Supporting information

for

Low-cost pentagonal NiX_2 (X=S, Se, and Te) monolayers with strong anisotropy as potential thermoelectric materials

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Contents

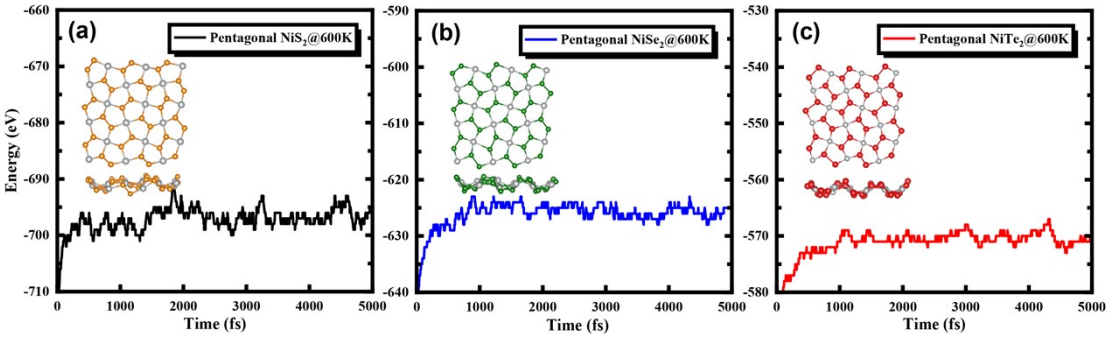

Figure S1. The snapshots of AIMD simulations of the pentagonal NiX_2 (X = S, Se, and Te) monolayers at 600K. The Ni, S, Se, and Te atoms are represented by the gray, yellow, green, and red balls, respectively.

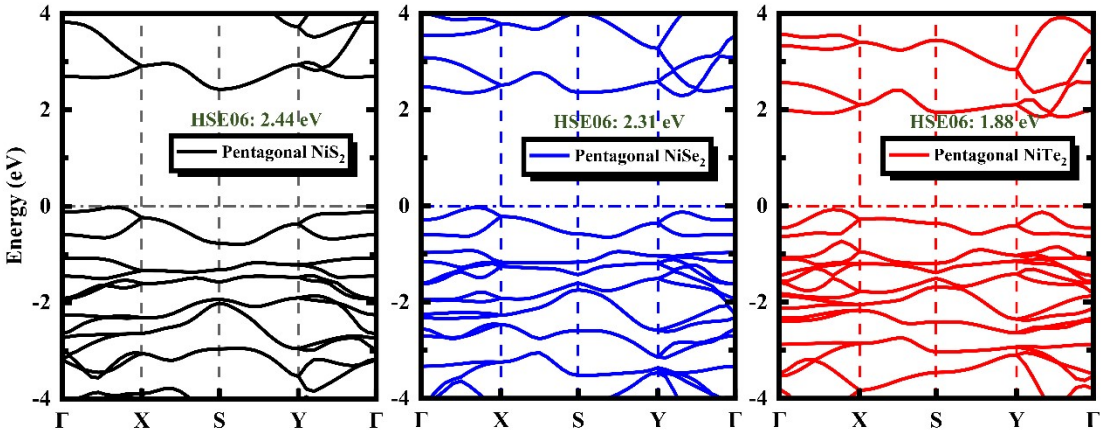

Figure S2. Electronic band diagrams of the pentagonal NiX_2 (X = S, Se, and Te) obtained by HSE06 method.

