Supplementary Materials for

Giant Rashba Splitting in One-Dimensional Atomic Tellurium Chains

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S1.PHONON SPECTRA AND DYNAMICS STABILITY

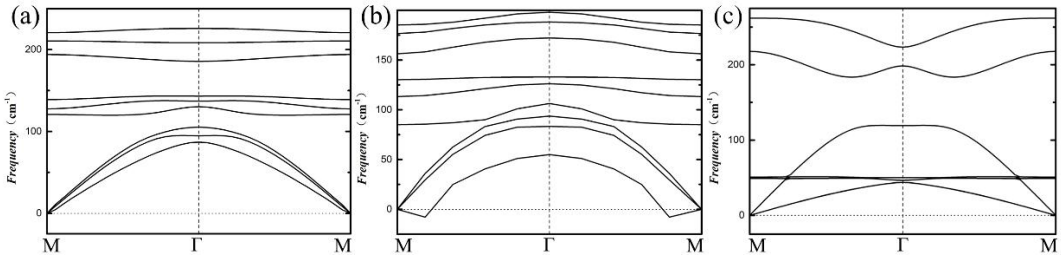

Figure. S1. The phonon spectra of (a) isolated helical Te chain. (b) mean-23.13%-stretched Te chain. (c) Stable linear Te chain.

To study the dynamics stability of isolated helical Te chain, ab inito 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.

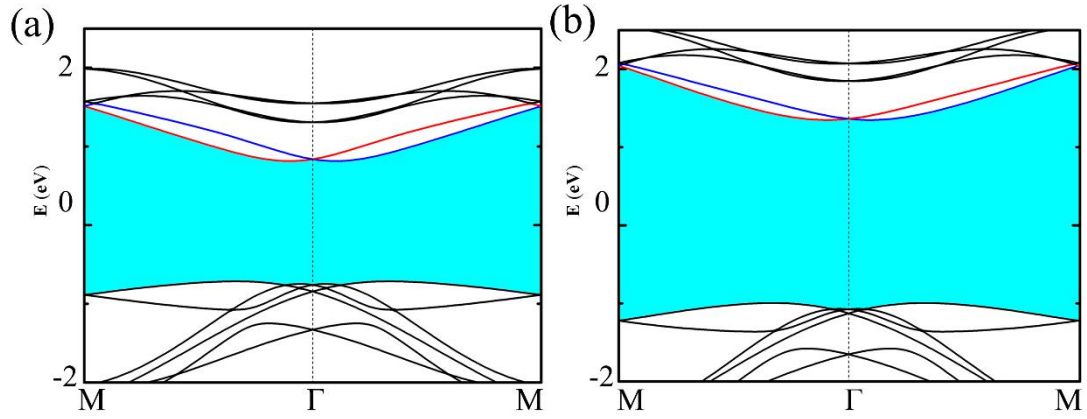

Figure. S2. The band structure of isolated helical Te chain by PBE+SOC (a) and HSE+SOC (b), which exhibits quasi-1D characters and is insensitive to the choice of exchange-correlation functional.

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

functionals	E_R (eV)	k_R (Å^{-1})	E_g (eV)
PBE+SOC	0.024	0.057	1.528
HSE+SOC	0.015	0.057	2.343

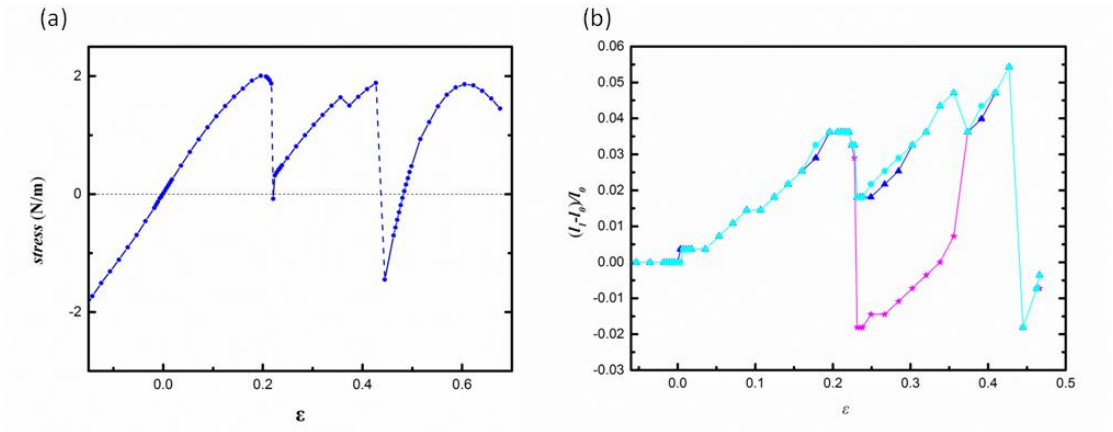

Figure. S3. (a) The stress as a function of tensile for helical Te chain. (b) The change (in percent) of bond length with respect to strain for helical Te chain.

