Supplementary Materials for

**Giant Rashba Splitting in One-Dimensional Atomic Tellurium Chains**

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S1.PHONON SPECTRA AND DYNAMICS STABILITY

Figure. S1. The phonon spectra of (a) isolated helical Te chain. (b) mean-23.13%-stretched Te chain. (c) Stable linear Te chain.

To study the dynamics stability of isolated helical Te chain, ab initio molecular dynamics simulations (AIMD) at the evaluated temperature of 300 K are performed, our 10 Ps AIMD calculations (with 1 fs time step), suggest that the equilibrium structure of isolated helical T chain can be hardly changed at room temperature, corresponding to a pronounced dynamic stability: Te-300K.mp4 represents the infinite isolated helical Te chain at 300K in side view.
Figure S2. The band structure of isolated helical Te chain by PBE+SOC (a) and HSE+SOC (b), which exhibits quasi-1D characters and is insensitive to the choice of exchange-correlation functional.

TABLE SI. Band structures parameters of isolated helical Te chain obtained by PBE+SOC functional and HSE+SOC functional.

<table>
<thead>
<tr>
<th>functionals</th>
<th>$E_R$ (eV)</th>
<th>$k_R$ (Å$^{-1}$)</th>
<th>$E_g$ (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PBE+SOC</td>
<td>0.024</td>
<td>0.057</td>
<td>1.528</td>
</tr>
<tr>
<td>HSE+SOC</td>
<td>0.015</td>
<td>0.057</td>
<td>2.343</td>
</tr>
</tbody>
</table>

Figure S3. (a) The stress as a function of tensile for helical Te chain. (b) The change (in percent) of bond length with respect to strain for helical Te chain.

Figure S4. The charge distribution of (a) isolated helical Te chain. (b) mean-23.13%-stretched Te chain. (c) Stable linear Te chain. In this figure, a loss of electrons is indicated in yellow, while electron enrichment is indicated in cyan.
Figure S5. The in-chain potential gradient of (a) isolated helical Te chain. (b) mean-23.13%-stretch Te chain.

Figure S6. (a) Top and (b) side view of the Te chain in 10-5 carbon nanotubes. (c) The band structure of the Te chain in 10-5 carbon nanotubes. (d) Top and (e) side view of the Te chain in 10-5 boron-nitrogen nanotubes. (c) The band structure of the Te chain in 10-5 boron-nitrogen nanotubes.