Electronic Supplementary Material (ESI) for Nanoscale.

[Supporting Information]

First Principles Study of 2D Ring-Te and its Electrical Contact with Topological Dirac Semimetal

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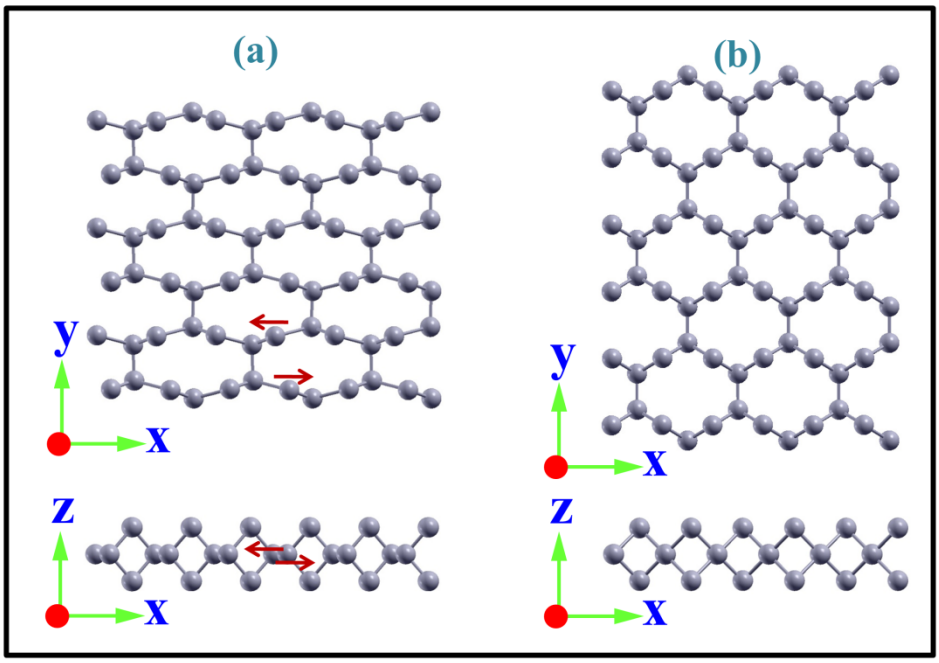

Fig. S1 Top and side views of ring-Te at critical strain of **(a)** 12% (x-direction) and **(b)** 26% (y-direction), respectively.

TABLE S1 The bond angles (Θ_1, Θ_2, Θ_3, Θ_4, Θ_5) and bond lengths (L_1, L_2, L_3) of relaxed and strain structures**.**

Strain	**Θ_1(°)**	**Θ_2(°)**	**Θ_3(°)**	**Θ_4(°)**	**Θ_5(°)**	**L_1(Å)**	**L_2(Å)**	**L_3(Å)**
Relaxed	88.44	88.62	85.32	103.44	91.46	3.02	2.80	3.02
ε_x= 12%	95.05 (7.47%)	71.61 (-19.19%)	91.07 (6.74%)	102.23 (-1.17%)	96.72 (5.75%)	2.82 (-6.62%)	2.77 (-1.07%)	3.56 (17.88%)
ε_y= 26%	80.05 (-9.49%)	81.76 (-7.74%)	79.71 (-6.58%)	114.62 (10.81%)	99.02 (8.27%)	3.07 (1.66%)	2.82 (0.71%)	3.07 (1.66%)