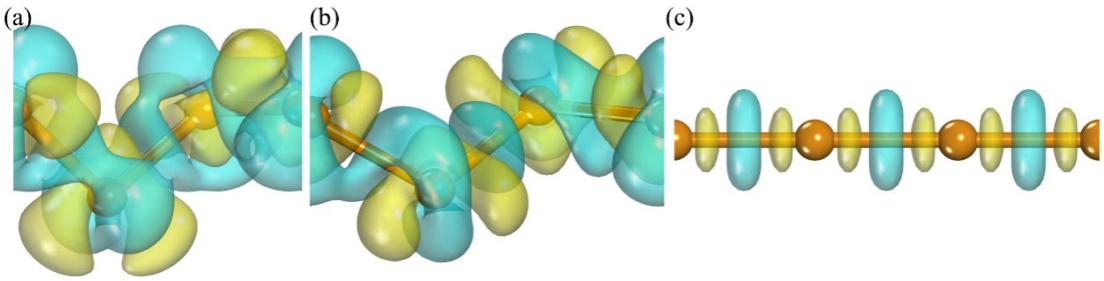

Figure. S4. The charge distribution of (a) isolated helical Te chain. (b) mean-23.13%-stretched Te chain. (c) Stable linear Te chain. In this figure, a loss of electrons is indicated in yellow, while electron enrichment is indicated in cyan.

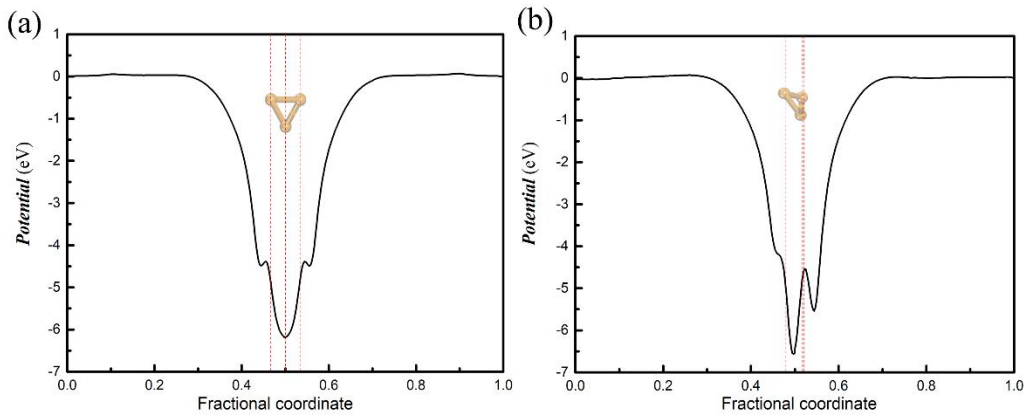

Figure. S5. The in-chain potential gradient of (a) isolated helical Te chain. (b) mean-23.13%-stretche Te chain.

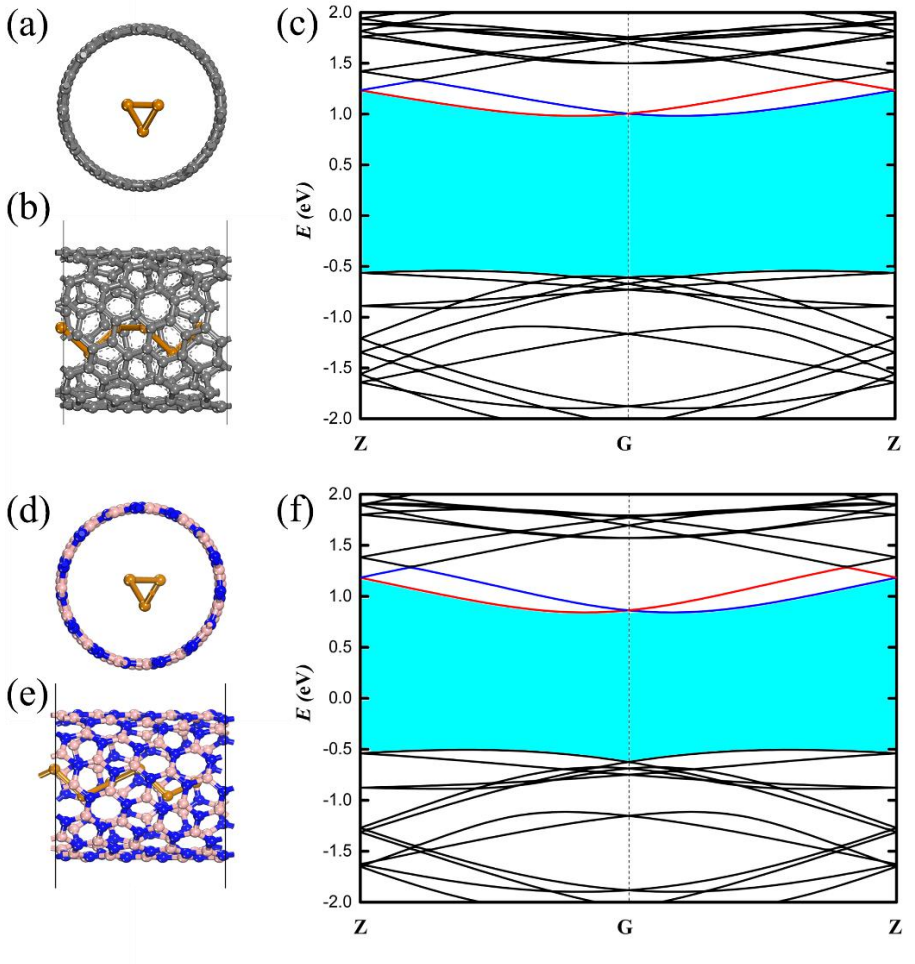

Figure. S6. (a) Top and (b) side view of the Te chain in 10-5 carbon nanotubes. (c) The band structure of the Te chain in 10-5 carbon nanotubes. (d) Top and (e) side view of the Te chain in 10-5 boron-nitrogen nanotubes. (c) The band structure of the Te chain in 10-5 boron-nitrogen nanotubes.