Supporting Information for

Robust 2D Topological Insulators in van der Waals Heterostructures

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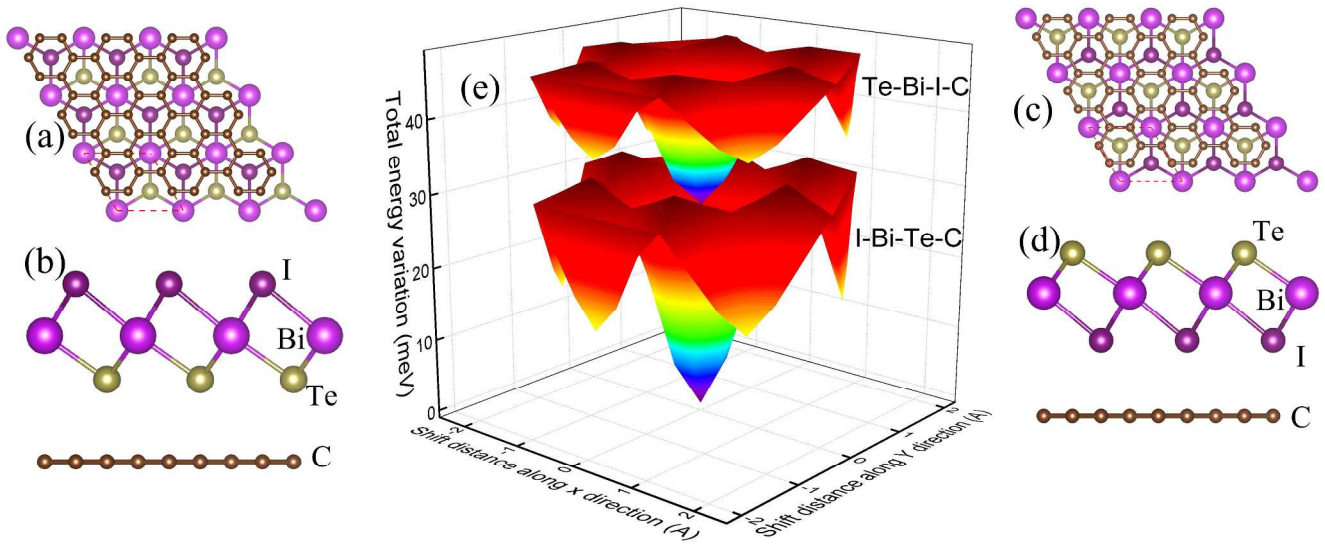

Figure S1. (a, c) Top view and (b, d) side view of the QW structural models with the I-Bi-Te-C and Te-Bi-I-C stacking sequence, respectively. The atom (Te or I) adjacent to the graphene layer is located at the carbon hexagon center in the initial stacking pattern, see (a) and (c). When shifting the graphene layer relative to the BiTeI layer, the total energy variation as a function of the shifted distance is displayed in (e). The total energy of the I-Bi-Te-C model with Te at the carbon hexagon center is set to zero as the reference point. It is clear that the I-Bi-Te-C configuration is more stable than the Te-Bi-I-C one, while in either case the configuration with the atom that is adjacent to the grapheme layer located at the carbon hexagon center is the most stable.