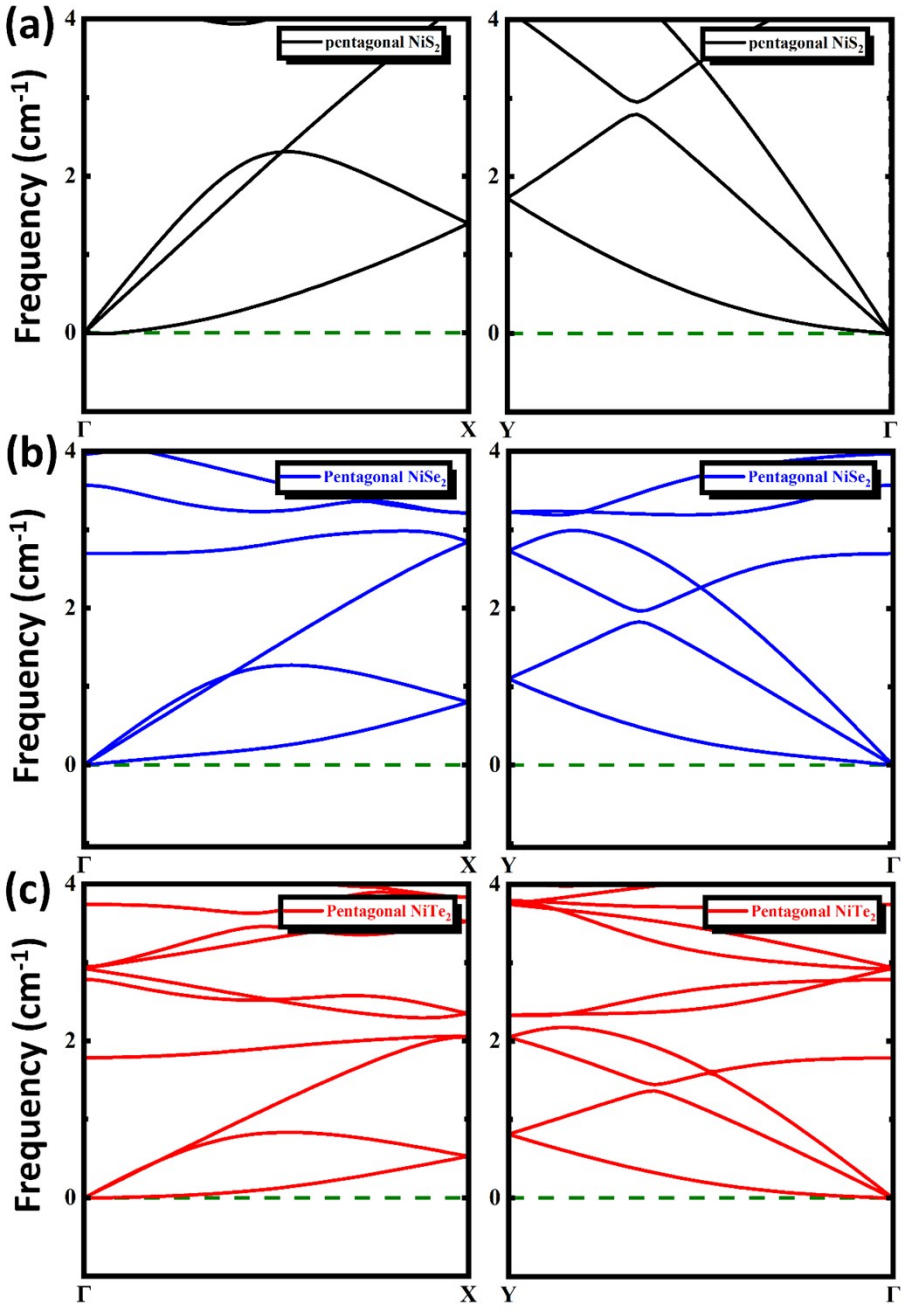

Figure S3. The magnified images of the lowest-lying acoustic frequencies in the phonon dispersion diagrams of the NiX_2 (X = S, Se, and Te) monolayers near the Γ point.