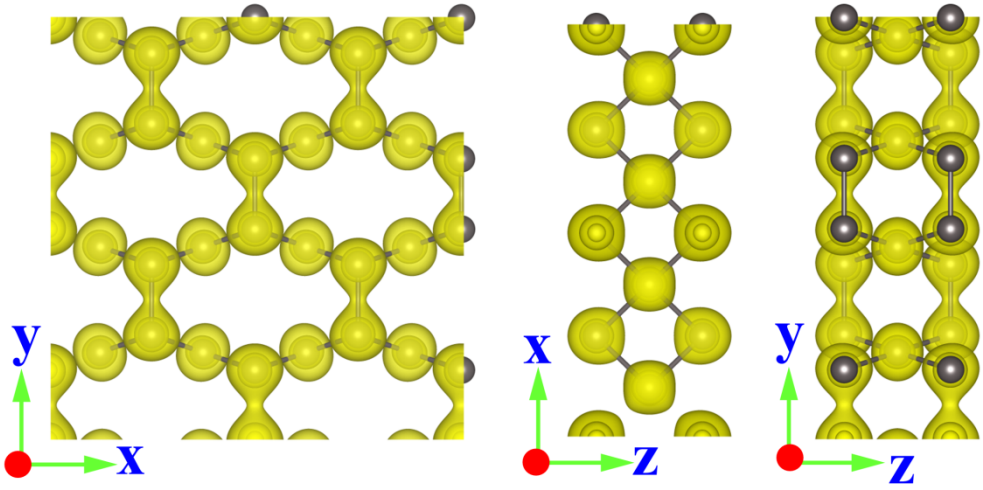

Fig. S2 The total charge density distribution of ring-Te. The isosurface value is 0.05 eÅ^{-3}.

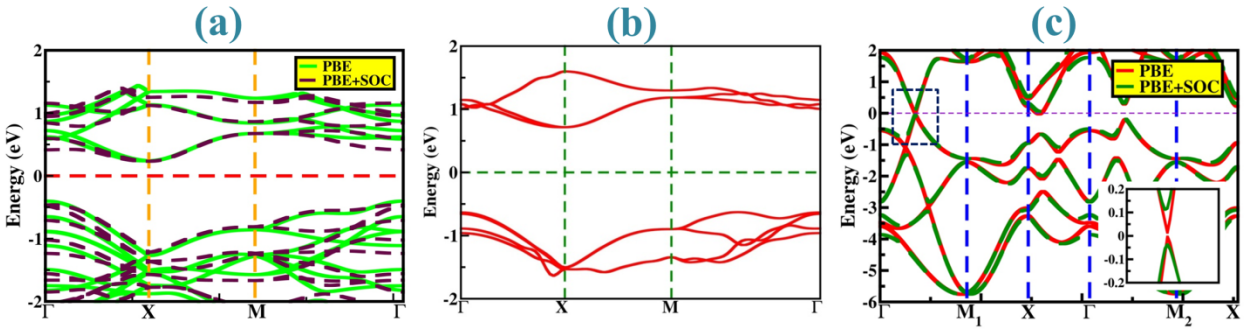

Fig. S3 Electronic band structures of ring-Te: **(a)** with PBE functional, **(b)** with G_0W_0 method and **(c)** sq-Te: with PBE functional.

