Supplementary Information

High mobility and enhanced photoelectric performance in two-dimensional ternary compounds NaCu*X* (*X*=S, Se, and Te)

Heming Li,[1,2] Xinxin Jiang,[a] Xuhui Xu,[a] Ge Xu,[a] Dongmei Li,[a] Chong Li,[3] Bin Cui*[a] and De-Sheng Liu*[a,4]

	a^{VASP}(Å)	a^{ATK}(Å)	E_g^{VASP} (eV)	E_g^{ATK}(eV)	E_{coh}^{VASP}(eV)	E_{coh}^{ATK}(eV)
NaCuTe	4.33	4.28	0.85	0.86	-2.90	-3.54
NaCuSe	4.03	4.01	0.30	0.32	-3.13	-3.70
NaCuS	3.83	3.80	0.31	0.32	-3.35	-4.14

Table. S1. Comparison of ATK and VASP calculations: optimized lattice constant, band gap and cohesive energy.

In order to compare the results calculated by VASP and ATK. On the basis of PBE functional, we calculate the band gap and binding energy after optimizing the lattice structure. It can be seen from table S1 that the results are consistent.
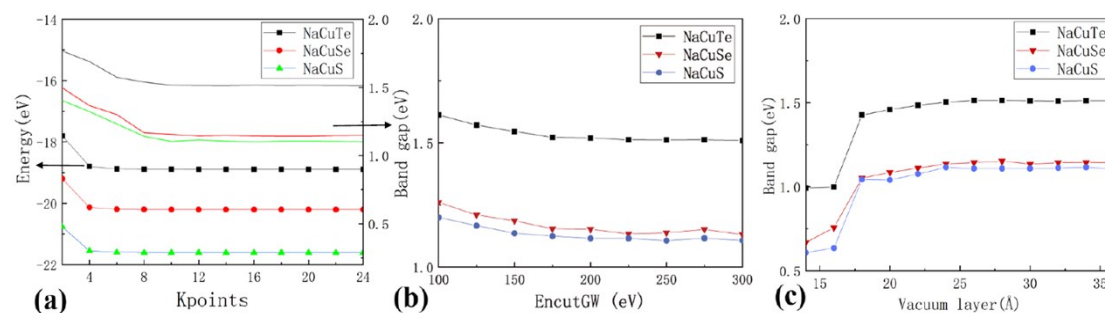

Fig. S1. Convergence test of GW parameters: (a) kpoints, (b) encutGW, (c) vacuum layer.

Through the convergence test in Fig. S1, the k-points in GW calculation was set to 12 × 12 × 1. The GW energy cut off was 250eV, which is converged to the band gap. The GW band gap are also sensitive to vacuum thickness. In order to get an accuracy result, we set the vacuum thickness to be 30Å.

