electronic supplementary information for

Strain-induced phase transition and piezoelectricity in monolayer tellurene

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#Equal contribution

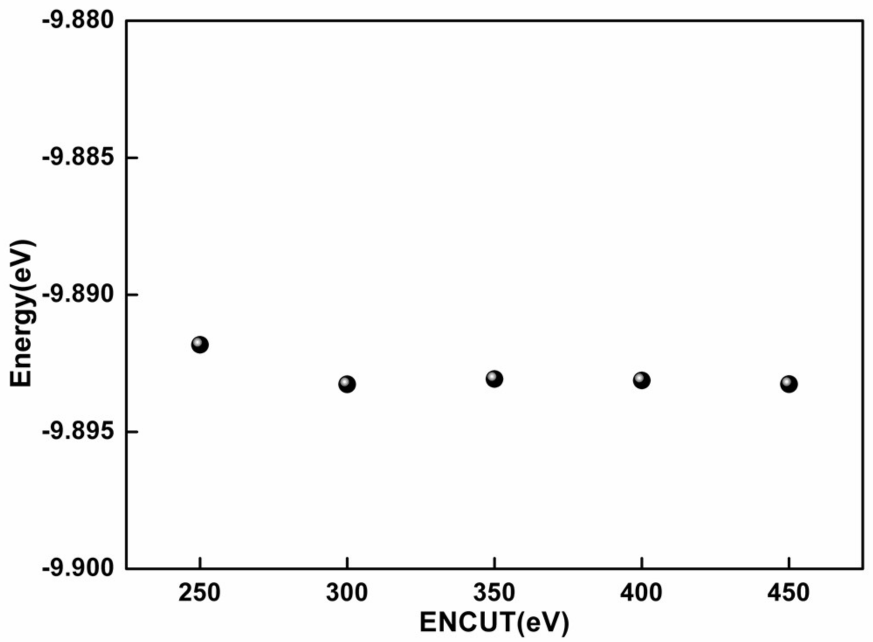

Fig. S1 The total energy convergence with plane wave cutoff ENCUT.

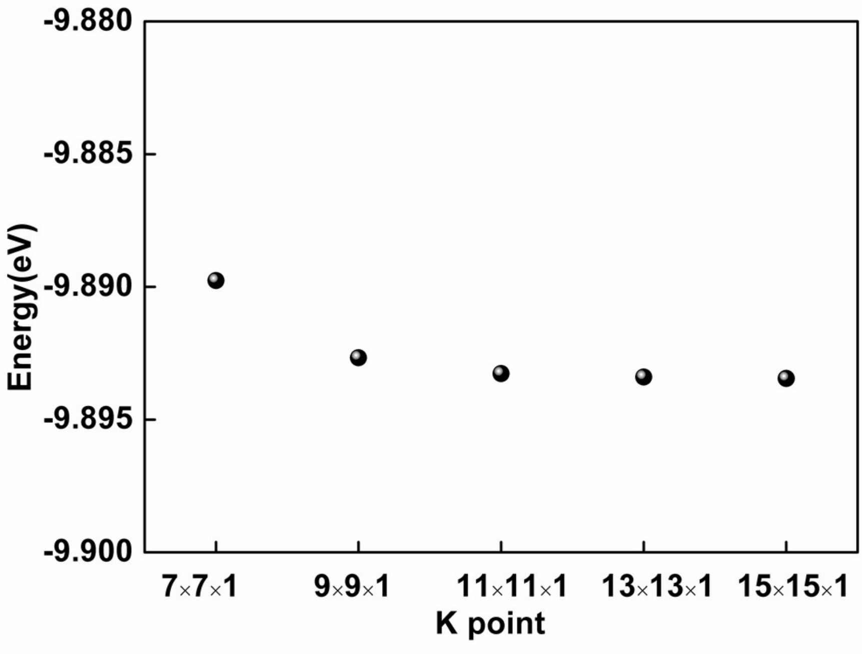

Fig. S2 The total energy convergence with K points.