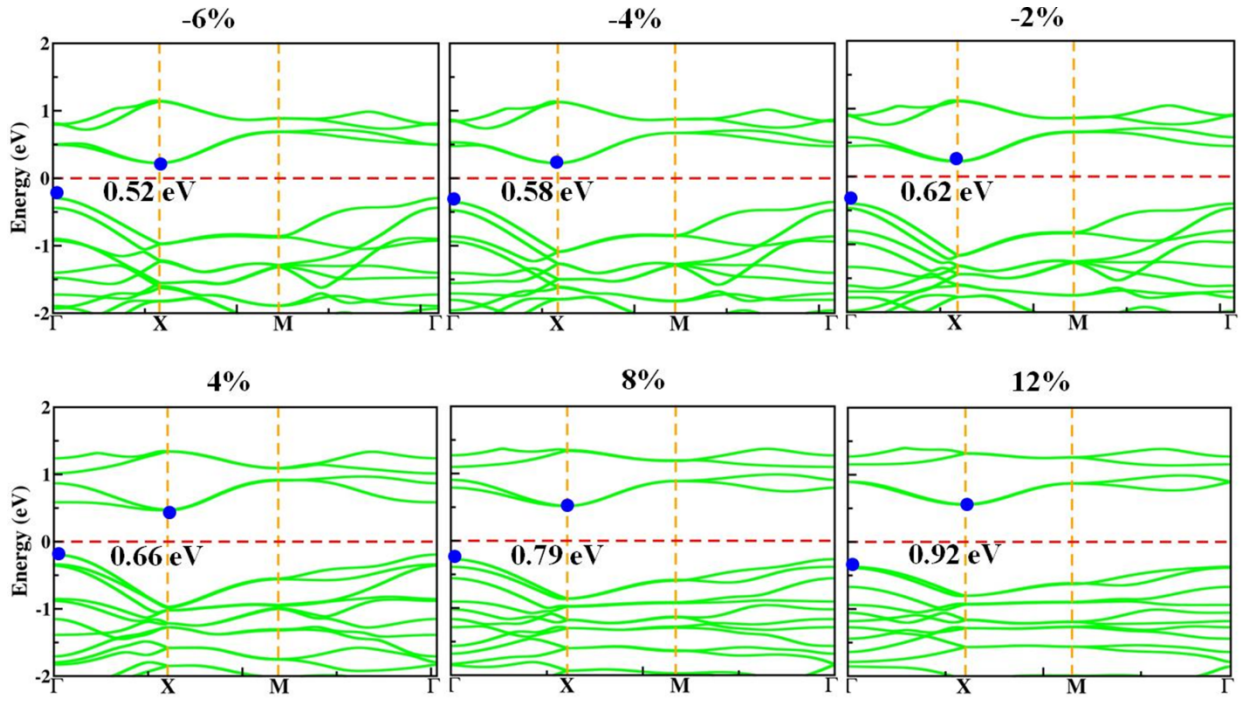

Fig. S4 Effect of strain on band structures of ring-Te along x-direction.

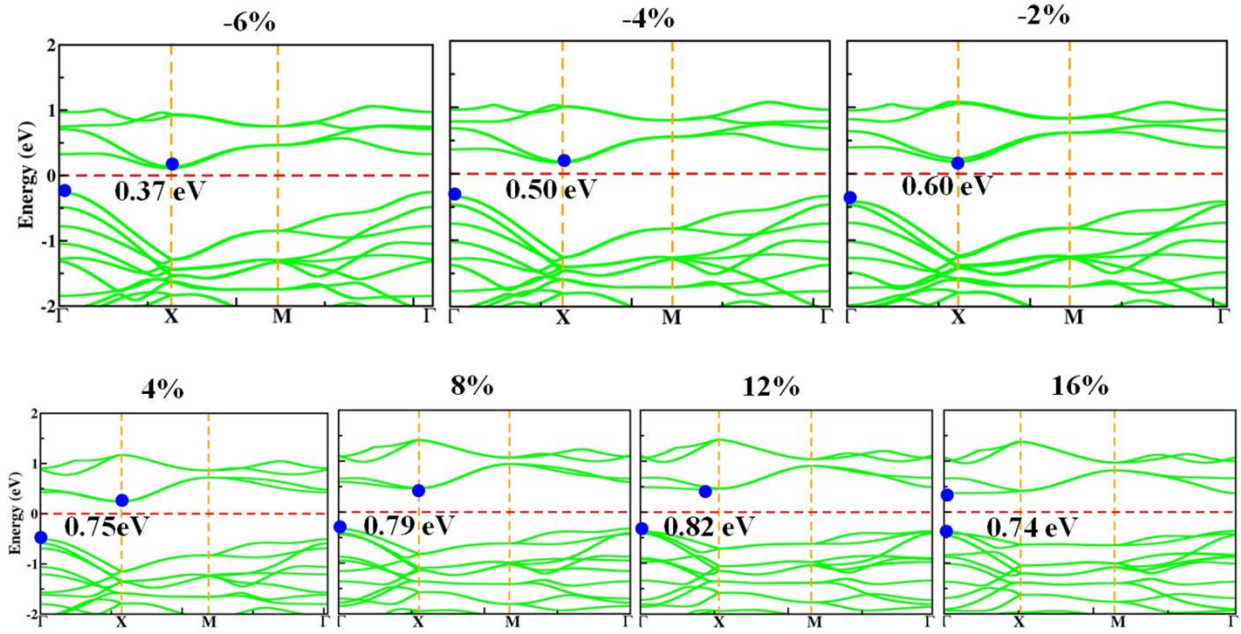

Fig. S5 Effect of strain on band structures of ring-Te along y-direction.

