Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.
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Supporting information for

Flexible chalcogenide perovskite $Ba_3Te_2S_7$ with high electron mobility and strong optical absorption ability

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The present supplemental material provides more details about the structural properties, electronic and optical properties of $Ba_3Te_2S_7$.

Table S1 The average equatorial and axial Te-S-Te angles for monolayer (ML), two-layer (2L), three-layer (3L), four-layer (4L) and bulk $Ba_3Te_2S_7$

Layer	ML	2L	3L	4L	Bulk
Equatorial Te-S-Te angle (°)	136.31	168.11	148.14	151.56	153.37
Axial Te-S-Te angle (°)	156.76	152.07	151.61	151.61	154.88

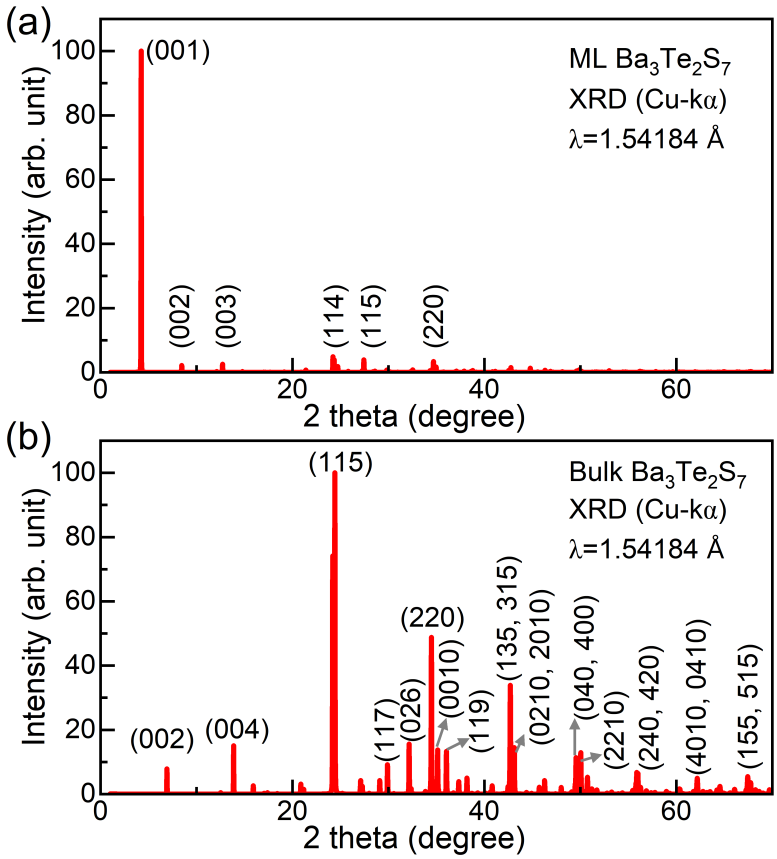

Fig. S1 (a) The calculated XRD patterns for the relaxed (a) monolayer (ML) and (b) bulk $Ba_3Te_2S_7$ from 10° to 70° by using the radiation wavelength λ=1.54184 Å(Cu-K_α). Several important peaks are marked with the corresponding Miller indices (hkl).

