Supporting Information

Quantum Spin-quantum Anomalous Hall Insulators and Topological Transitions in Functionalized Sb(111) Monolayers

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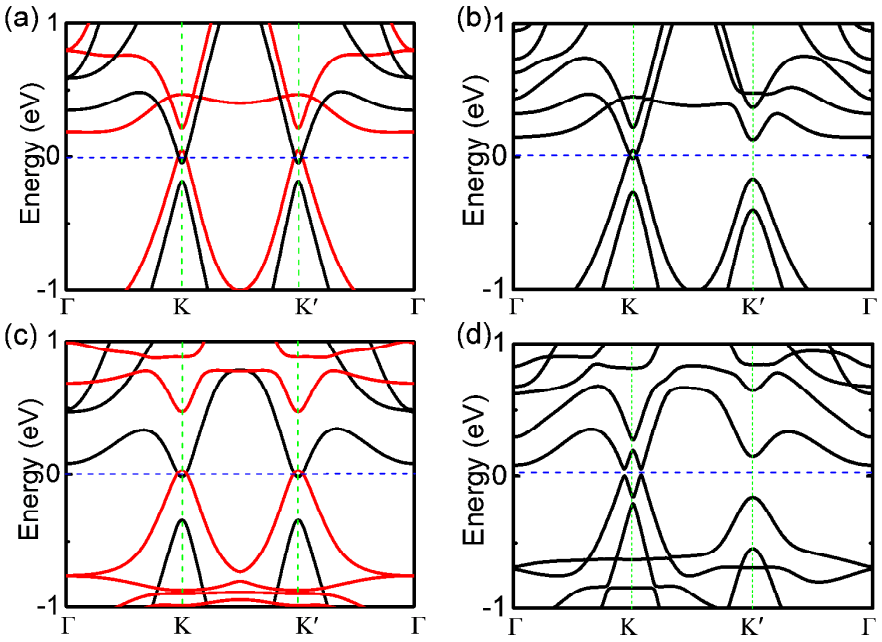

Figure S1. (a) and (b) Band structures for the 1×1 unit cell of Cr@SbH with a 5% tensile strain applied, without and with SOC considered, respectively. The red and black curves denote the spin-up and spin-down states, respectively. (c) and (d) are the same as (a) and (b) except for W@SbH.

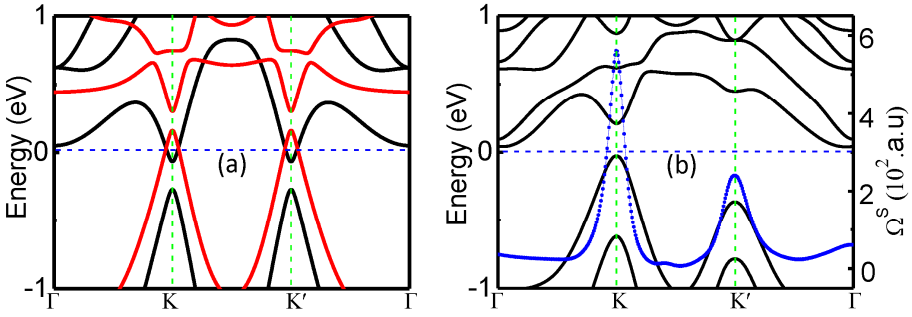

Figure S2. (a) and (b) Band structures for the 1×1 unit cell of Mo@BiH without and with SOC, respectively. The red and black curves in (a) denote the spin-up and spin-down states, respectively. The blue dots in (b) denote the spin Berry curvatures for the whole valence bands. Chern number and spin Chern number of the system are 0 and ~1, respectively.

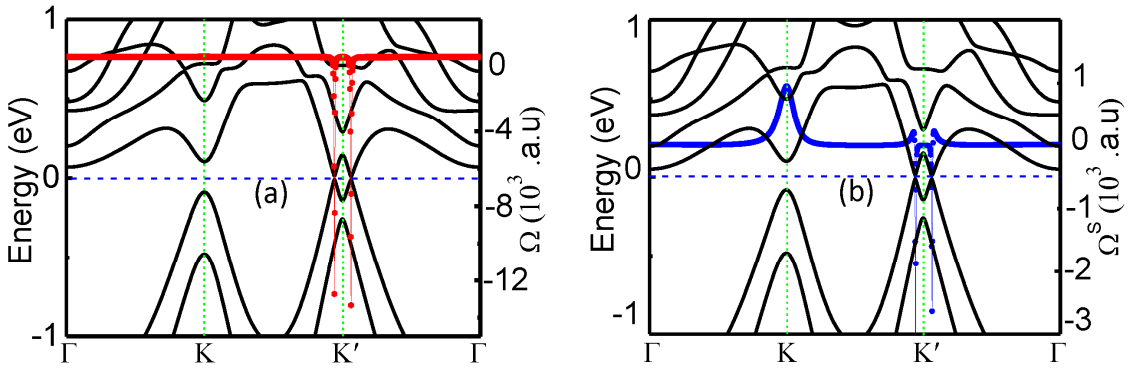

Figure S3. (a) and (b) Band structures (black solid curves) for the SbH sheet with one Mo atom deposited on Sb_A atom in the 1×1 unit cell with a 3% tensile strain. The red dots in (a) and blue dots in (b) denote the Berry curvatures and spin Berry curvatures for the whole valence bands, respectively.

