Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information for

Super high-performance 7-atomic-layer thermoelectric materials $ZrGe_2N_4$

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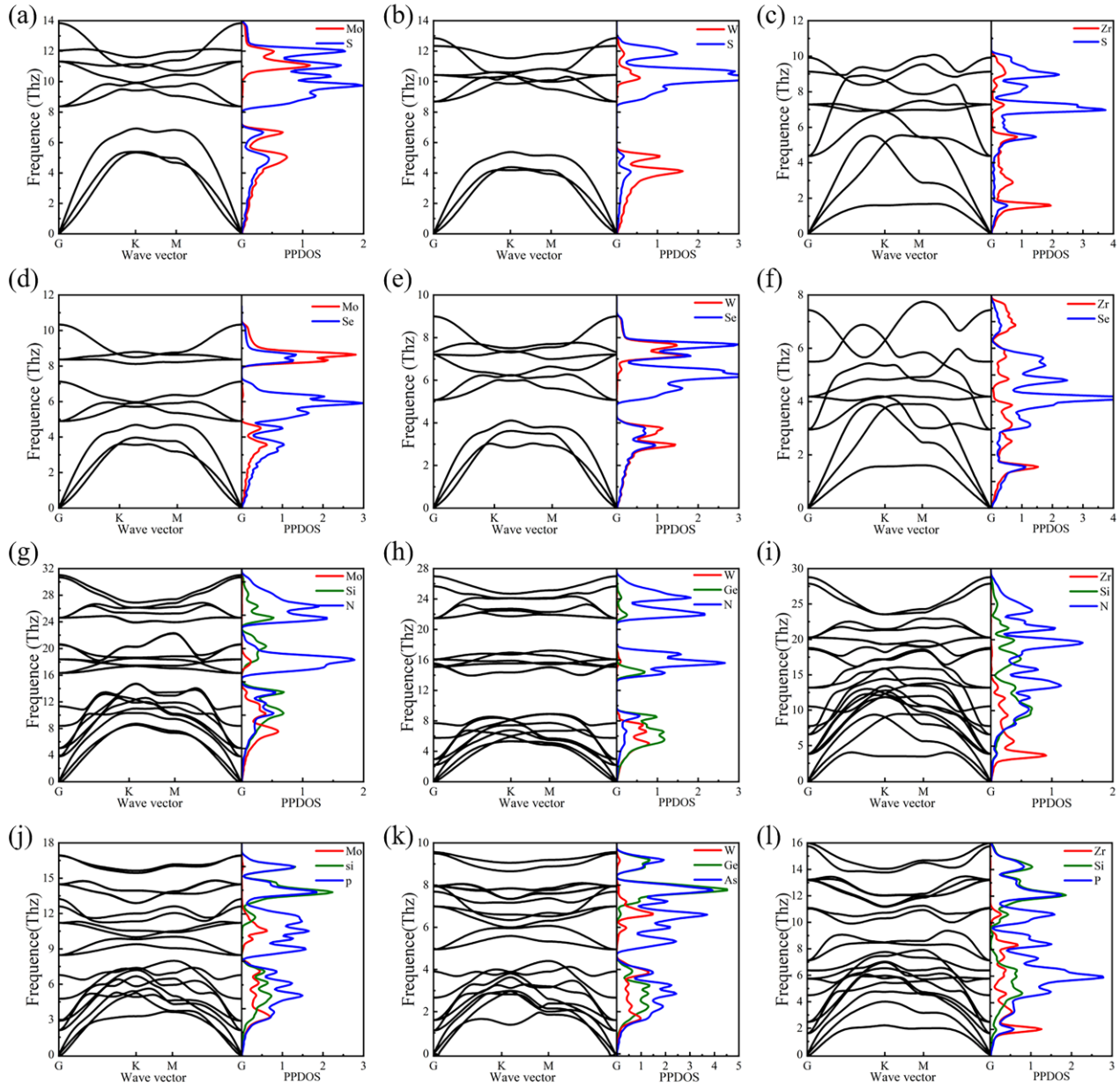

Figure S1. Phonon spectra and phonon projection density of states (PPDOS) of (a) 3-atomic-layer MoS_2, (b) 3-atomic-layer WS_2, (c) 3-atomic-layer ZrS_2, (d) 3-atomic-layer $MoSe_2$, (e) 3-atomic-layer WSe_2, (f) 3-atomic-layer $ZrSe_2$, (g) 7-atomic-layer $MoSi_2N_4$, (h) 7-atomic-layer WGe_2N_4, (i) 7-atomic-layer $ZrSi_2N_4$, (j) 7-atomic-layer $MoSi_2P_4$, (k) 7-atomic-layer WGe_2As_4 and (l) 7-atomic-layer $ZrSi_2P_4$.

