Supplementary Information

New Topological States in HgTe Quantum Wells from Defect Patterning

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(1) The band structures of the HgTe QW ribbon with two flat boundaries and a row of hexagonal holes.

In Figure S1, we construct an HgTe QW nanoribbon with the width of 57*a*, where *a* is lattice constant and adopted as 5 nm. This ribbon configuration has two flat boundaries and a row of hexagonal holes near to the upside edge of the QW ribbon. The numerical results show that in this model only as $M < 0$, i.e., the QW thickness d is larger than the critical value d_c which denotes the occurrence of the band inversion, the Dirac cone appears as shown in Figures (e)~(h).

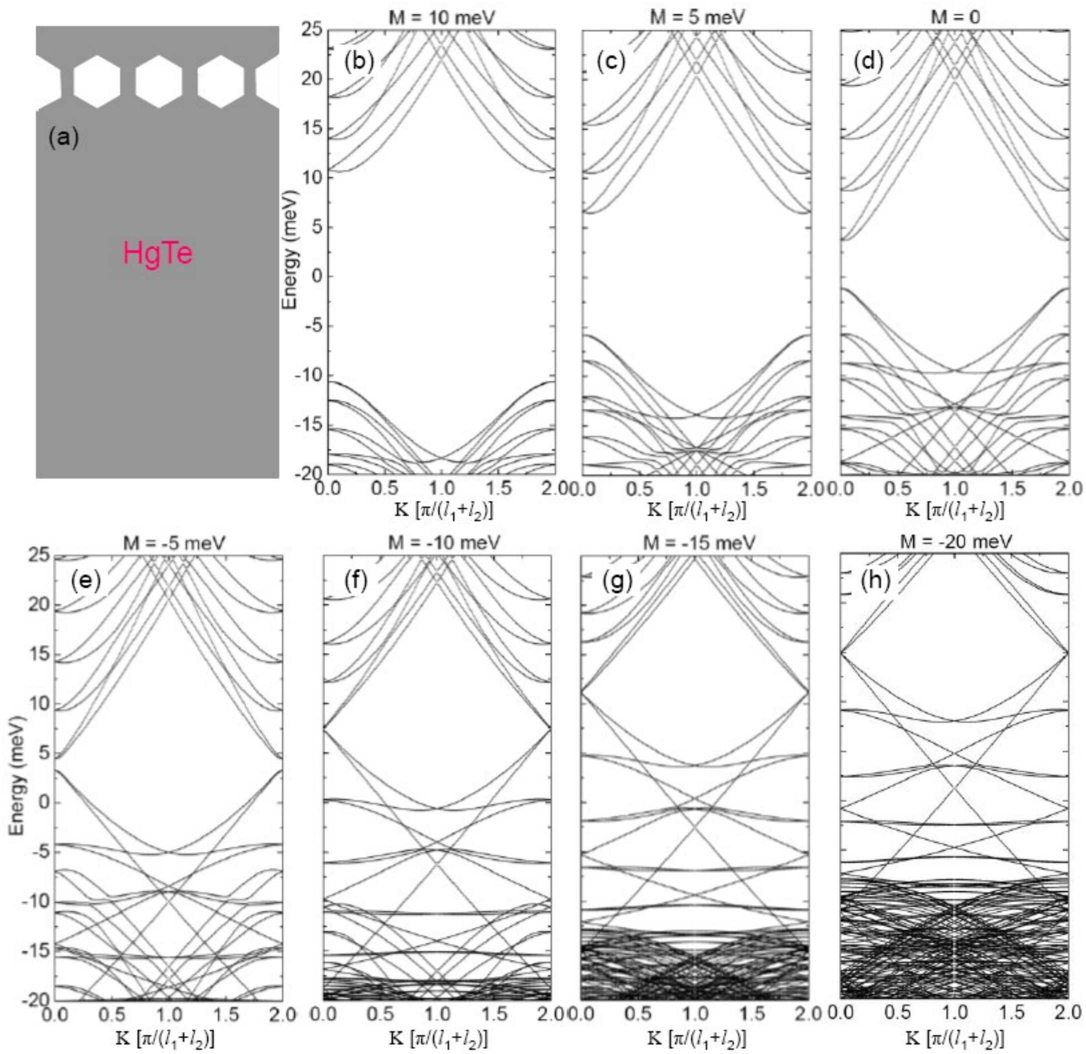

Figure S1. (a) The model configuration of the HgTe QW ribbon with two flat boundaries and a row of hexagonal holes (upside). (b)-(h) The related band structures of the ribbon versus decreasing *M* from 10 to -20 meV. The width of every hexagonal hole is set as 6*a* (= 30 nm), and the distance between two nearest holes is set as 4*a* (= 20 nm).

