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

Exfoliable and self-healable two-dimensional materials from wurtzite zinc chalcogenides as building blocks of nanodevices

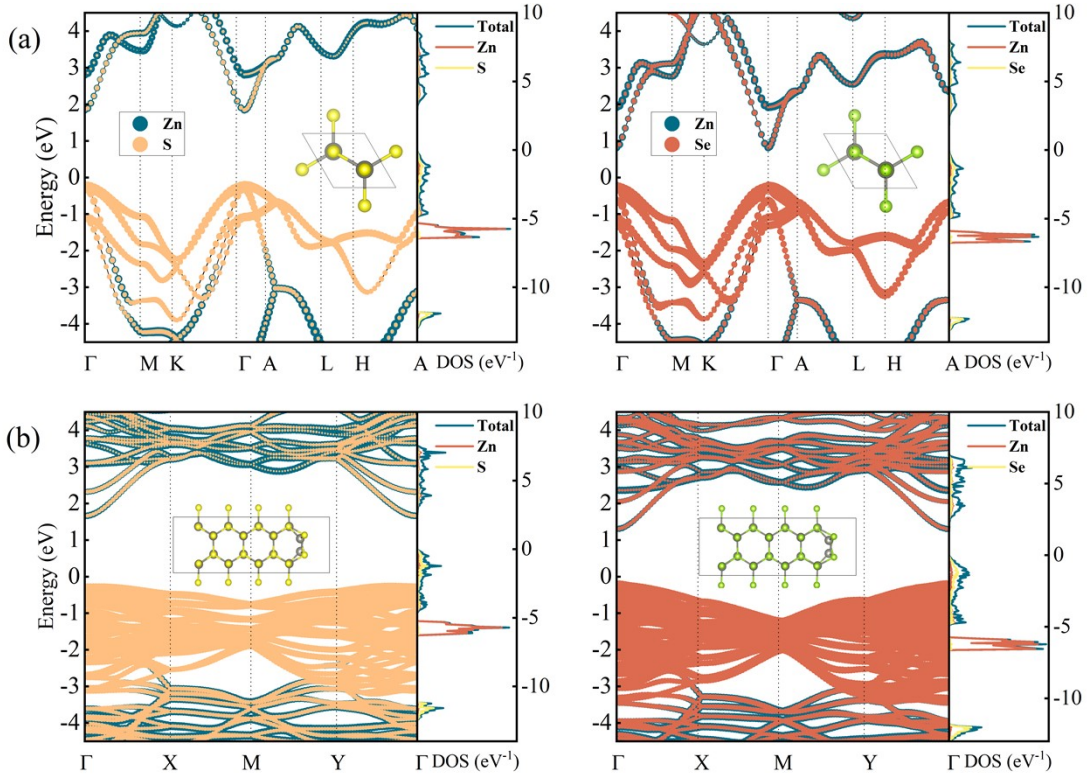

Figure S1 (a) and (b) Element-projected electronic band and DOS of bulk and multilayer Zn*X*. The Fermi level (E_F) is set to zero

According to reference[6], the exfoliation energy (EE) is defined as the difference between the ground-state energy of an N-layer-thick slab, the exfoliated layer, and the remaining (N−1)-layer slab for the traditional slab model. As shown in Figure S2, the EE is described as the energy difference between the original structure (I), the exfoliated layer (II), and the remaining structure (III). Namely, the exfoliation energy per unit area E_{exf} is defined as:

$$E_{exf} = (E_{II} + E_{III} - E_I)/A$$

where A refers to the in-plane area of the surface unit cell.

We calculate the exfoliation energy according to the methods introduced previously[6]. The exfoliation energy is 0.52 J/m^2 for ZnS and 0.43 J/m^2 for ZnSe. Our calculated exfoliation energy obtained by formula (2) is consistent with previous reports [6].