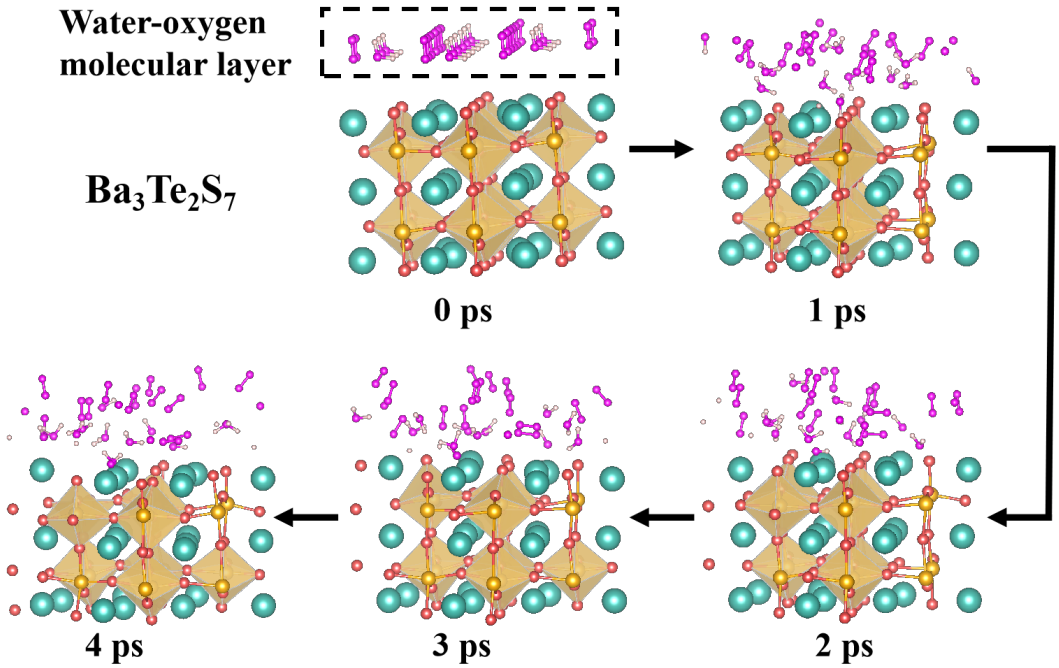

Fig. S2 Snapshots of AIMD trajectories of $Ba_3Te_2S_7$ with a water-oxygen molecular layer following 4 ps AIMD simulation at 300 K.

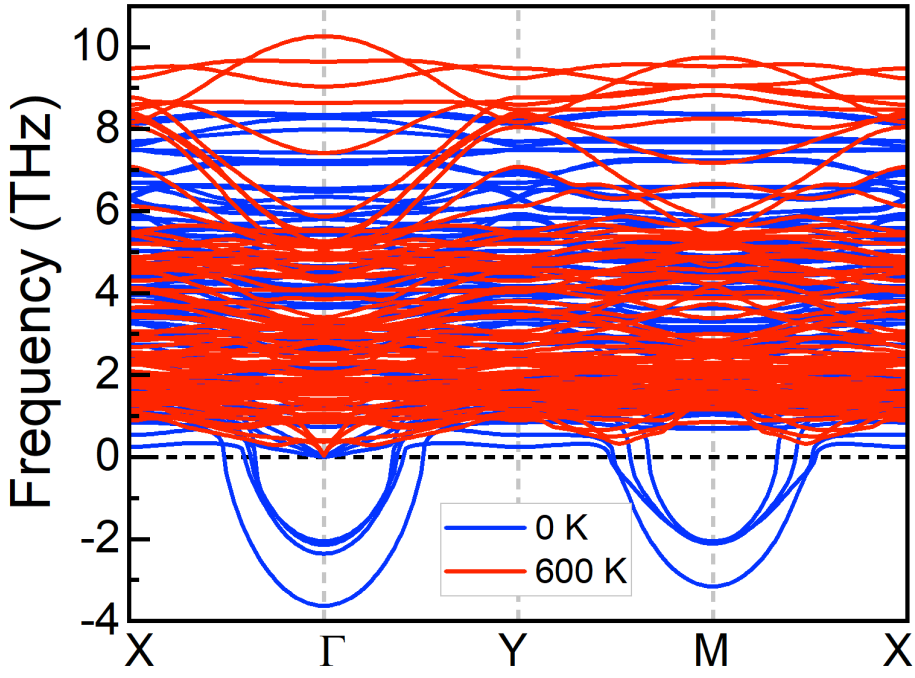

Fig. S3 Calculated phonon spectrum of $Ba_3Te_2S_7$ at 0 K and 600 K.