[1] *School of Physics, State Key Laboratory of Crystal Materials, Shandong University, Jinan 250100, China.*
[2] *School of Intelligent Engineering, Shandong Management University, Jinan 250357, China*
[3] *School of Physics and Microelectronics, Zhengzhou University, Zhengzhou 450001, China*
[4] *Department of Physics, Jining University, Qufu 273155, China.*
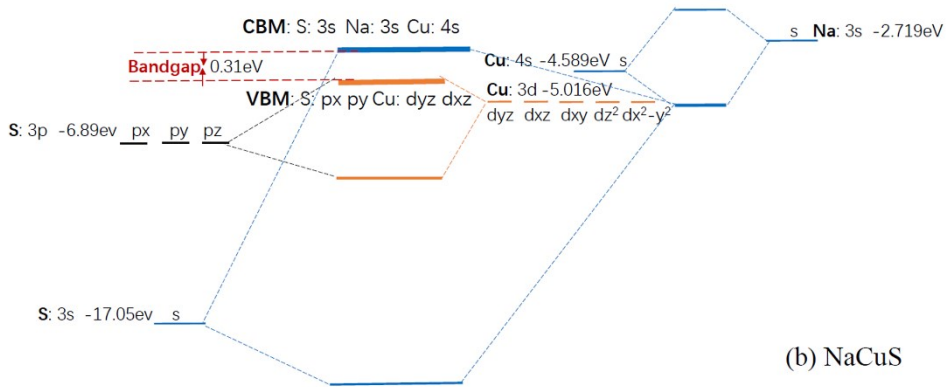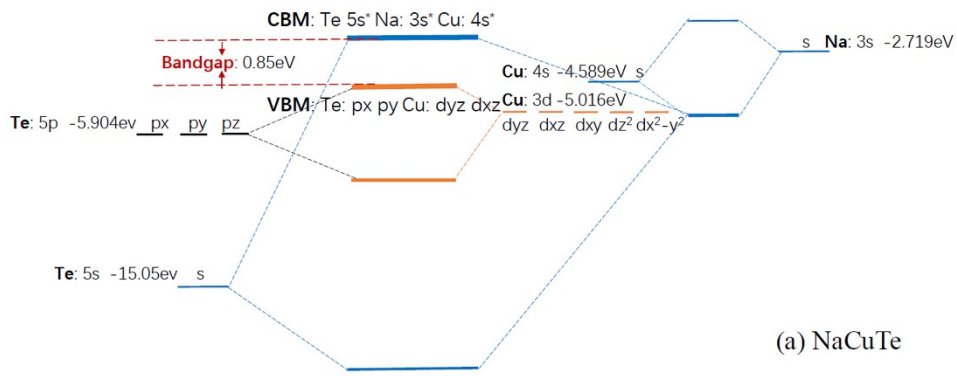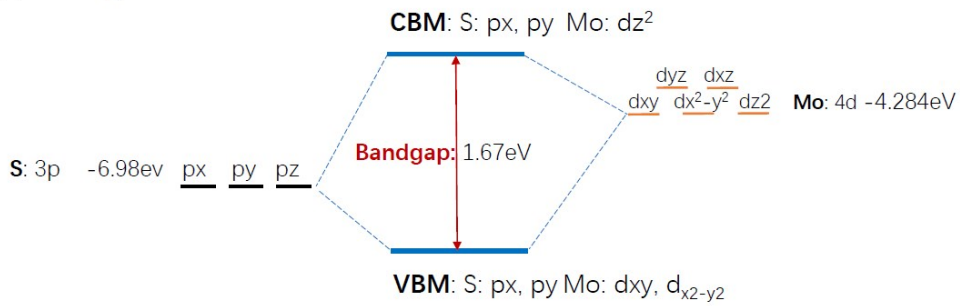*Email: cuibin@sdu.edu.cn ,liuds@sdu.edu.cn*

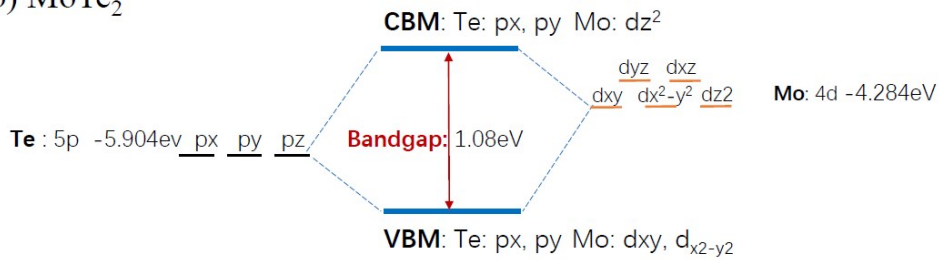Fig. S2. Schematic illustration of the hybridization of NaCuTe and NaCuS.

Fig. S3. Schematic illustration of the hybridization of MoS_2 and $MoTe_2$.