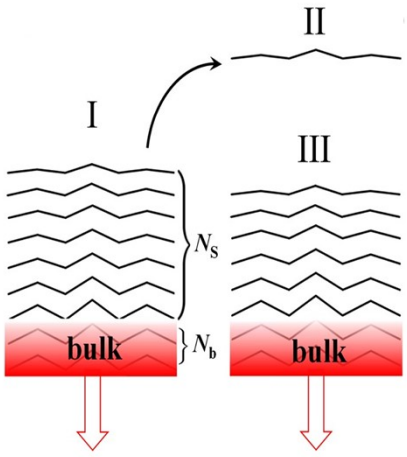

Figure S2. Schematic of the Green's function surface model for calculating the exfoliation energies. I (III) is the original (remaining) structure and II is the exfoliated layer. Nb and NS refer to the numbers of atomic layers in the bulk and surface regions, respectively[6]

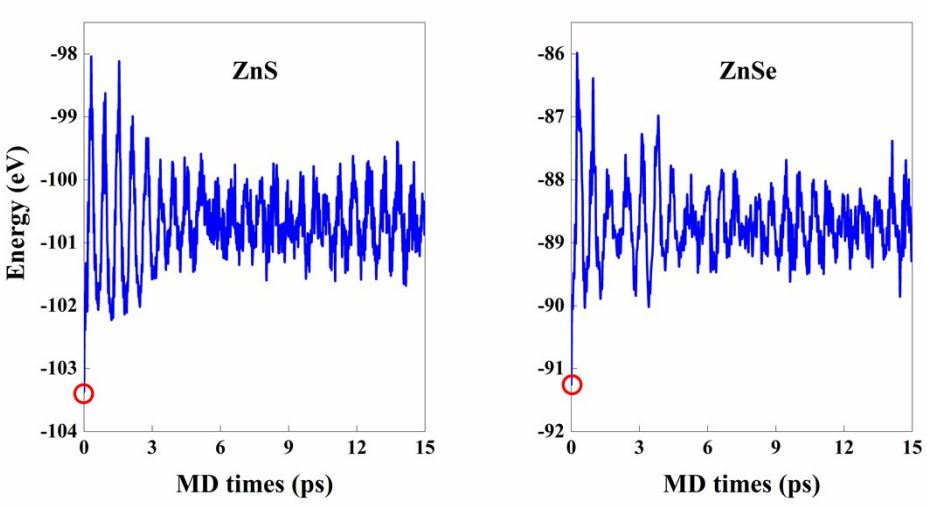

Figure S3. Ab initio MD simulations of Zn*X* at 600 K

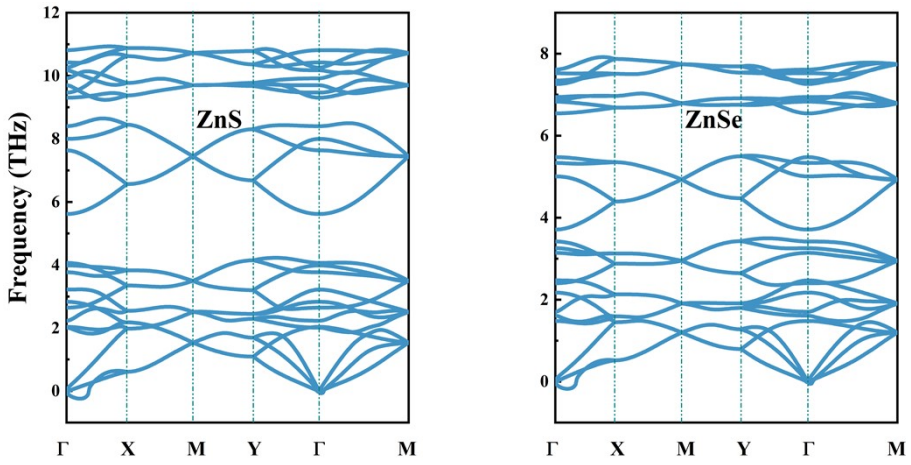

Figure S4. Calculated Phonon band structure of Zn*X*

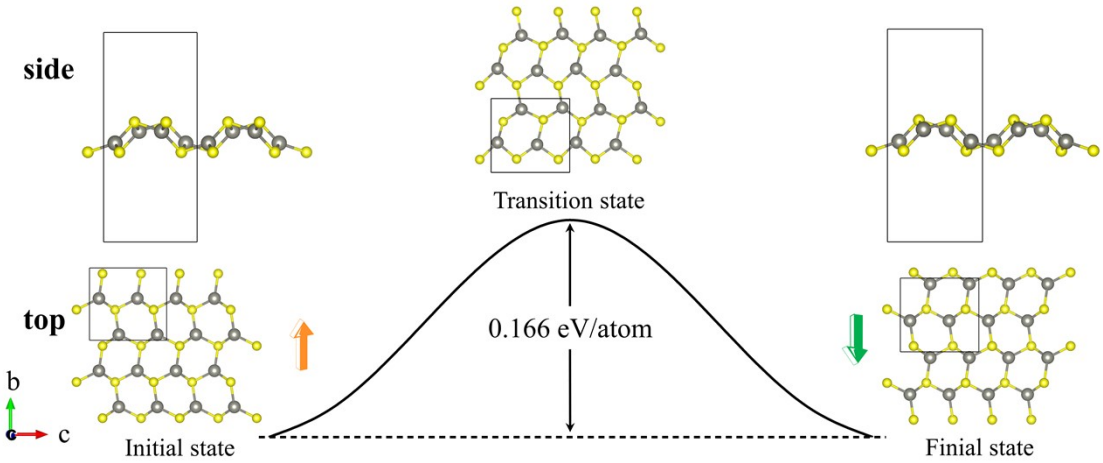

Figure S5. Evolution of the total energy of ZnS phase transforming from the initial state (left) to the finial state (right) by a direct shifting process