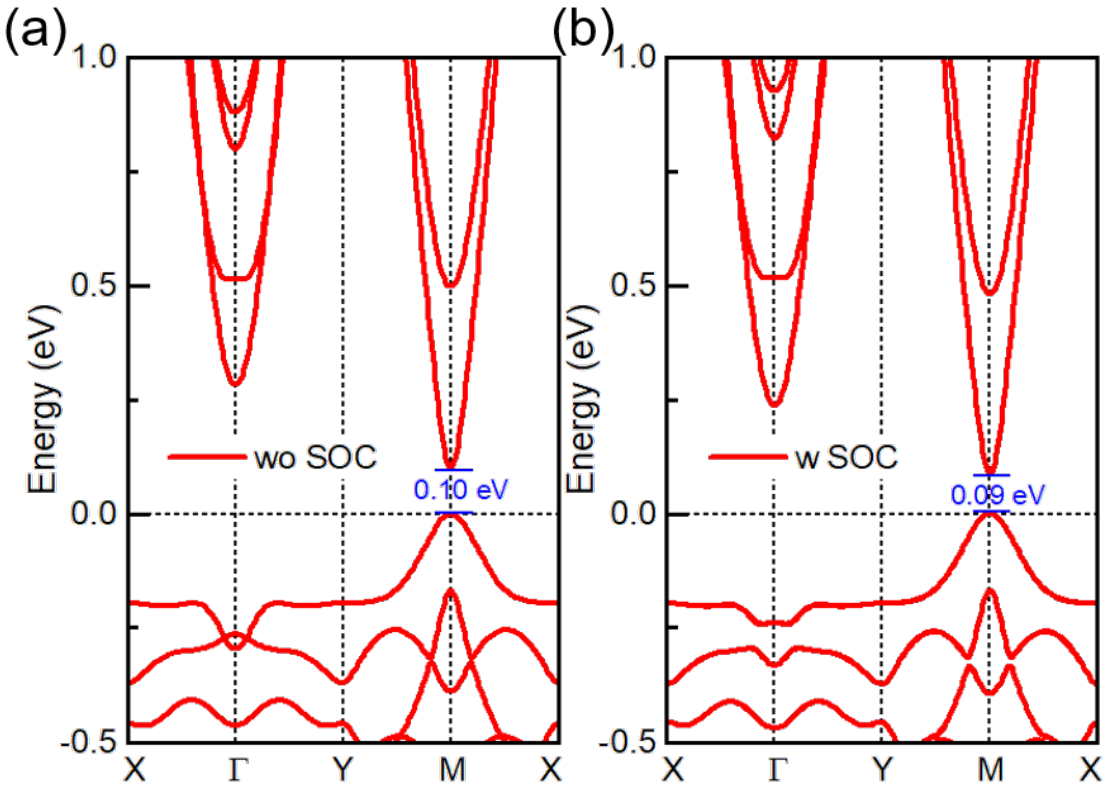

Fig. S4 The computed band structure of ML $Ba_3Te_2S_7$ (a) without (wo) and (b) with (w) the spin-orbital coupling (SOC) effect using PBE functional. It is shown that the SOC effect has little influence on the band structure, except for a very small bandgap difference of 10 meV, which can be ignored indeed. Here X (0.5, 0.0, 0.0), Γ (0.0, 0.0, 0.0), Y (0.0, 0.5, 0.0) and M (0.5, 0.5, 0.0) refer to the special high-symmetry points in the first Brillouin zone. The top of the valence bands is chosen as the zero energy.