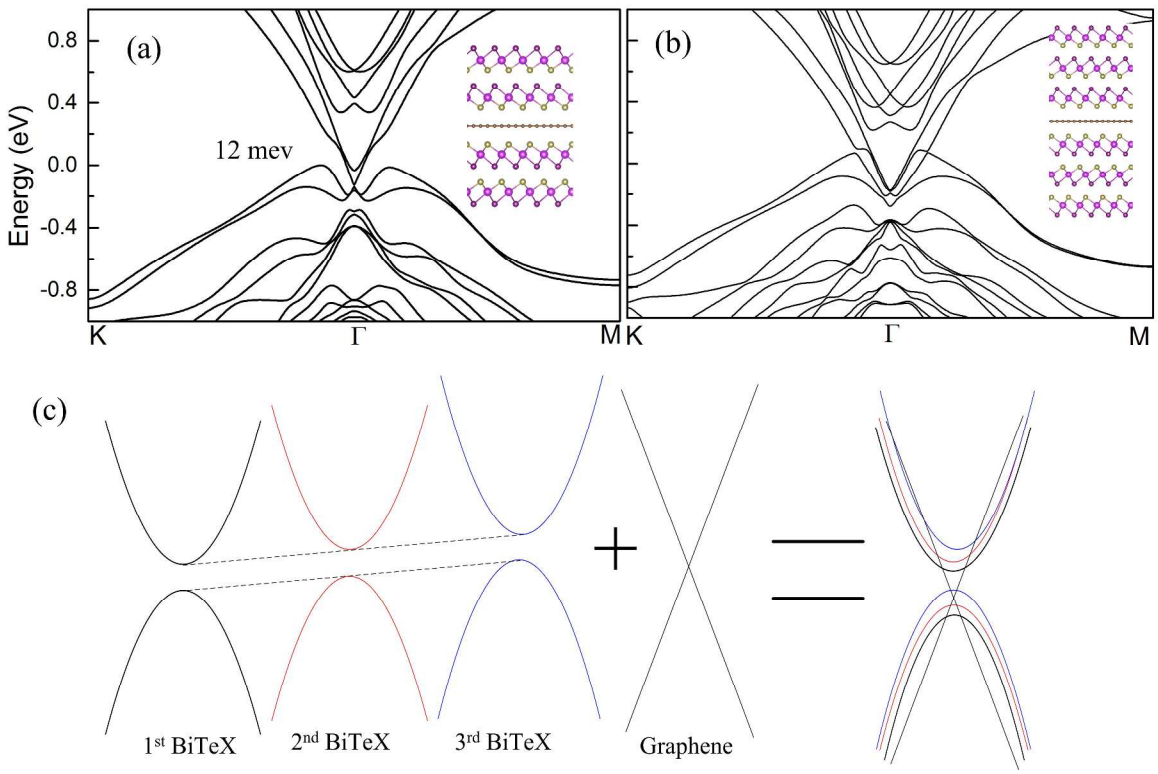

Figure S2. Electronic band structures of the BiTeI/Graph QW with (a) double and (b) triple cladding layers. The structural models are shown as insets. With the double cladding layer, the gap at the Γ point is preserved (12 meV) although part of the valance states away from the Γ point is raised into the conduction band region. A Z_2 index check indicates that the structure is still a 2D TI. When an additional BiTeI layer is added, the topological feature is broken. An illustration of the mechanism of the layer dependence of band topology in the BiTeI/Graph QW is shown in (c). Due to the intrinsic dipole moments in BiTeI, both the valance and conduction bands of each additional BiTeI layer are shifted upwards. When graphene is sandwiched between multilayers of BiTeI, the valance bands will gradually move into the conduction band region of graphene as the number of the cladding layers of BiTeI increases.

