Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information For

Propose two dimensional Sb_2Te_2X (X= S, Se) with isotropic electron mobility and remarkable visible light response

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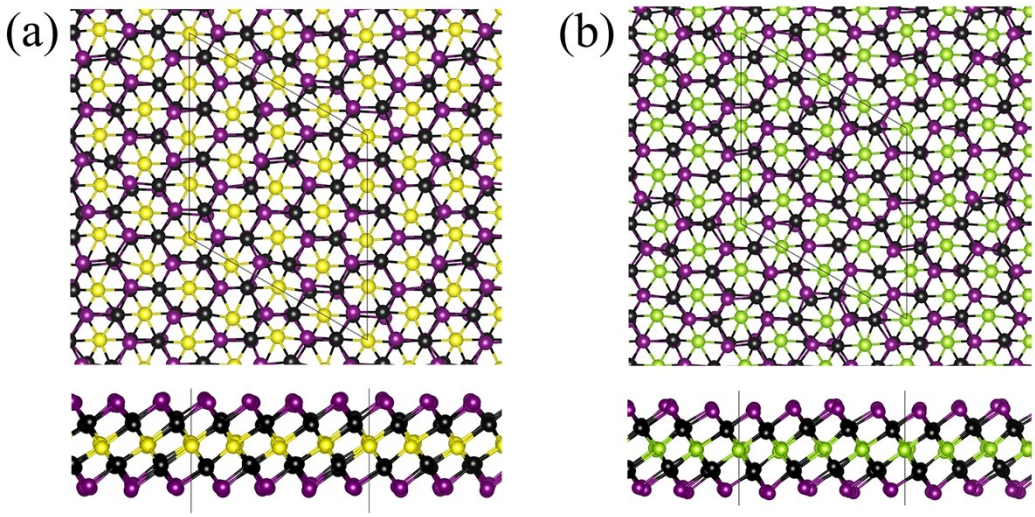

Fig.S1 Top and side views of snapshot at 7.5 ps of the BOMD simulations for monolayer (a) Sb_2Te_2S and (b) Sb_2Te_2Se.

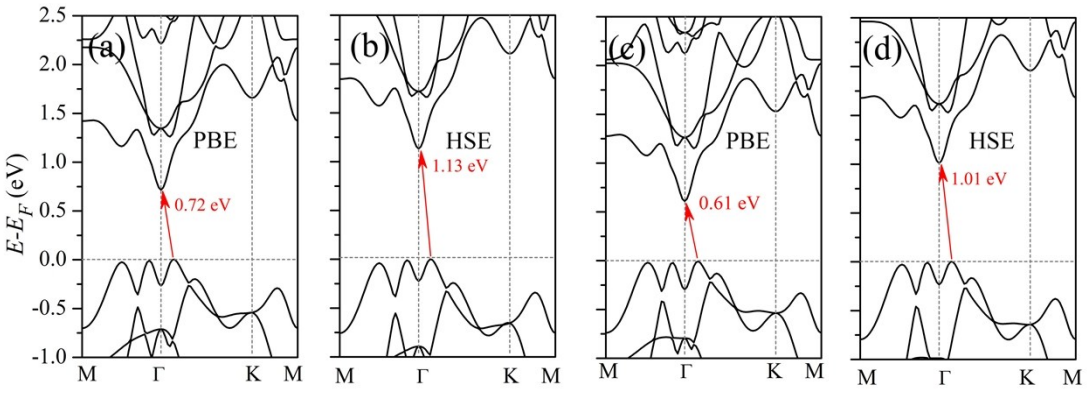

Fig.S2 PBE and HSE band structures of (a-b) Sb_2Te_2S and (c-d) Sb_2Te_2Se monolayers.