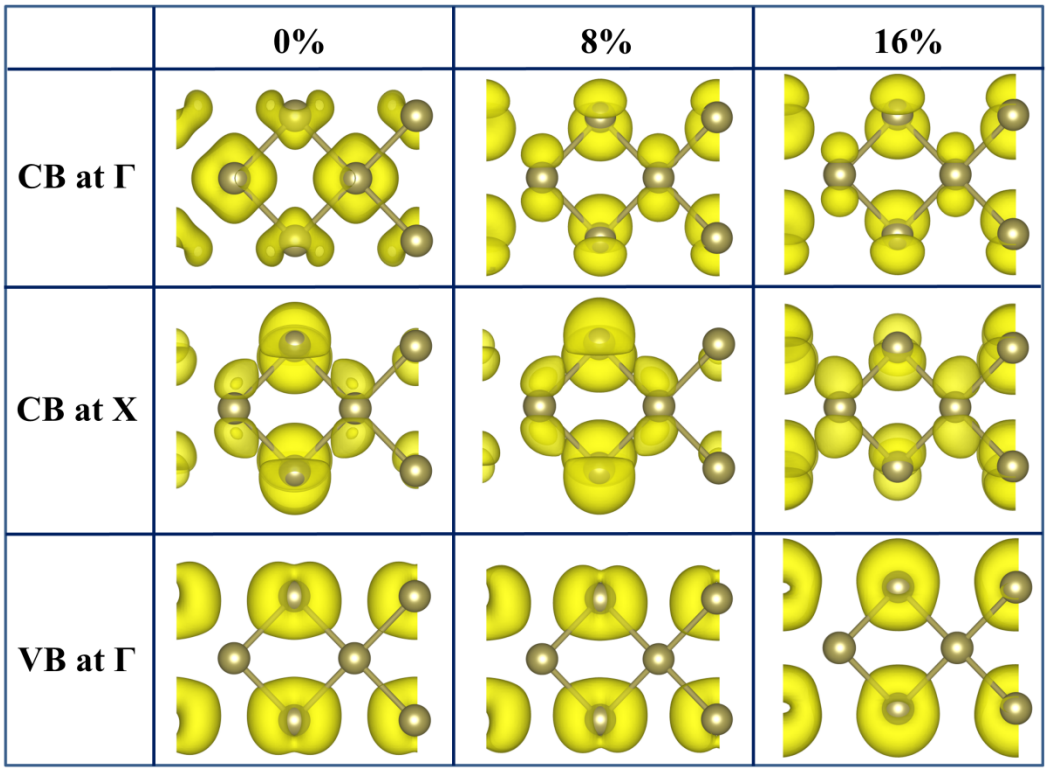

Fig. S6 Band decomposed charge densities of ring-Te (side view) corresponding to the valence band maximum (at Γ point) and conduction band minimum (at X and Γ point) under the uniaxial strain along y-direction. The isosurface value is 0.0007 eÅ^{-3}.

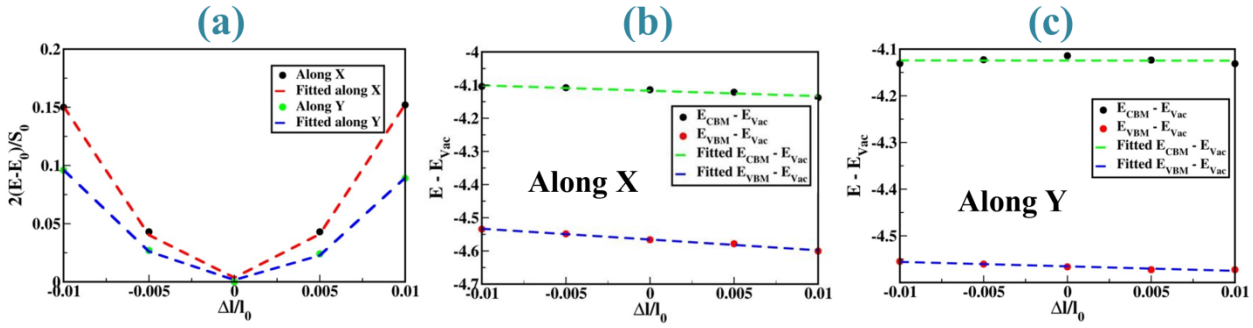

Fig. S7 Variation of (**a**) $\frac{2(E-E_0)}{S_0}$ and (**b, c**) $E-E_{vac}$ w.r.t strain i.e. $\frac{\Delta l}{l_0}$ with their parabolic and straight fitting, respectively of ring-Te. $E-E_0$ is the difference in the total energy of stable and

strained structure, S_0 is the surface area of monolayer slab and $E - E_{vac}$ is the difference in the energy of i^{th} band and vacuum energy.