Efficient Absorption of Cu_2WX_4 (X = S, Se, Te) for Photovoltaic Application: A Theoretical Study

[1,2]Jiaxi Zhang, [1]Zhenghao Li, [1]Fengxiao Che, [1]Chong Li, [1]Kai Han*, [1]Hongchao Yang*

[1]School of Physics and Electronic Information, Weifang University, Weifang 261061, China

[2]School of Electronic Information Engineering, Shandong University of Science and Technology, Qingdao 266590, China

*Corresponding authors: hc_yang90@163.com; hankai@wfu.edu.cn

Computational methods

According to the DP theory, the 2D carrier mobility μ can be described by the following equation:[1]

$$\mu = \frac{e\hbar^3 C}{3k_B T|m_{e/h}^*|^2 (E_d)^2}$$

where e, $\hbar$, k_B, and T are the electron charge, the reduced Planck constant, the Boltzmann constant, and the temperature, respectively. C is the elastic modulus and E_d is the deformation potential. $m_{e/h}^* = \pm \hbar^2 (\frac{d^2 E_k}{dk^2})^{-1}$ is the effective mass.

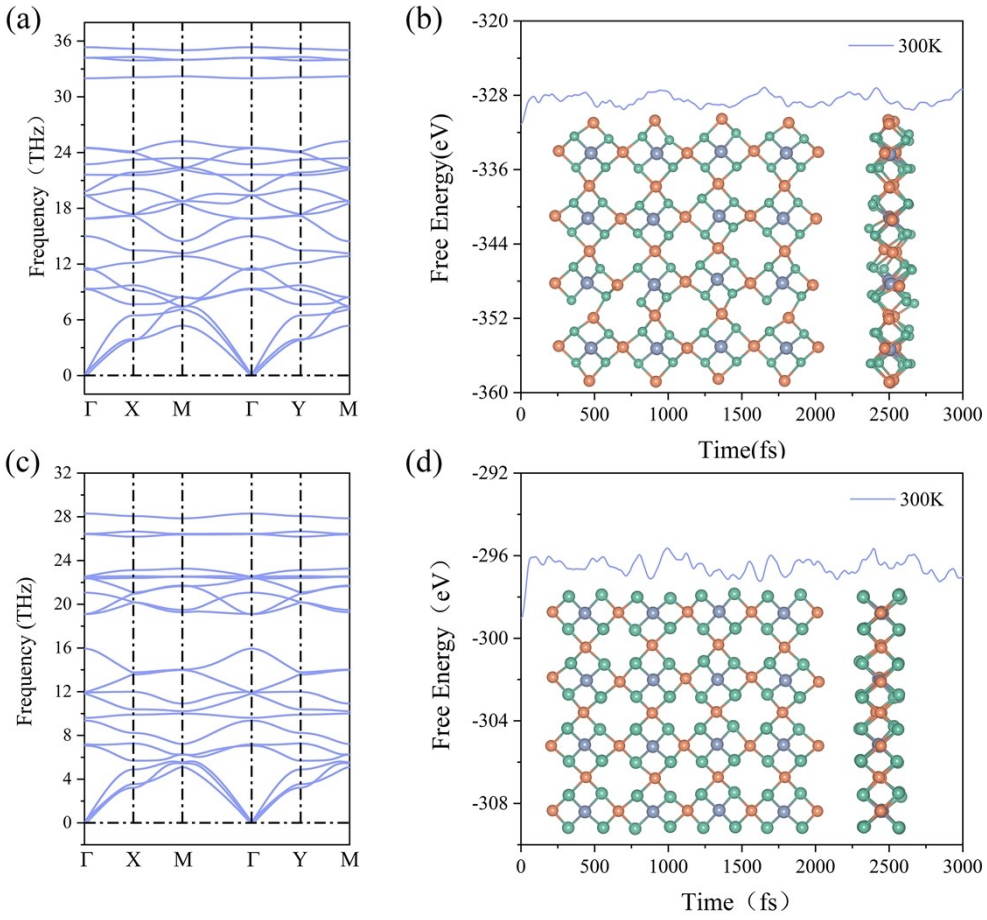

Fig. S1 (a) Phonon spectrum and (b) variation of total energy of the Cu_2WSe_4 monolayer. (c) Phonon spectrum and (d) variation of total energy of the Cu_2WTe_4 monolayer. The insets in (b) and (d) are top and side views of the snapshot at the end of simulation of Cu_2WSe_4 and Cu_2WTe_4, respectively.

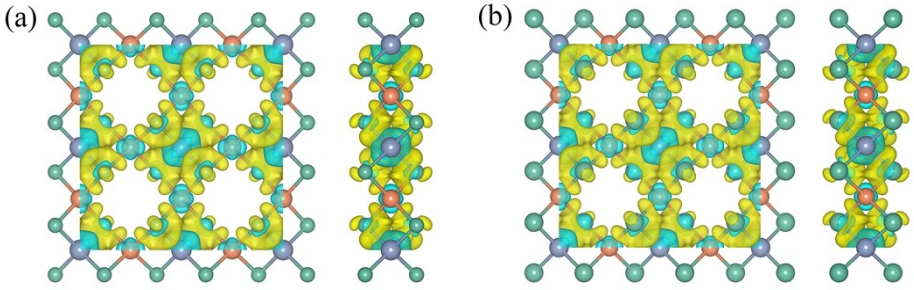

Fig. S2 The calculated charge density difference of (a) Cu_2WSe_4 and (b) Cu_2WTe_4. The isosurface value is set to 0.06 eÅ^{-3}. The cyan and yellow regions represent electron depletion and accumulation, respectively.

Reference

1 J. Bardeen and W. Shockley, *Phys. Rev.*, 1950, **80(1)**, 72.