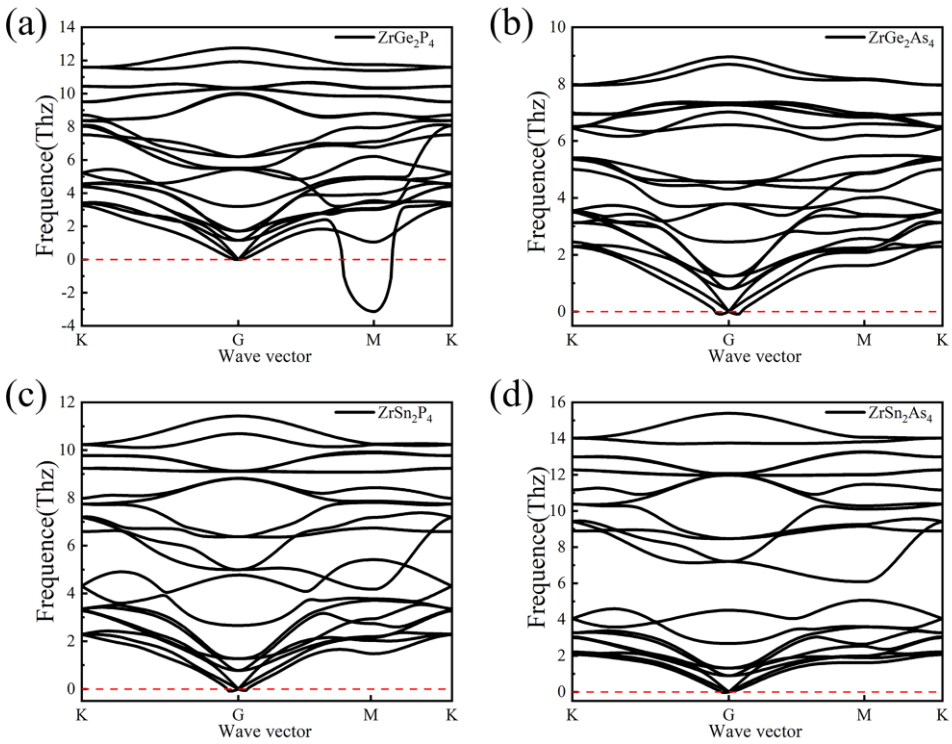

Figure S2. Phonon spectra of (a) 7-atomic-layer $ZrGe_2P_4$, (b) 7-atomic-layer $ZrGe_2As_4$, (c) 7-atomic-layer $ZrSn_2P_4$, (d) 7-atomic-layer $ZrSn_2As_4$.