(2) The band structures of Model 3 with the further increasing of HgTe QW thickness.

In Figure S2, we provide some additional numerical calculations on the band structures of Model 3 drawn in Figure 1c, in which the structure parameter M is decreased from -20 to -35 meV. It clearly shows that the formation of a new Dirac cone with the increasing of the QW thickness, since some bands highlighted by the red dash elliptical circles become more and more linear. Note that the all structural parameters are adopted as the same as those in the main article.

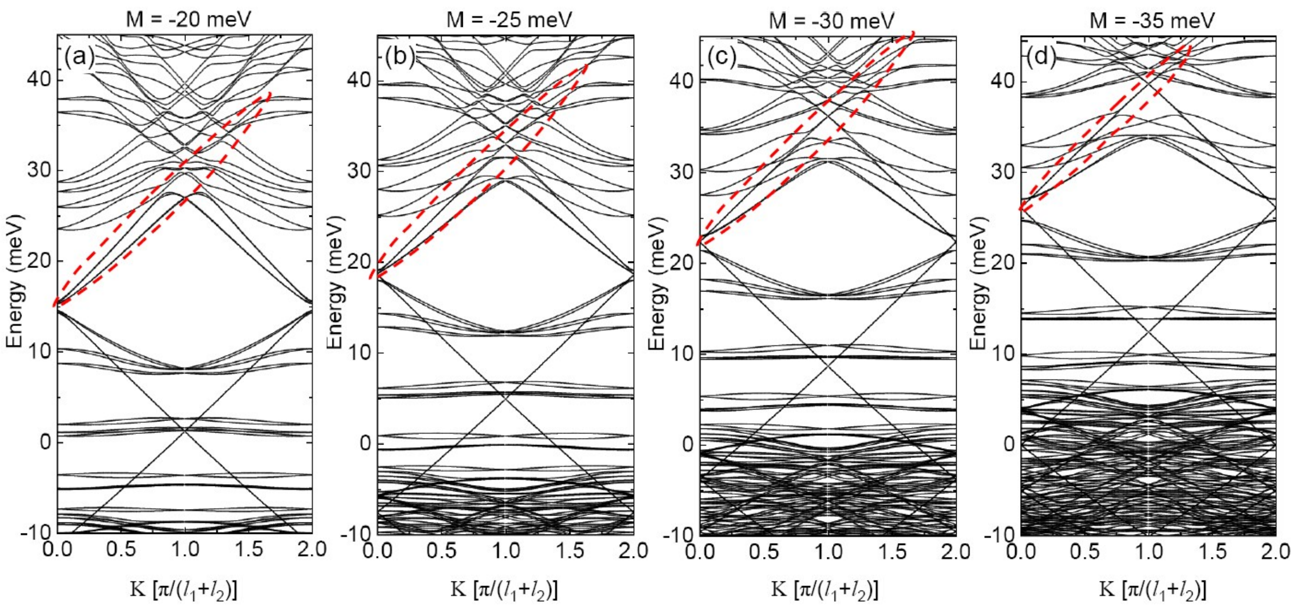

Figure S2. (a)-(d) The band structures of Model 3 as drawn in Figure 1c, where only three rows of holes are dug in the HgTe QW ribbon and the structural parameter M is increased from -20 to -35 meV. The QW width W is 57a (= 285 nm) and the distance between the upside ribbon boundary and the nearest row of holes W_c is 15a (= 75 nm).

