Supporting Information

Two-dimensional ferroelasticity and negative Poisson's ratios in monolayer YbX (X=S, Se, Te)

Qingwen Lan[1], Changpeng Chen[1,2,*]
1.School of Science, Wuhan University of Technology, Wuhan 430070, P. R. China
2.Research Center of Materials Genome Engineering, Wuhan University of Technology, Wuhan 430070, P. R. China
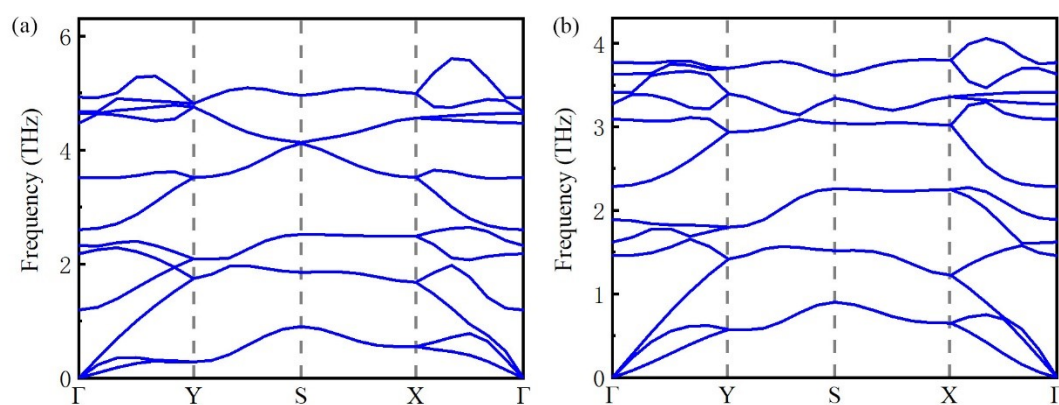
Fig. S1. (a) Phonon spectra of ML YbSe. (b) Phonon spectra of ML YbTe.
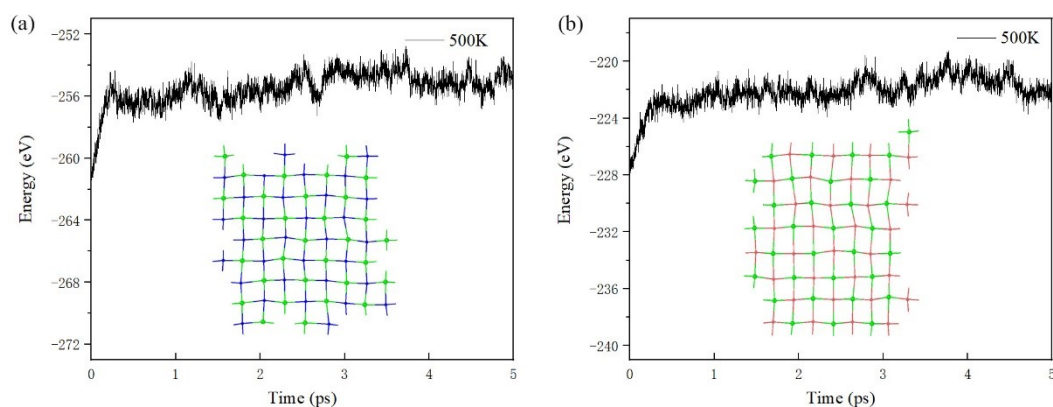

