Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

SUPPLEMENTARY MATERIALS

Novel *p*-type thermoelectric materials Cu_3MCh_4 (M = V, Nb, Ta; Ch = Se, Te): High band degeneracy

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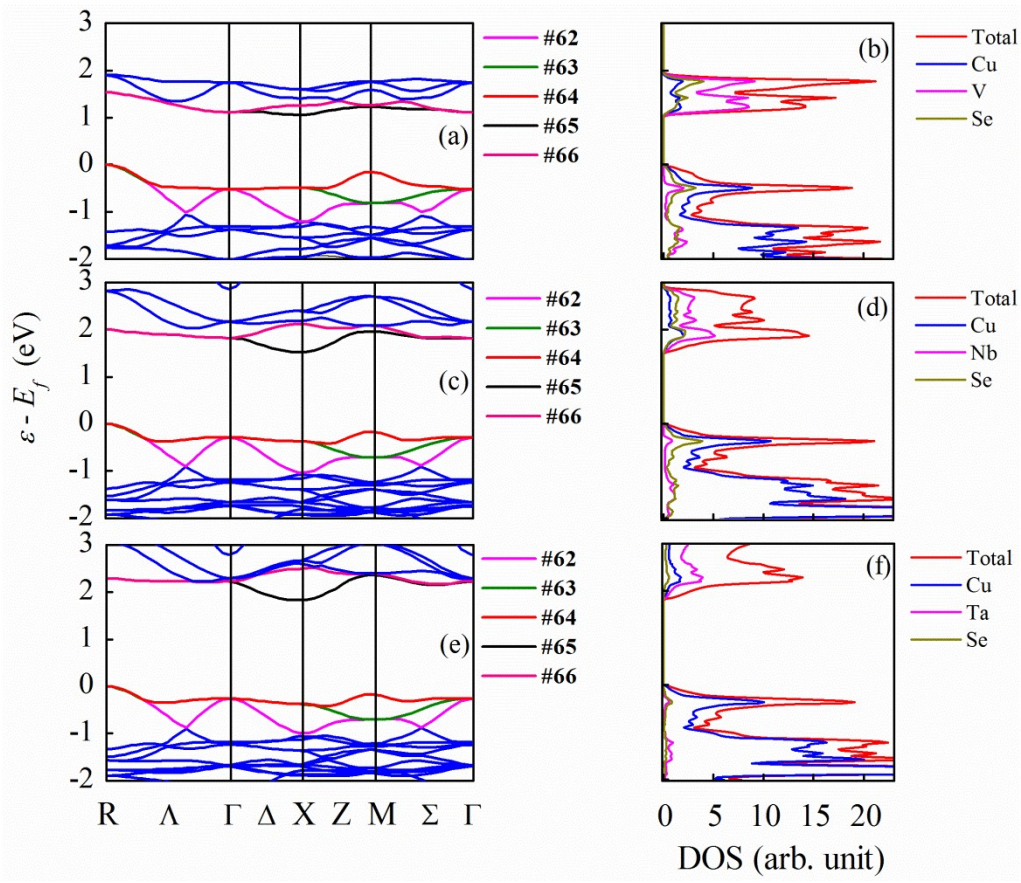

Figure S1. The calculated band structure of Cu_3VSe_4 (a), Cu_3NbSe_4 (c), and Cu_3TaSe_4 (e), as well as the calculated total and partial DOS data of Cu_3VSe_4 (b), Cu_3NbSe_4 (d), and Cu_3TaSe_4 (f), respectively.