(3) Transition from the flat bands to the Dirac bands.

Here, we construct Model 4 in which an HgTe QW nanoribbon with only one role of holes to show the formation of the topological edge states around the holes. The ribbon model is drawn in the inset of Figure S3a, where a row of holes are localized near to the upside boundary of the HgTe QW ribbon. The distance between two boundaries of the nearest holes is set as l_2, and the structure parameter M is set as -20 meV. The numerical results show that as l_2 is decreased, a new Dirac cone appears in the band structures and the new topological edge states appear in the boundaries of the row of the holes.

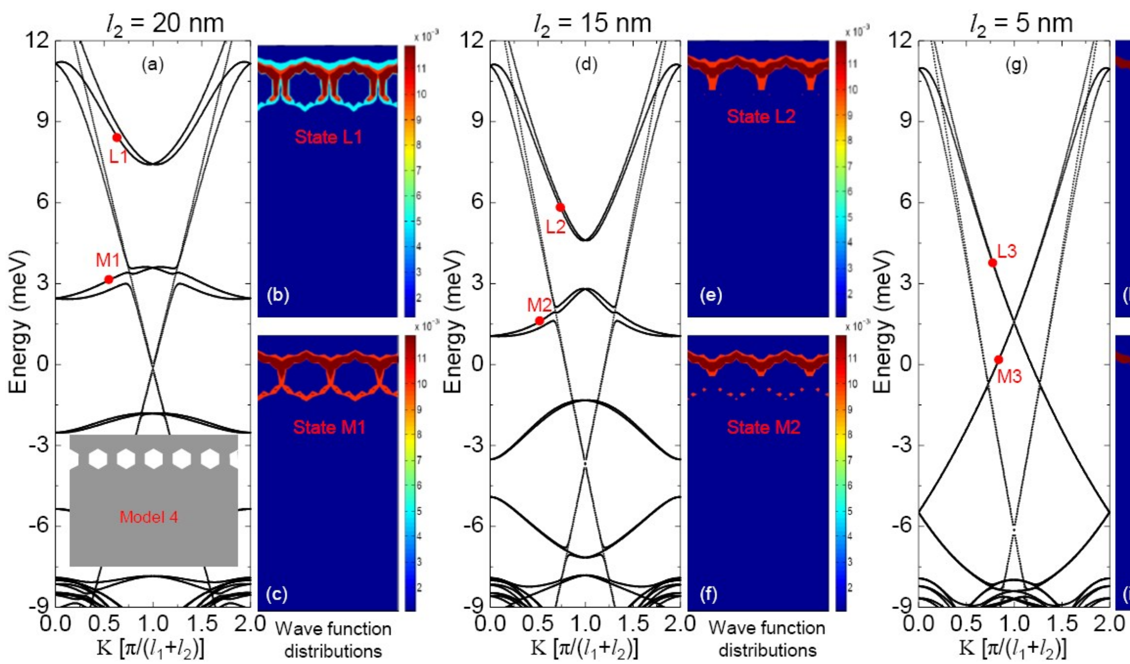

Figure S3. (a), (d) and (g) The band structures of Model 4 (see the inset of Figure a) as the distance between two boundaries of the nearest holes, l_2, is set as 20, 15 and 5 nm. The states **L1-M3** are six states are chosen in the bands as plotted in the figures. In the right panels of each figure, the wave function distributions of these states are drawn along the ribbon direction, where three repeating units are adopted and the parameter M is set as -20 meV. It is clearly shown that the states in the nearly flat bands are related to the circulating edge states (CESs) around the holes. As the distance of two nearest CESs is decreased, CESs will couple with each other, and the flat bands are converted gradually into the Dirac ones.