Supporting Information

Novel layered As_2Ge with pentagonal structure for potential thermoelectrics

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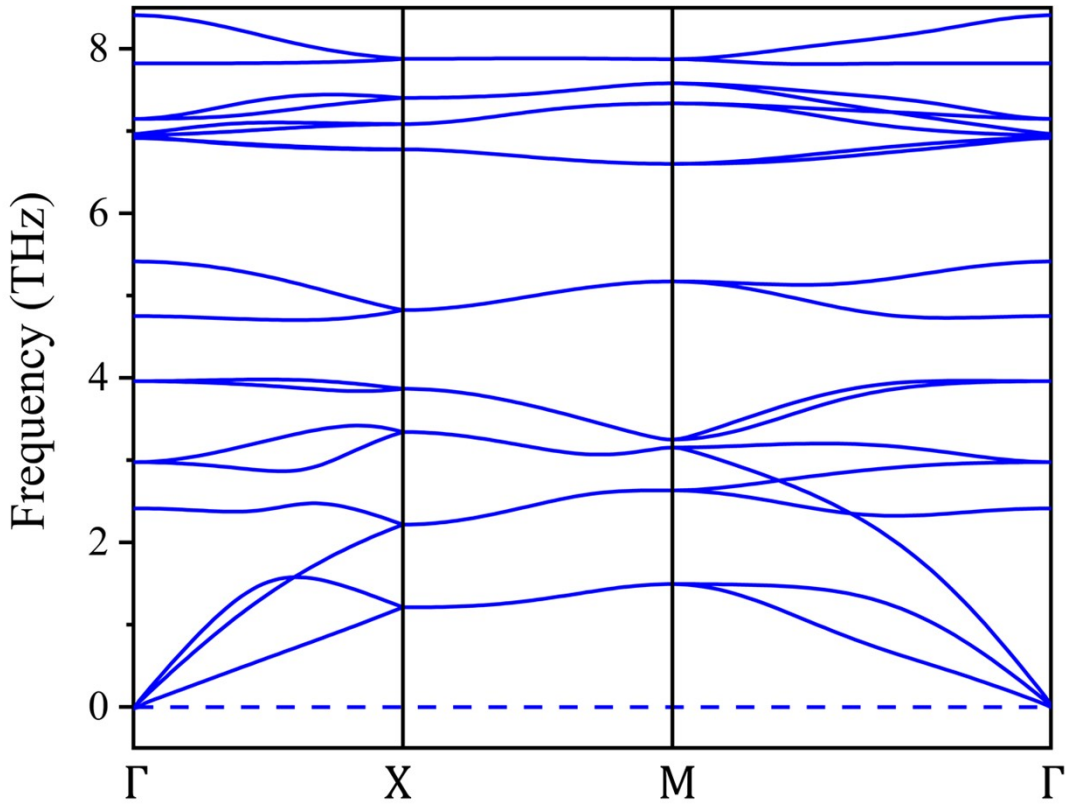

Fig. S1 Phonon dispersion of the As_2Ge monolayer.