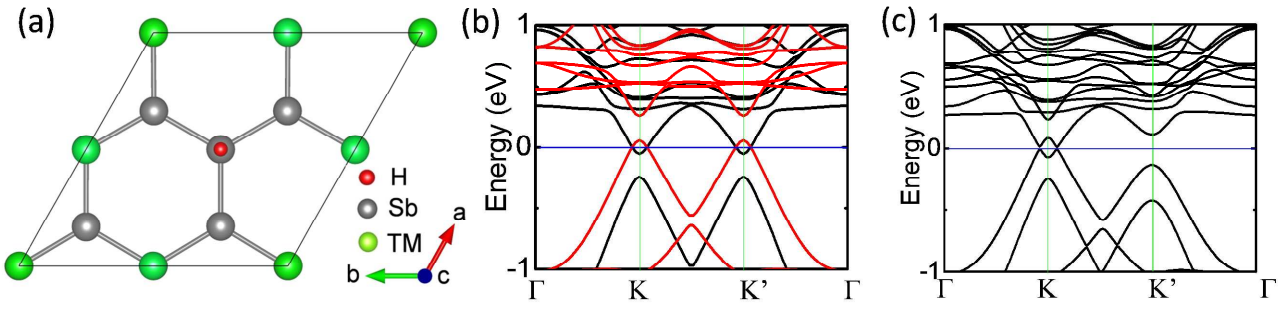

Figure S4. (a) The atomic structure of Mo@SbH with a defect (one missing Mo atom) in a 2×2 supercell (the defect concentration is 25%). (b) and (c) Band structures for the Mo@SbH with a defect in a 2×2 supercell without and with SOC, respectively. The red and black curves in (b) denote the spin-up and spin-down states, respectively. The obtained bands without and with SOC indicate that the QSQAH state remains intact, consistent with the results obtained from the SbH sheet with one Mo atom doped in the 2×2 unit cell. The QSQAH state is robust despite the defects with certain concentrations.

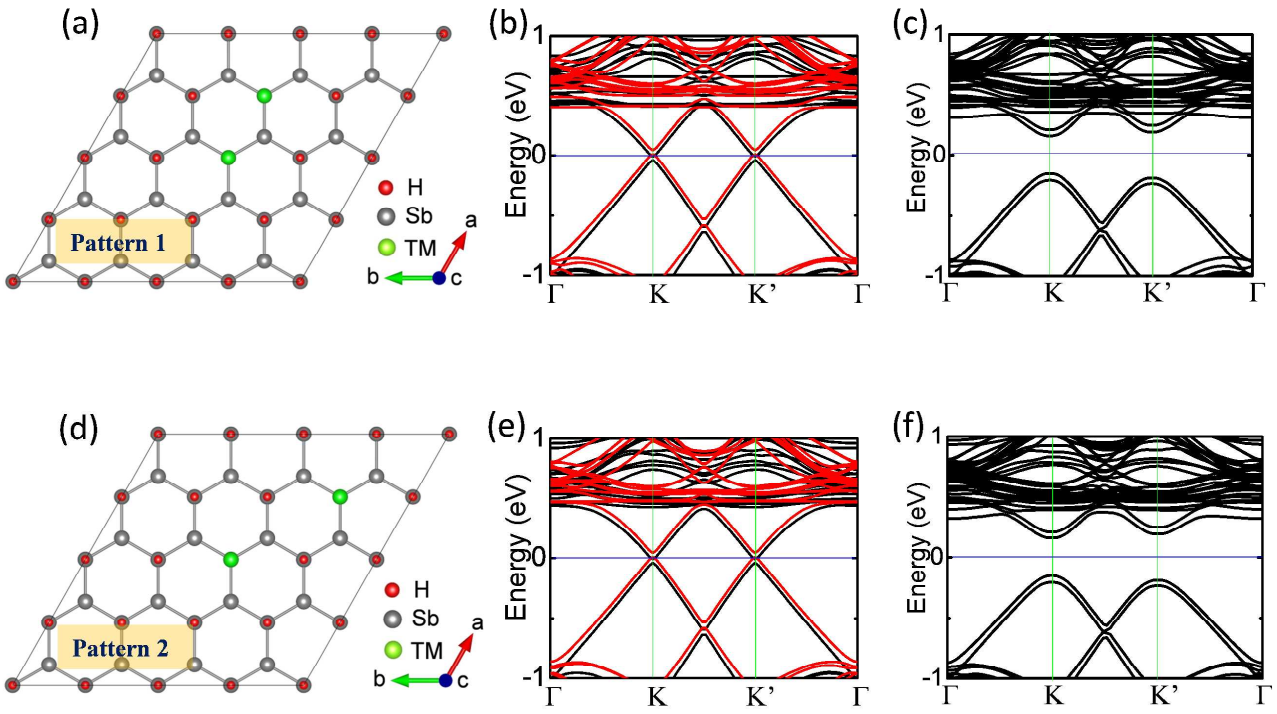

Figure S5. (a) The atomic structure for Mo@SbH with two Mo atoms in Pattern 1 configuration in a 4 ×4 supercell. (b) and (c) The corresponding band structures for the system without and with SOC, respectively. The red and black curves in (b) denote the spin-up and spin-down states, respectively. (d), (e), and (f) are the same as in (a), (b), and (c), respectively, except for Mo@SbH with two Mo atoms in Pattern 2 configuration. The calculations show that the TRSB-QSH state remains intact in the both cases. Moreover, there are no obvious differences in the bands for the two patterns, meaning the randomization of the TM atoms does not affect much the results obtained.