Fig. S2. Total energy variations as well as the top view of the snapshots from the AIMD simulation for (a) ML YbSe and (b) ML YbTe.
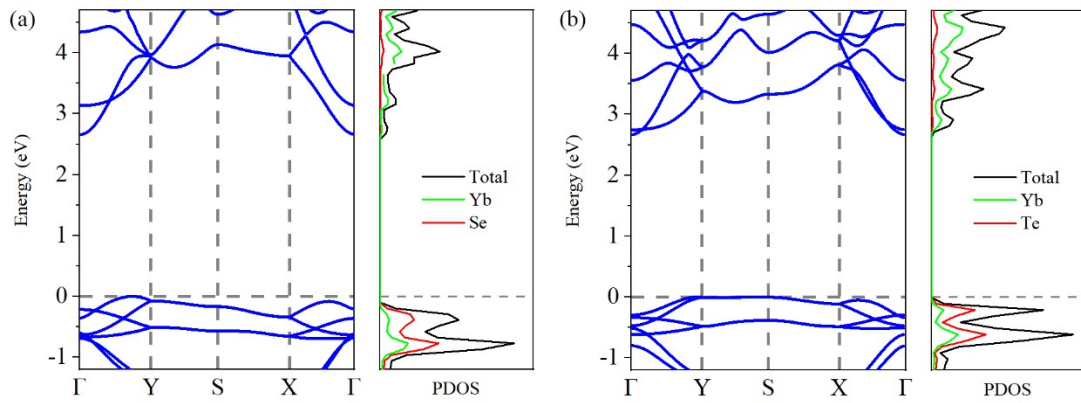
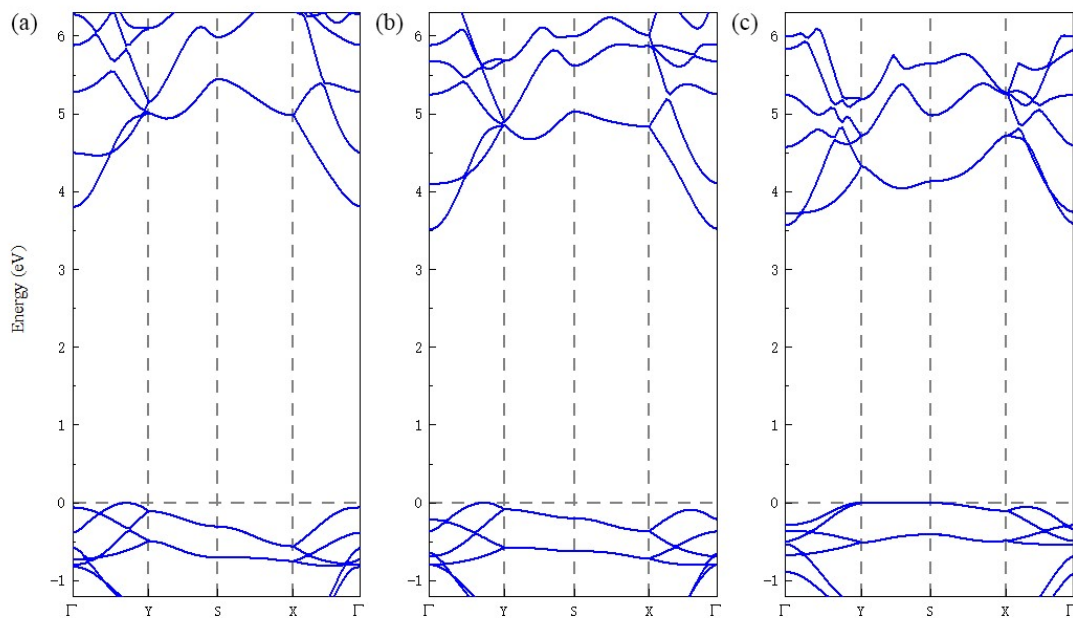Fig. S3. The PBE level band structure and projected density of states (PDOS) of ML (a) YbSe and (b) YbTe.