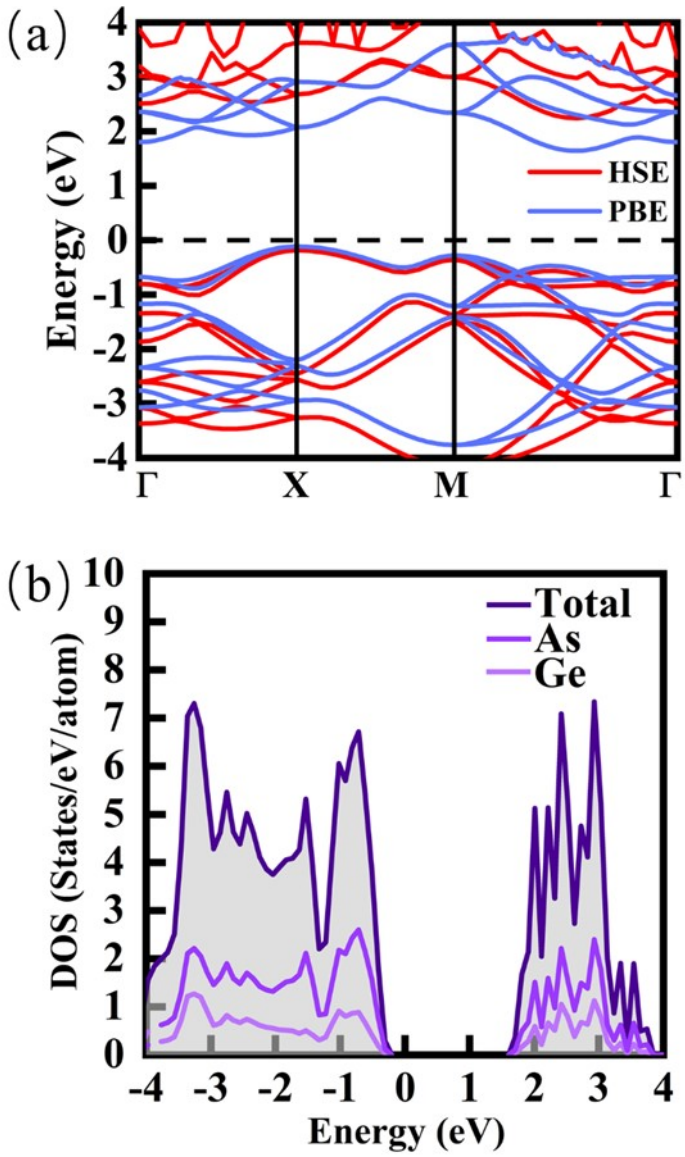

Fig. S2 (a) PBE and HSE band structure of As_2Ge monolayer and (b) corresponding partial and total state of density.