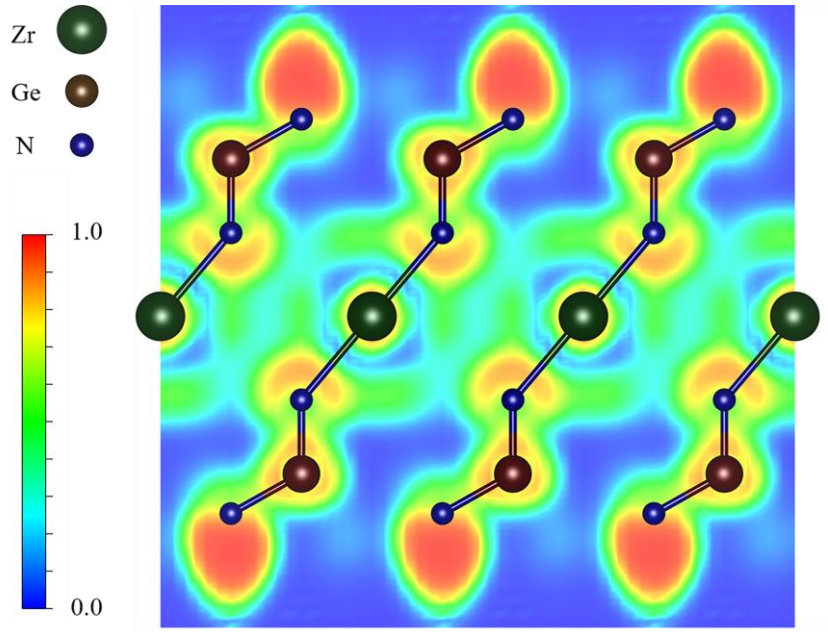

Figure S3. 2D view of the electron localization function (ELF) of $ZrGe_2N_4$, 1 and 0 correspond to the areas with perfectly localized and vanished electron density, respectively

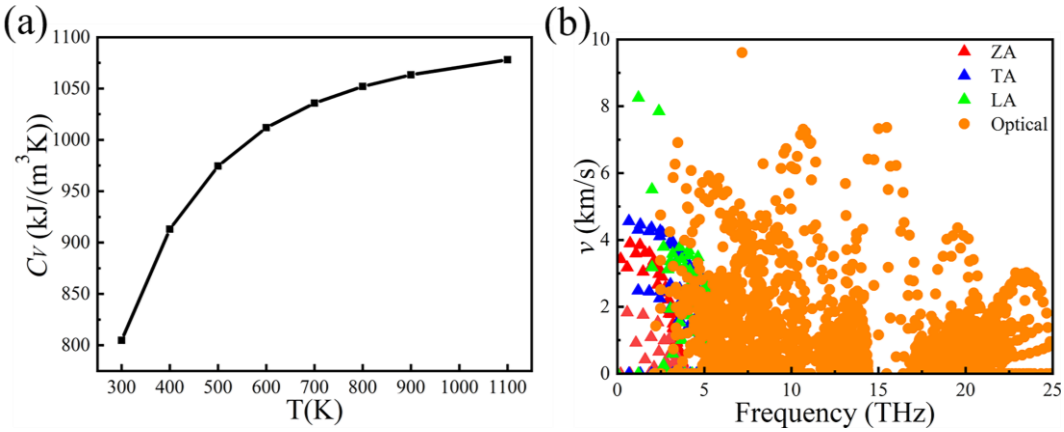

Figure S4. (a) Specific heat capacity (C_V) of 7-atomic-layer $ZrGe_2N_4$. (b) Phonon group velocity (ν) of 7-atomic-layer $ZrGe_2N_4$

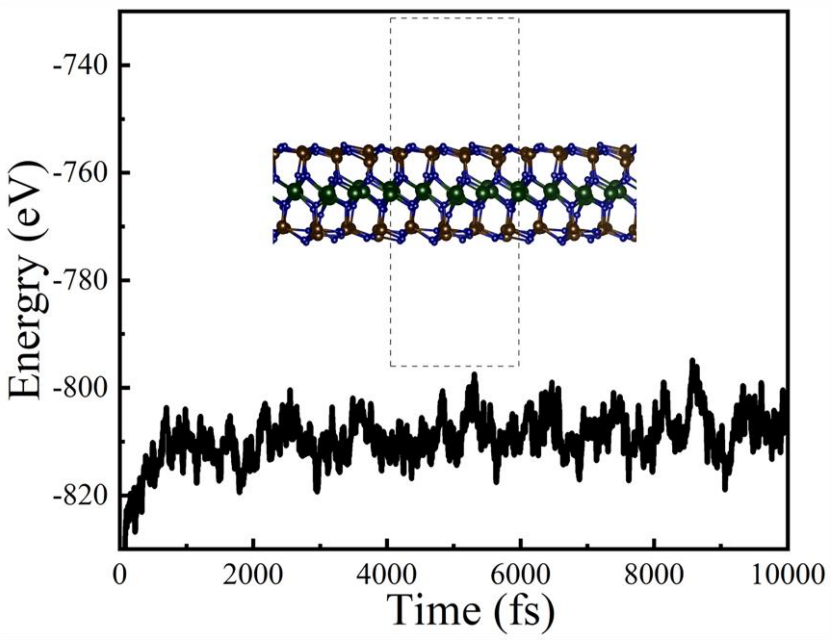

Figure S5. Time-dependent energy of 7-atomic-layer $ZrGe_2N_4$ at 2000 K. Inset: Relaxation structure at 2000 K.