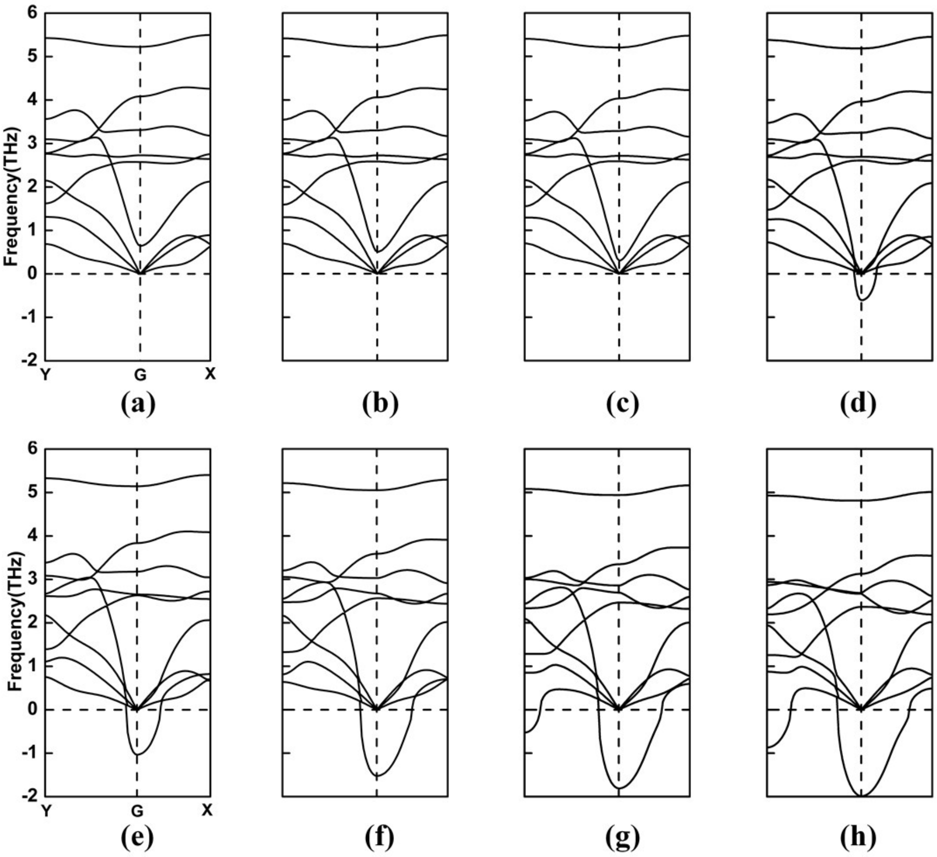

Fig. S3 Phonon spectra for β tellurene under different biaxial tensile strains: (a)0%; (b)0.2%; (c)0.4%; (d)1%; (e)2%; (f)4%; (g)6%; (h)8%

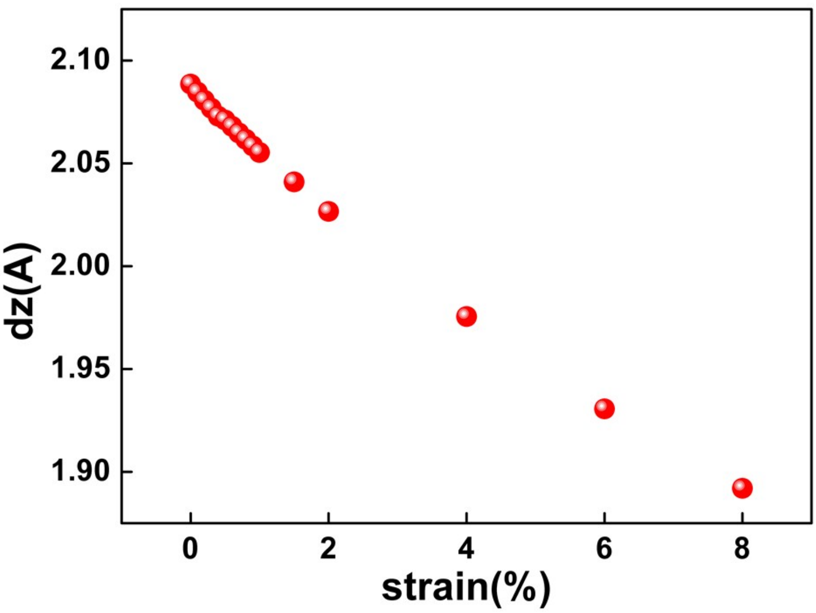

Fig. S4 The variation of dz under different strain. dz represents the height of buckling.