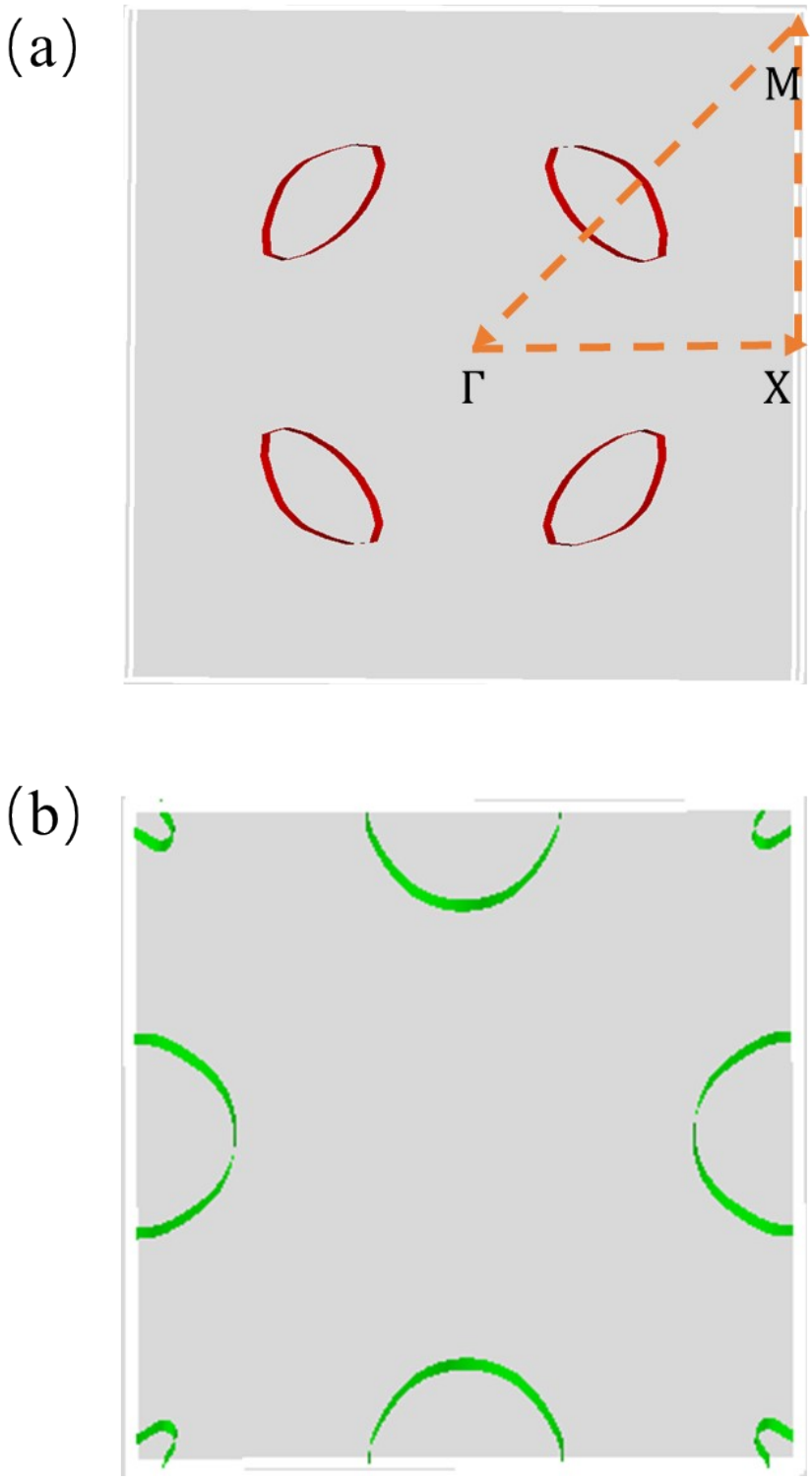

Fig. S3 Calculated constant energy surfaces for As_2Ge monolayer with (a) the energy level of 0.1 eV higher than CBM and with (b) energy level of 0.2 eV lower than VBM.

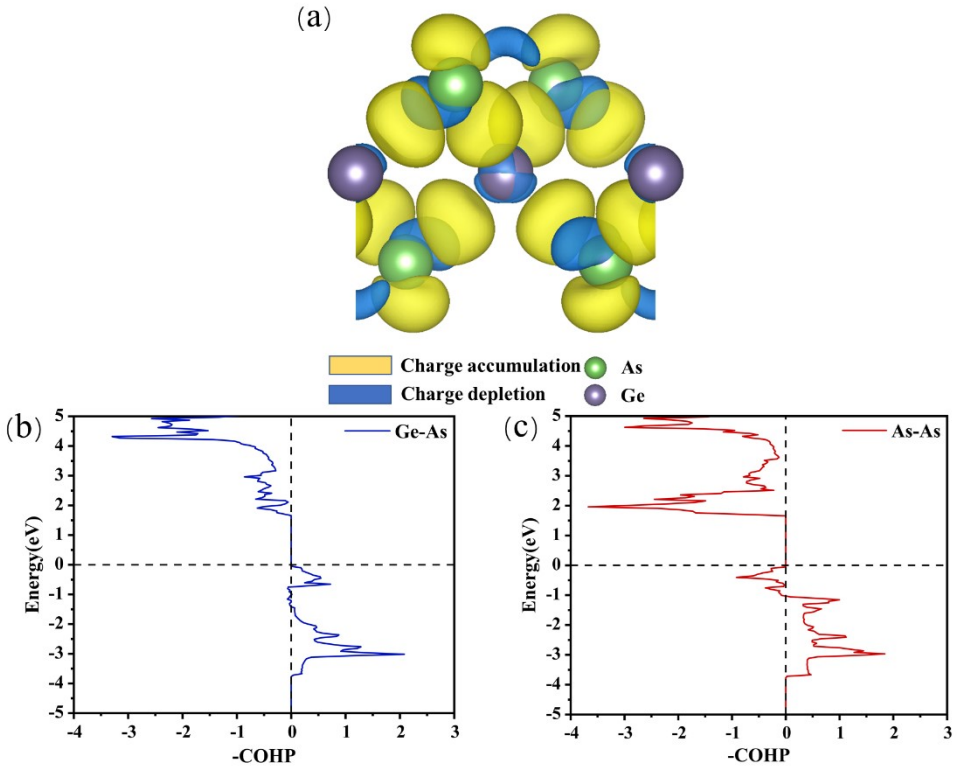

Fig. S4 (a) The charge density difference, and -COHP curves of (b) Ge-As and (c) As-As bonds.