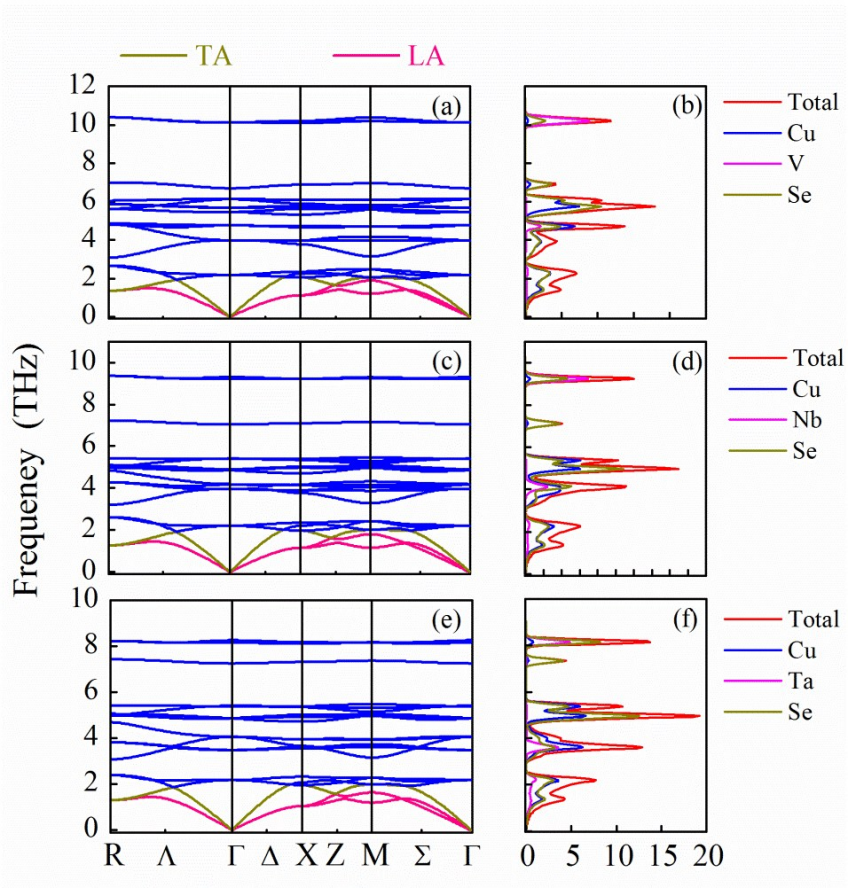

Figure S2. The calculated phonon spectra of Cu_3VSe_4 (a), Cu_3NbSe_4 (c), and Cu_3TaSe_4 (e), as well as the calculated total and partial phonon DOS data of Cu_3VSe_4 (b), Cu_3NbSe_4 (d), and Cu_3TaSe_4 (f).

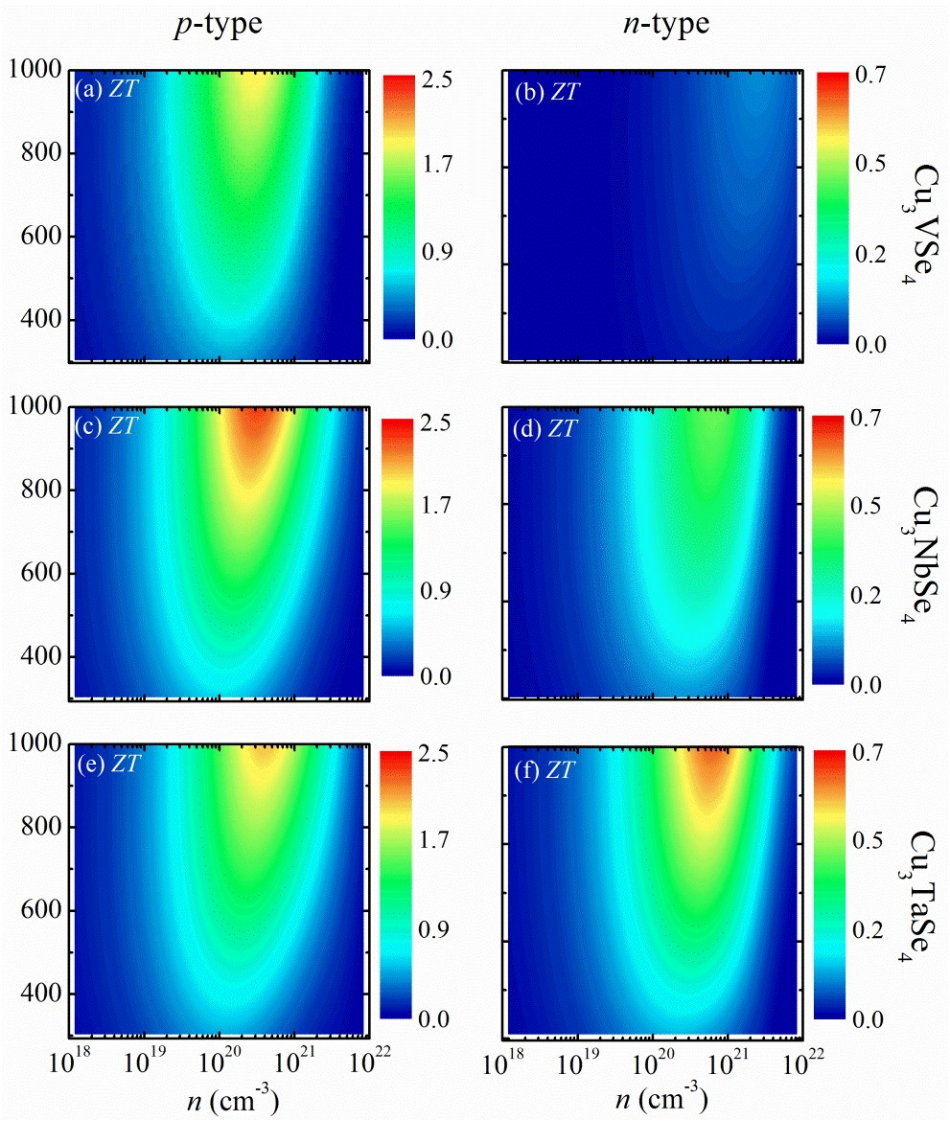

Figure S3. The temperature *T* and carrier density *n* dependences of the *ZT* values of the *p*-type Cu_3VSe_4 (a), Cu_3NbSe_4 (c), and Cu_3NbSe_4 (e), as well as the *n*-type Cu_3VSe_4 (b), Cu_3NbSe_4 (d), Cu_3NbSe_4 (f).