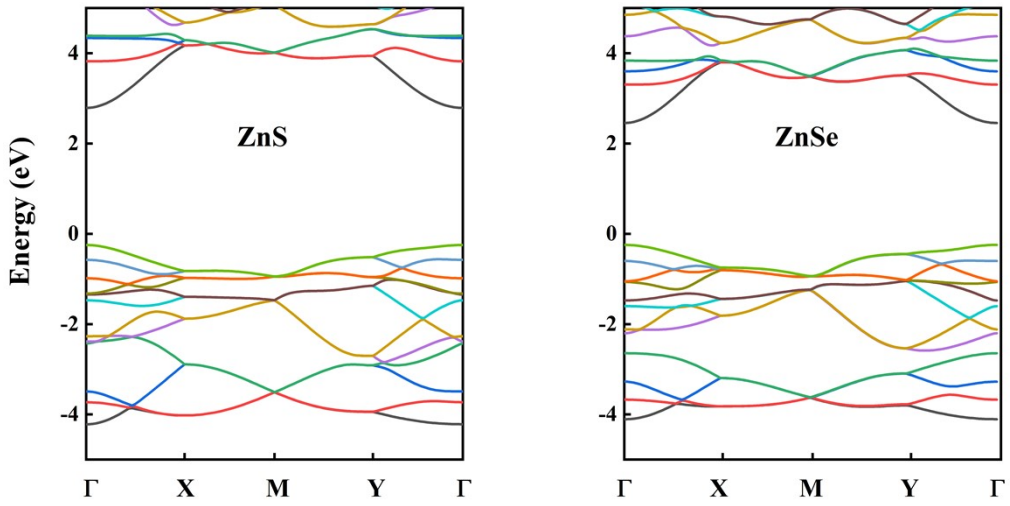

Figure S6. Non-SOC band structures of 2D monolayer Zn*X* unit cell

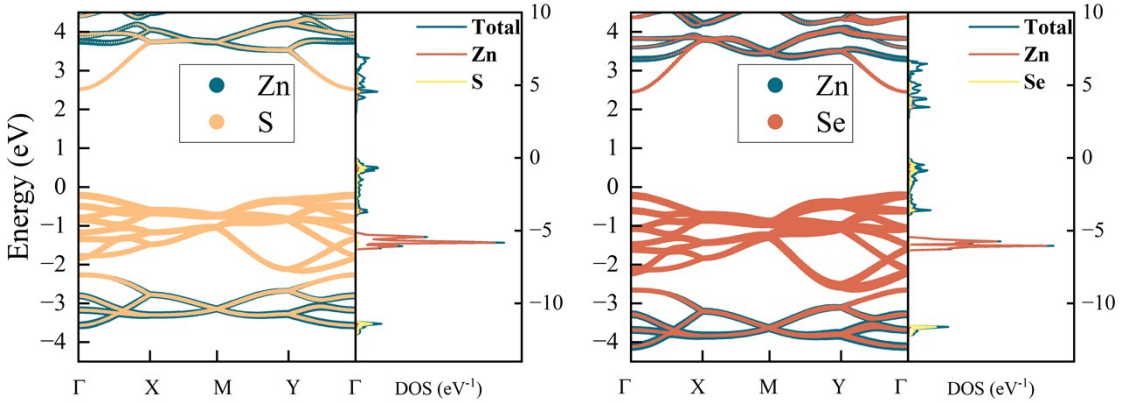

Figure S7. Element-projected electronic band and DOS of 2D monolayer Zn*X* unit cell. The Fermi level (E_F) is set to zero

