Supporting Information For

Propose two dimensional Sb$_2$Te$_2$X (X= S, Se) with isotropic electron mobility and remarkable visible light response

Yan Liang,† Jianwei Li,‡ Hao Jin,*‡ Baibiao Huang† and Ying Dai *,†

†School of Physics, State Key Laboratory of Crystal Materials, Shandong University, Shandanan Str. 27, Jinan 250100, People's Republic of China

‡ Shenzhen Key Laboratory of Advanced Thin Films and Applications, College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen 518060, People's Republic of China

*Corresponding authors: jh@szu.edu.cn (H. J.); daiy60@sina.com (Y. D)
Fig. S1 Top and side views of snapshot at 7.5 ps of the BOMD simulations for monolayer (a) Sb$_2$Te$_2$S and (b) Sb$_2$Te$_2$Se.

Fig. S2 PBE and HSE band structures of (a-b) Sb$_2$Te$_2$S and (c-d) Sb$_2$Te$_2$Se monolayers.
Fig. S3 Linear fitting of band edges and quadratic fitting of total energy as a function of uniaxial strain for (a) Sb$_2$Te$_2$S and (b) Sb$_2$Te$_2$Se monolayers.

Fig. S4 Strain-dependent band structures of monolayer (a) Sb$_2$Te$_2$S and (b) Sb$_2$Te$_2$Se.
Fig. S5 Orbital-resolved band structure for Sb$_2$Te$_2$S, the green and purple circles represent Sb-$p$ and Sb-$s$ states, respectively.

Fig. S6 Set Sb$_2$Te$_2$S 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.