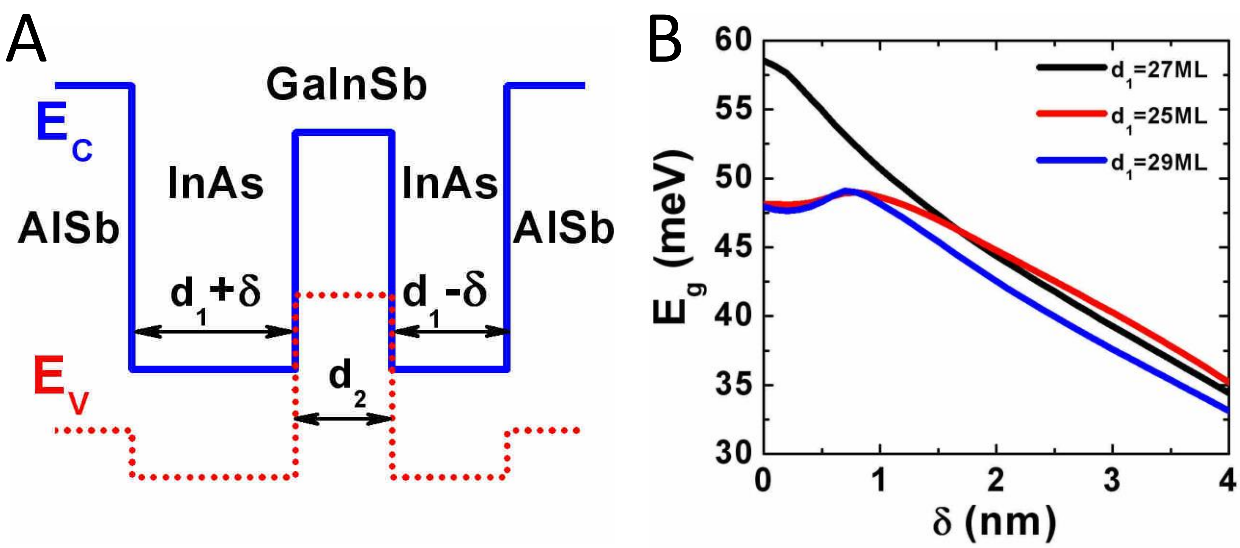

fig. S2. Bandgap in QSHI state in asymmetrical three-layer InAs/GaInSb QWs. (**A**) Schematic representation of asymmetrical three-layer InAs/GaInSb QWs with InAs-geometry. (**B**) A bandgap in QSHI state as a function of δ for the InAs/$Ga_{0.6}In_{0.4}Sb$ QWs with different values of d_1 and d_2 = 11 ML grown on $Ga_{0.68}In_{0.32}Sb$ buffer. A 3D plot of the band dispersion for the case of d_1 = 27 ML and δ = 0 is shown in Fig. 6C in the main text.

table S1. Parameters involved in the effective Hamiltonian $H_{InAs}(k_x, k_y)$ for three-layer InAs/GaSb QWs with InAs geometry grown on GaSb buffer. The thicknesses of InAs and GaSb layers for trivial band insulator (BI) and quantum spin Hall insulator (QSHI) states are also presented by open blue symbols in Fig. 1C in the main text.

	d_1, nm	d_2, nm	C, meV	Δ_{E1E2}, meV	M, meV	A, meV·nm
Band insulator	7.63	4.27	–32.74	14.58	18.17	88.23
Dirac cone	9.64	4.00	–56.40	20.25	0	108.79
QSHI	11.6	4.27	–60.69	70.40	–9.76	95.67

	R, meV·nm^2	S, meV·nm	B_{E1}, meV·nm^2	B_{H1}, meV·nm^2	B_{E2} meV·nm^2
Band insulator	22.84	37.08	1046.44	–837.68	740.55
Dirac cone	19.93	33.04	1084.26	–383.26	860.50
QSHI	19.55	30.21	924.04	–317.38	875.29

table S2. Parameters of the effective 2D Hamiltonian $H_{GaSb}(k_x, k_y)$ for three-layer InAs/GaSb QWs with GaSb geometry grown on GaSb buffer. The thicknesses of InAs and GaSb layers for BI and bilayer graphene (BG) states are also presented by open blue symbols in Fig. 3C in the main text.

	d_1, nm	d_2, nm	C, meV	M, meV	A, meV·nm
Band insulator	9.15	6.10	-22.55	4.49	61.64
Dirac cone	10.00	5.33	–33.54	0	55.17
BG state	9.76	6.41	–26.21	–1.24	52.18

	R, meV·nm^2	B_{E1}, meV·nm^2	B_{H1}, meV·nm^2	B_{H2}, meV·nm^2
Band insulator	66.09	735.98	–517.44	–345.32
Dirac cone	68.22	681.41	–440.51	–425.56
BG state	66.72	– 231.01	659.25	–380.06