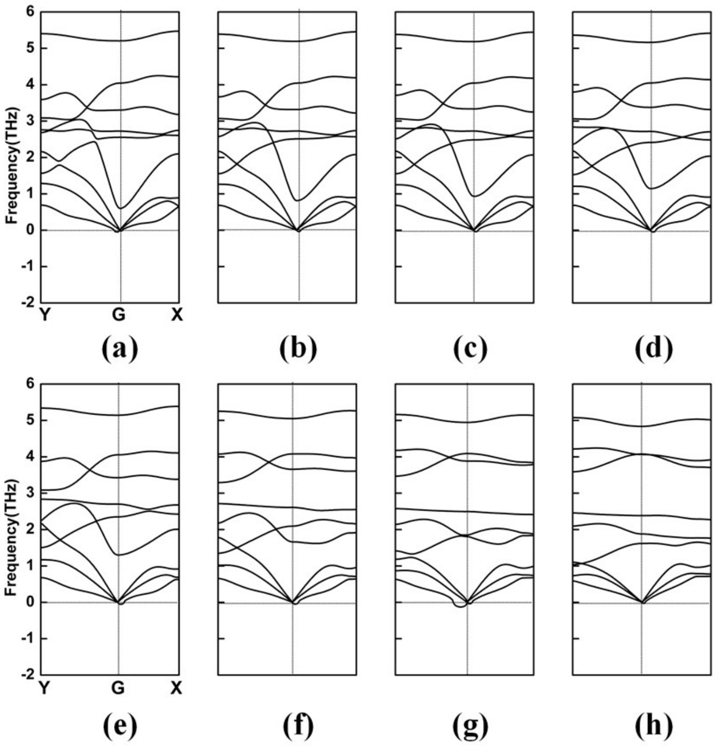

Fig.S5 Phonon spectra for α tellurene under different biaxial strains: (a)0.5%; (b)0.8%; (c)1%; (d)1.5%; (e)2%; (f)4%; (g)6%; (h)8%.

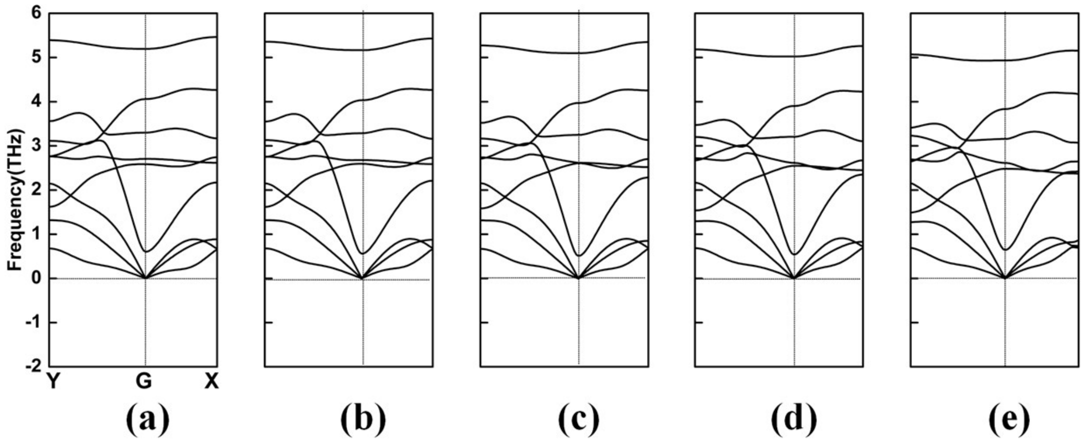

Fig.S6 Phonon spectra for β tellurene under different uniaxial strains in x direction: (a)1%; (b)2%; (c)4%; (d)6%; (e)8%. The imaginary frequency free spectrums indicate the stability of the β phase tellurene under strain along x-axis.