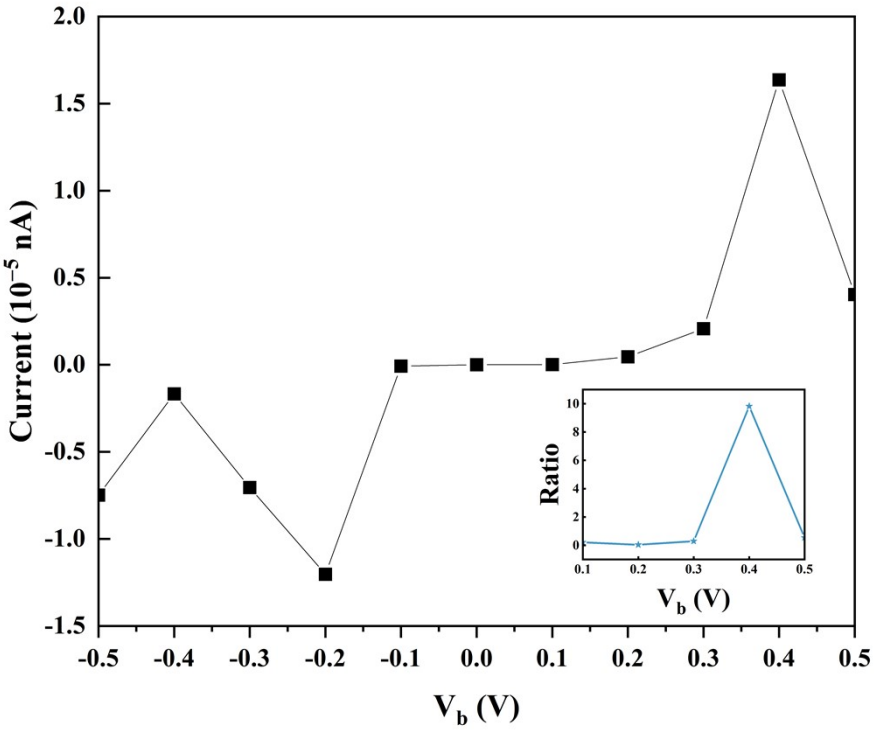

Figure S8. *I–V* characteristics change with the applied bias for model ZnS. Inset is the rectification ratio

	ZnS (eV)	**ZnSe (eV)**
xx	(4.38, 5.43)	(3.94, 4.55)
yy	(3.66, 5.52)	(3.33, 4.48)
zz	(3.39, 4.88)	(3.00, 4.57)

Table S1. Values of absorption peaks