## Supplementary On-Line Material for: High thermoelectric performance in two-dimensional tellurium: An *ab initio* study

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Figure S1: Electronic band structure of  $\alpha$ -Te at HSE06 level, which narrows the range of electronic energy in Figure 1(c) in the main text from [-4 eV, 4 eV] to [-2 eV, 2 eV]. The lowest (highest) point in conduction (valence) band is tagged with capital letter A (B).



Figure S2: Effective masses m\* along the x or y direction in the isotropic  $\alpha$ -Te material, calculated as m\* =  $\hbar^2 (\partial^2 E/k^2)^{-1}$  by fitting (a) conduction band minimum around A point and (b) valence band maximum around B point to a quadratic function.