By analyzing the energy band composition, we found that the CBMs (VBMs) of NaCuX are formed by the s orbitals of Na, Cu, and X atoms (d orbitals of Cu and p orbitals of X atoms), while, those of MoX_2 are composed by the d orbital of Mo and the p orbitals of X atoms (d orbitals of Mo and p orbitals of X atoms). Then we plot the schematic diagram of the energy levels at the Γ-point of NaCuX and MoX_2.

For NaCuX, the energy difference of the outmost s and p orbitals of X atoms majorly determines the bandgap tendency. From S to Te, the s-orbital enhancement is bigger than that of p orbital, and therefore, the CBM is of a bigger raise than the VBM. So, the bandgap increases from NaCuS to NaCuTe, as depicted in Fig S2.

On the contrast, for MoX_2, the energy distance of the p orbitals of X and d orbitals of Mo atoms is responsible for the band gap trend. As the p orbital increases from S to Te, the bandgap shrinks accordingly, as shown in Fig. S3.
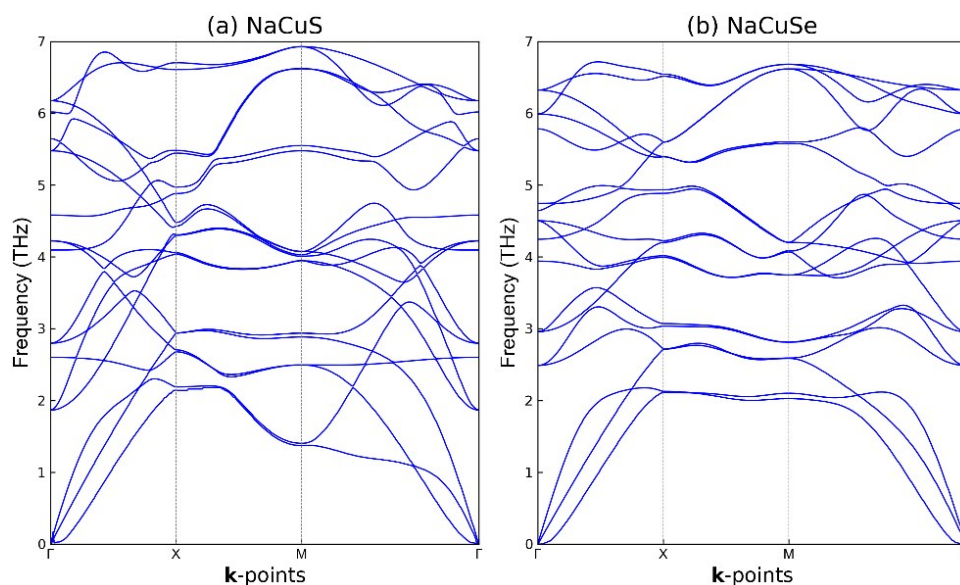

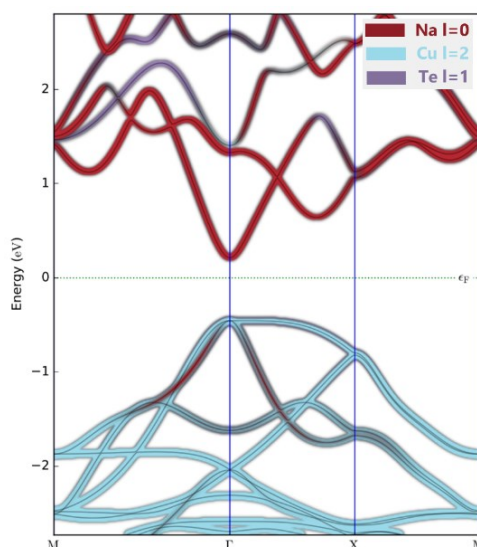Fig. S4. Phonon dispersion curves of the NaCuS and NaCuSe monolayer.

Fig. S5. Projected bandstructure of NaCuTe. Red, light blue, and violet colors respectively represent s orbital of Na atom, d orbital of Cu atom, and p orbital of Te atom.