Fig. S4. The band structure of ML (a) YbS (b) YbSe and (c) YbTe obtained from HSE06 hybrid functional calculations.
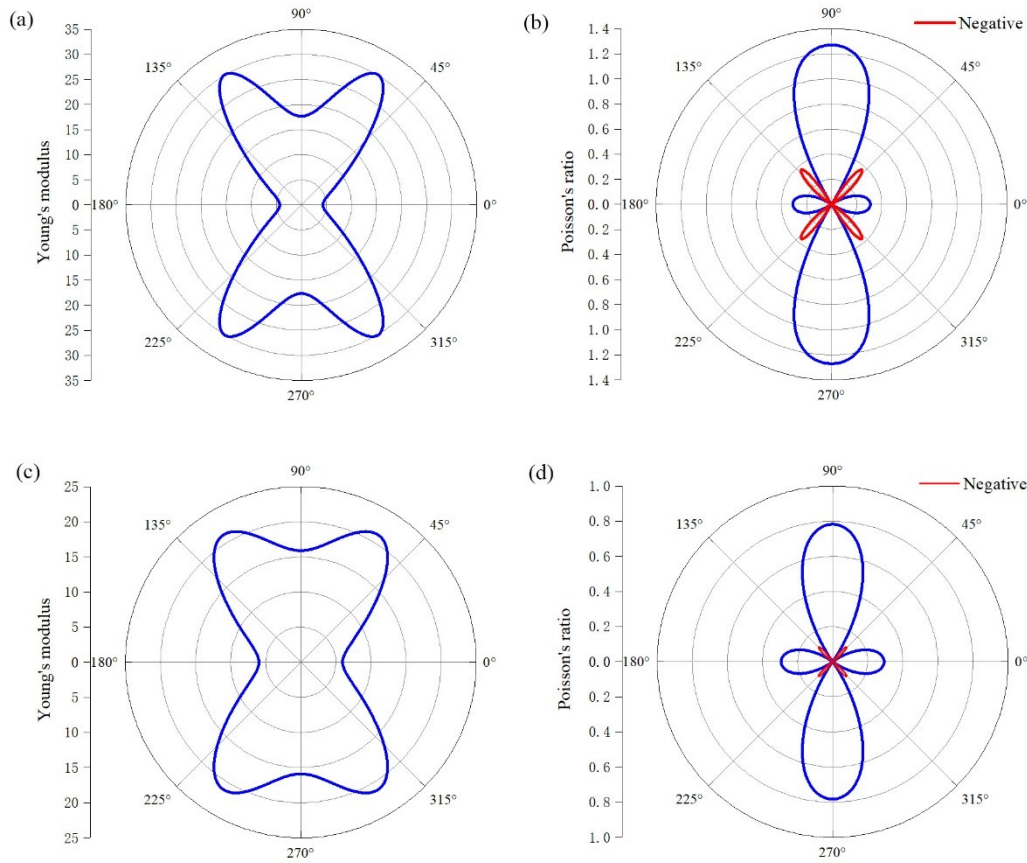
Fig. S5. (a,c) Young's modulus and (b,d) Poisson's ratio of ML YbSe and YbTe as a function of the angle θ, respectively. θ = 0° corresponds to the x-axis. NPR is represented with wine red, while PPR is shown with blue.
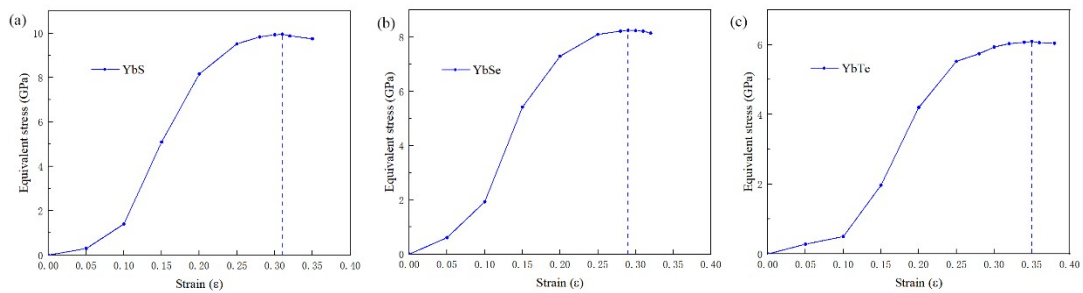

Fig. S6. The equivalent stress as a function of strain along the a direction. The strain-stress curve for (a) YbS, (b) YbSe and (c) YbTe (layer distance d_0=4.44, 4.82, 5.52 eV respectively). The critical strain is 31%, 29%, 35% and the breaking strength is 9.95, 8.25, 6.09 GPa respectively.