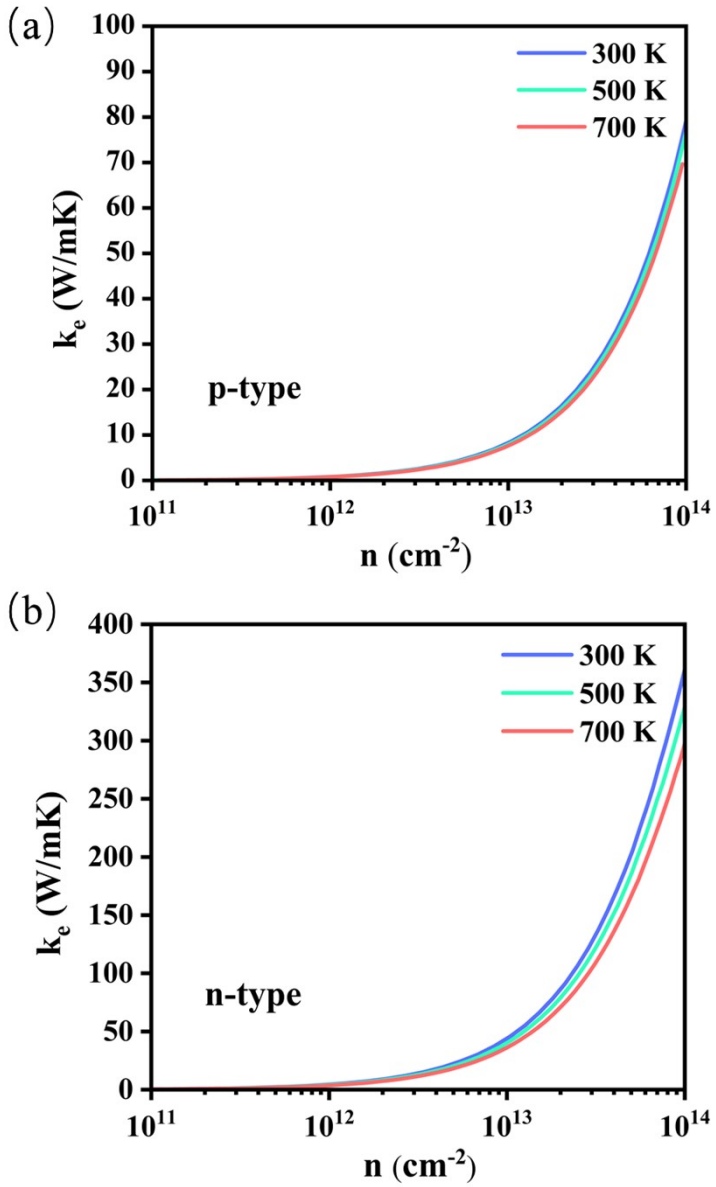

Fig. S5 Calculated electronic thermal conductivity (κ_e) for both (a) p-type and (b) n-type as the functions of carrier concentration of the As_2Ge monolayer.

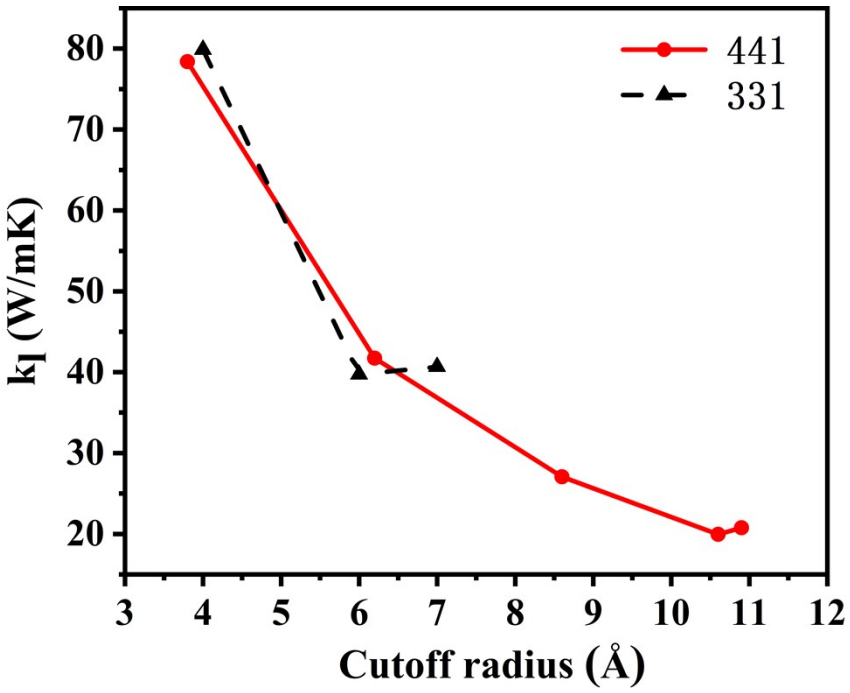

Fig. S6 At 300K, As_2Ge exhibits lattice thermal conductivities of 3 × 3 × 1 and 4 × 4 × 1 supercells in relation to the cutoff radius.