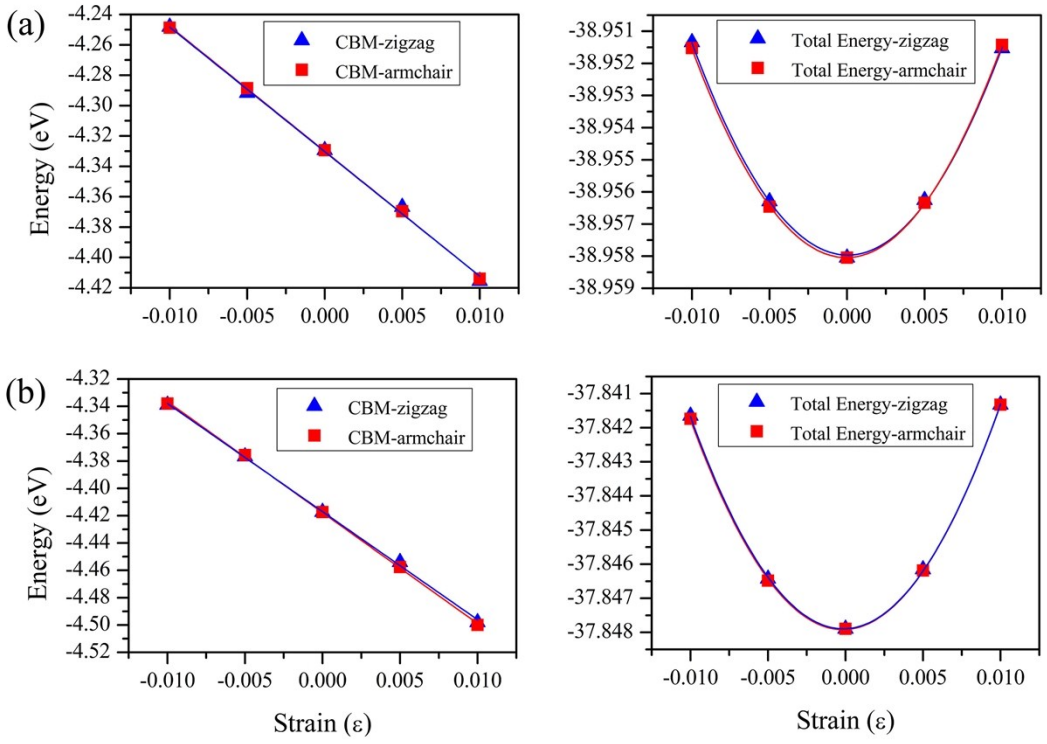

Fig.S3 Linear fitting of band edges and quadratic fitting of total energy as a function of uniaxial strain for (a) Sb_2Te_2S and (b) Sb_2Te_2Se monolayers.

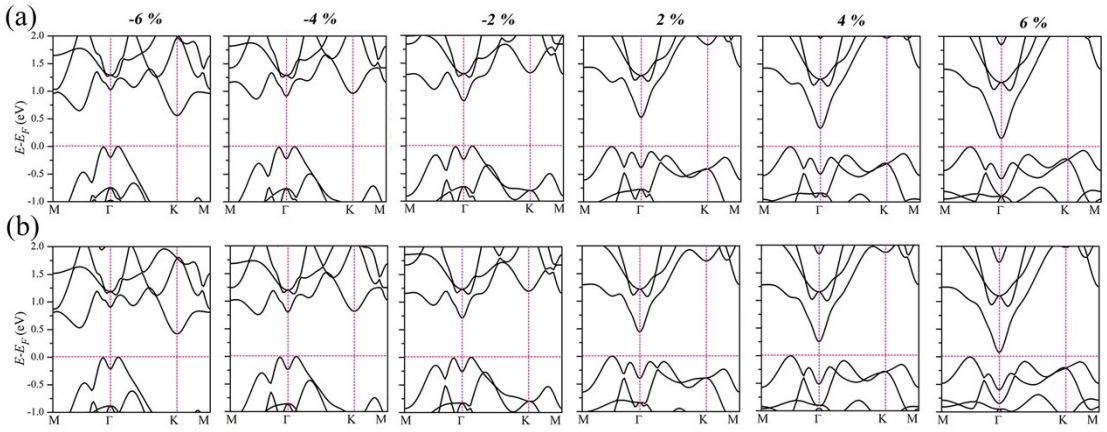

Fig.S4 Strain-dependent band structures of monolayer (a) Sb_2Te_2S and (b) Sb_2Te_2Se.

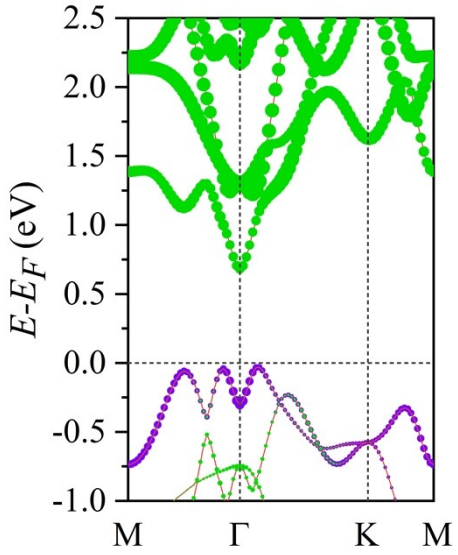

Fig.S5 Orbital-resolved band structure for Sb_2Te_2S, the green and purple circles represent Sb-*p* and Sb-*s* states, respectively.

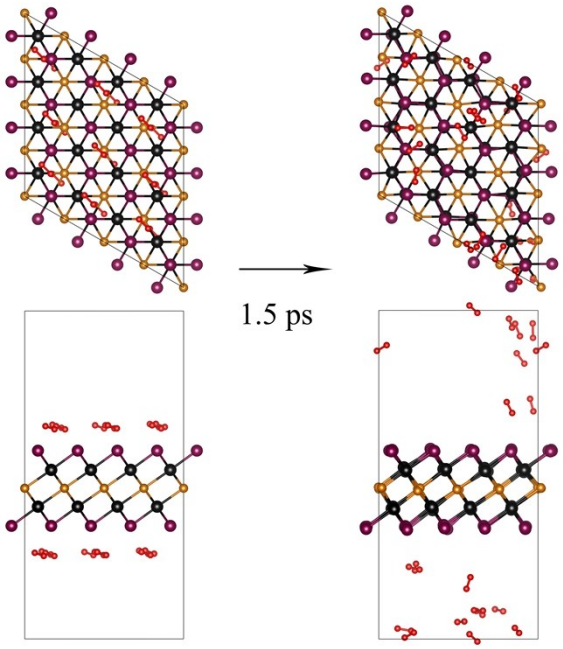

Fig.S6 Set Sb_2Te_2S as an example, we have verified their chemical stability by conducting BOMD simulation with 18 O_2 molecules at room temperature (300 K).We

found O_2 molecules move away from basal plane without dissociating into oxygen atoms, and without mechanical degradation and breakdown after 1.5 ps, indicating that they are chemically stable in the air at room temperature.