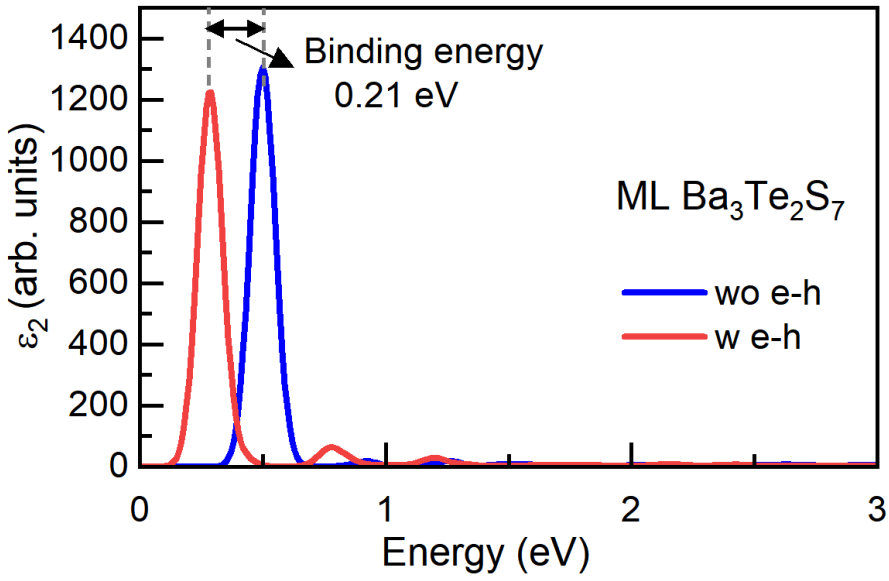

Fig. S5 Calculated imaginary part of the dielectric function ε_2 for ML $Ba_3Te_2S_7$ with (w) and without (wo) the electron-hole (e-h) interaction. The exciton binding energy is estimated to be 0.21 eV.

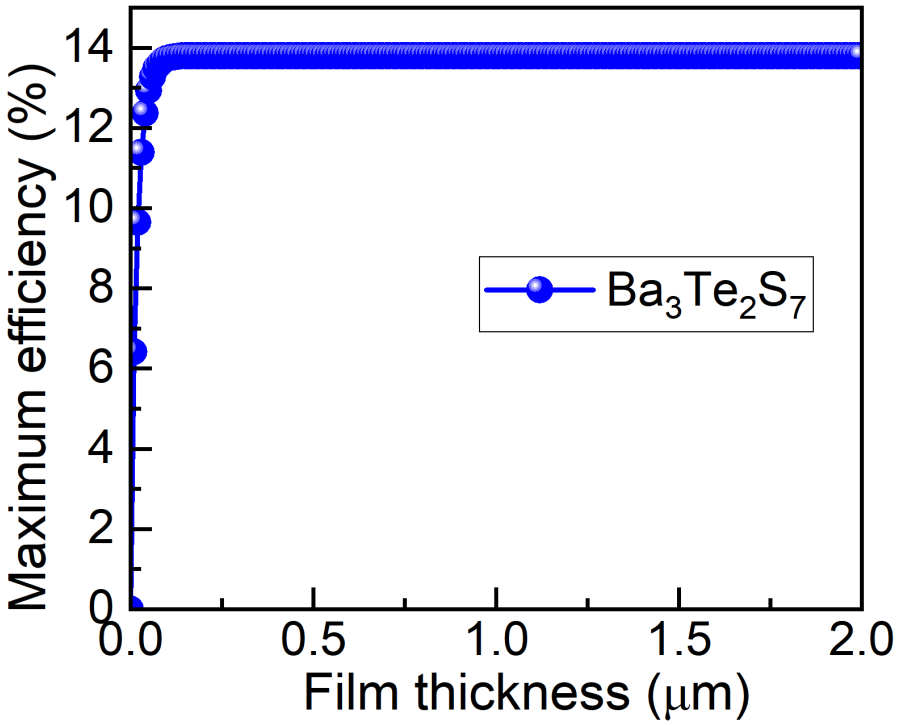

Fig. S6 The simulated maximum power conversion efficiency (PCE) of $Ba_3Te_2S_7$ as a function of the film thickness.