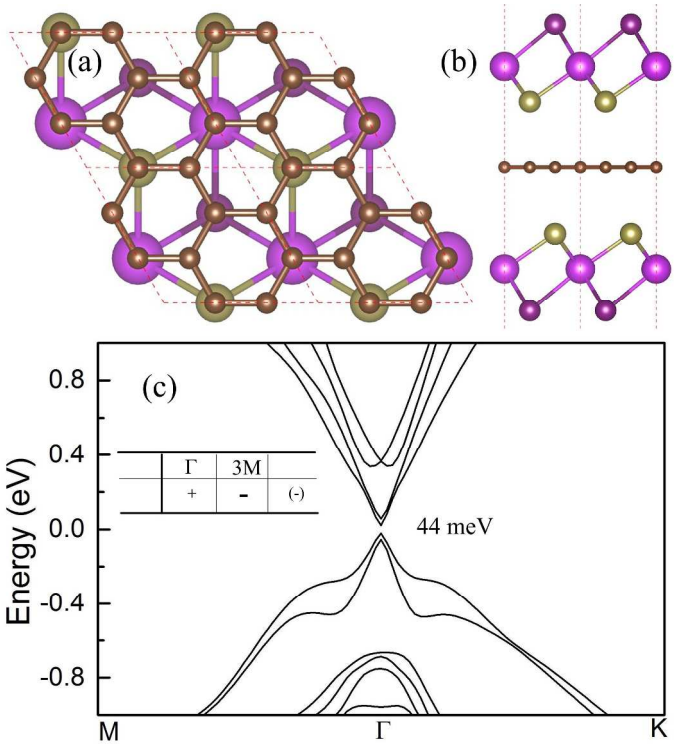

Figure S3. The top view (a) and side view (b) of BiTeI/Graphene/BiTeI with Te atom on top of carbon atoms. The corresponding bandstructure is shown in (c).

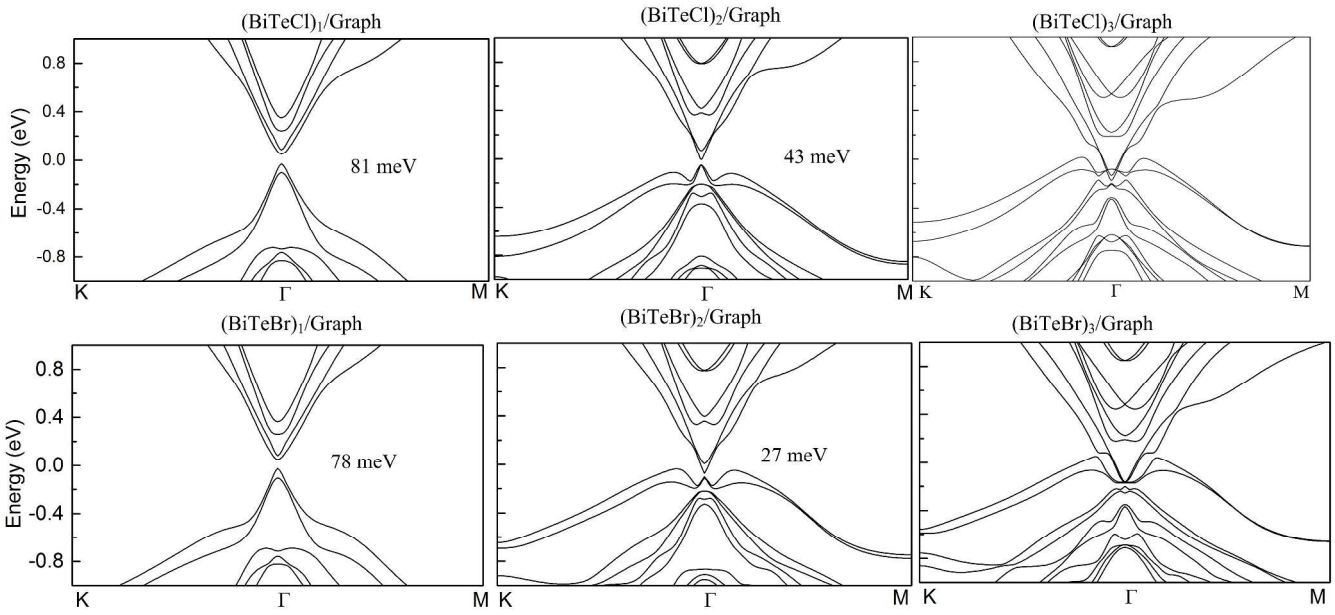

Figure S4. Electronic band structures of BiTeCl/Graph QWs (upper panels) and BiTeBr/Graph QWs (lower panels). The subscript in $(BiTeX)_n$/Graph indicates the number of the cladding layers.