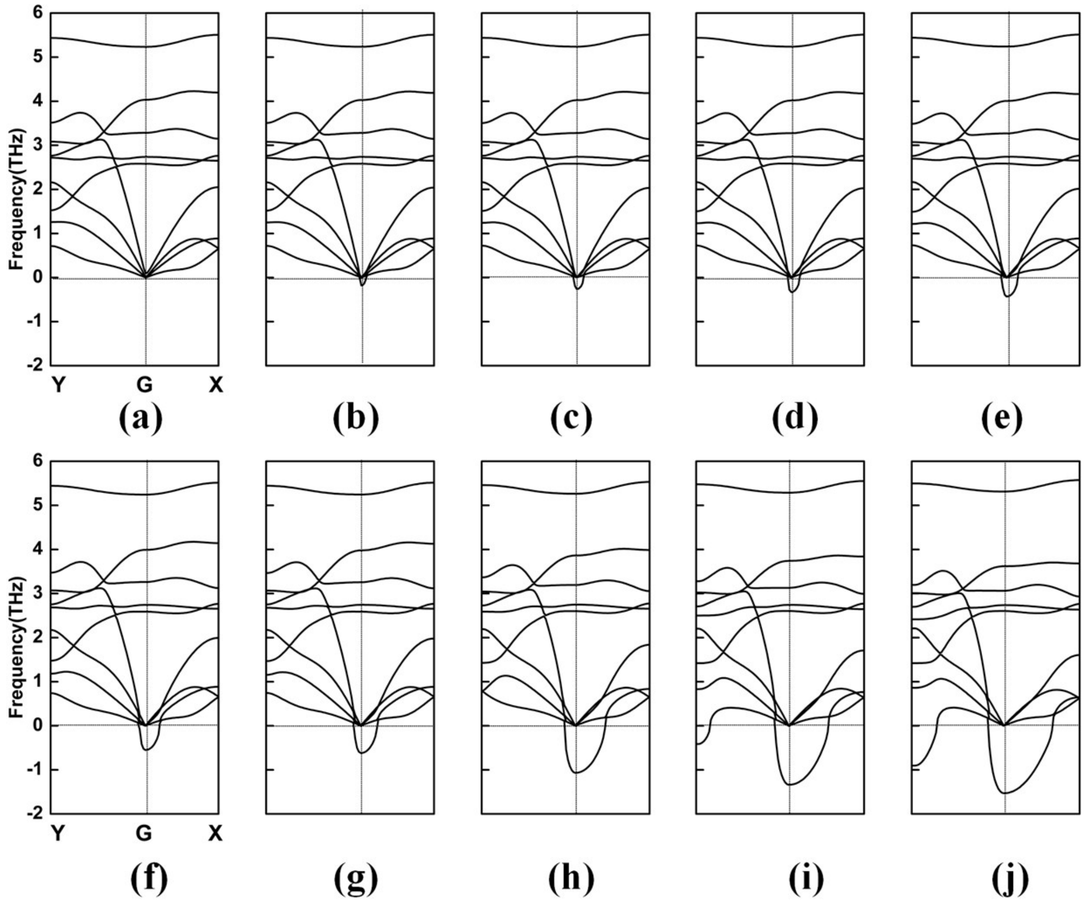

Fig.S7 Phonon spectra for β tellurene under different uniaxial strains in y direction: (a)1%; (b)1.1%; (c)1.2%; (d)1.3%; (e)1.5%;(f)1.8%;(g)2%;(h)4%;(i)6%;(j)8%.

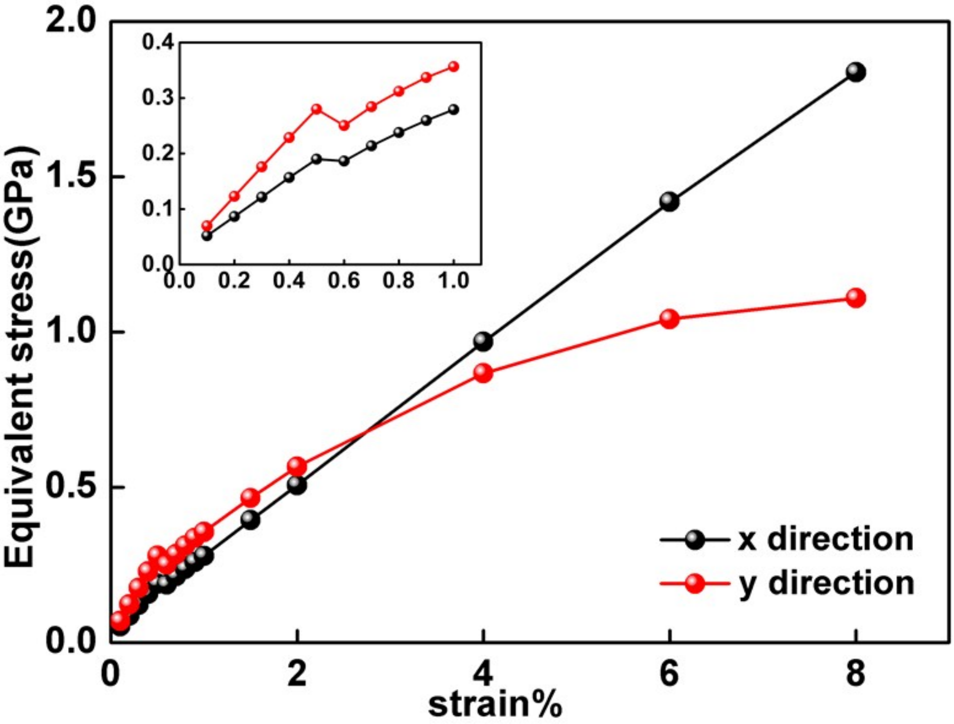

Fig.S8 The relationship between stress and strain under biaxial strain. The stresses in x direction and y direction are represented by black and red dots respectively. For the exsistance of vaccum space, the equivalent stress is adjusted by multiplying L/d, where L is the total length of lattice (include vaccum space), d is the thickness of tellurene (summation of buckling height and vdW radius of Te atom).