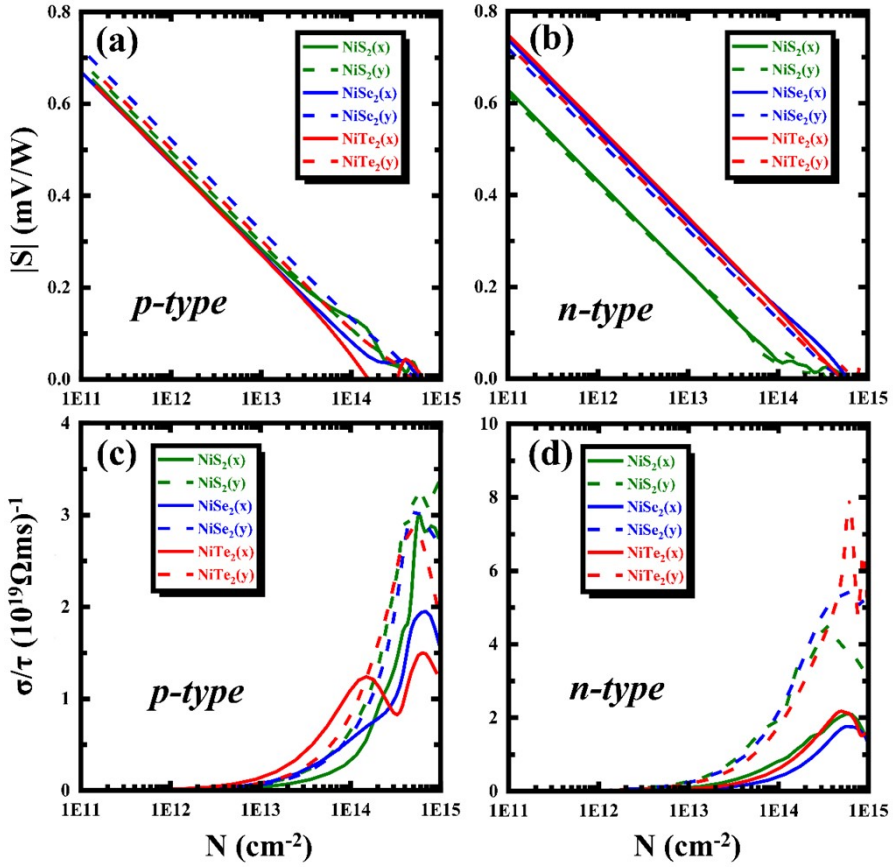

Figure S4. Seebeck coefficient (*S*) and electronic conductivity corresponding to relaxation time (σ/τ) as a function of carrier concentration for the *p*-type (a, c) and *n*-type (b, d) pentagonal NiX_2 (X = S, Se, and Te) monolayers at 300K.

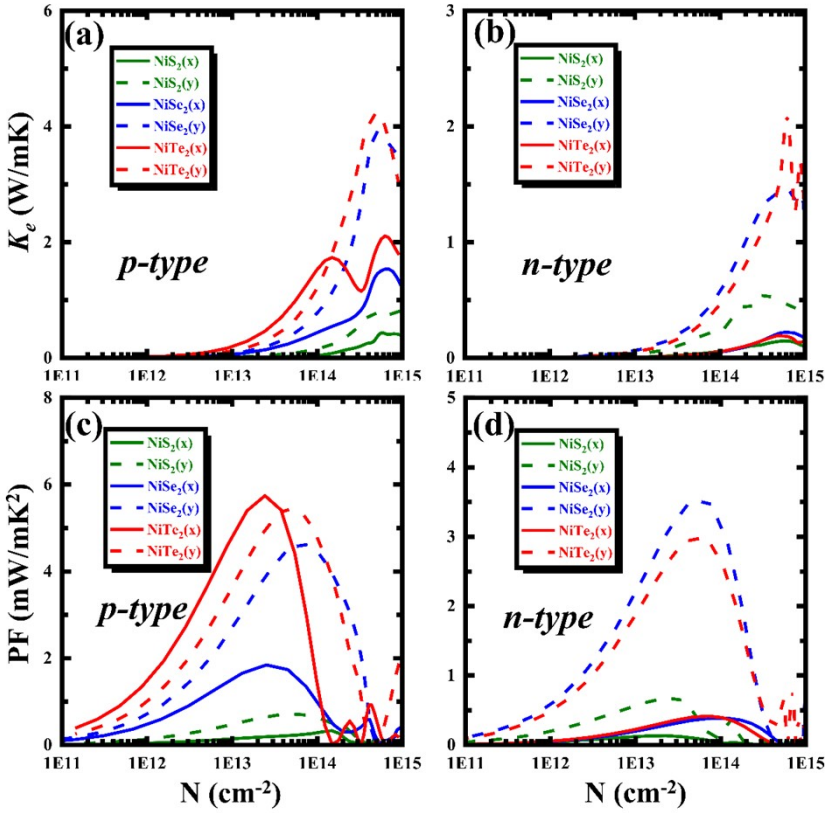

Figure S5. Electronic thermal conductivity (K_e) and Power factor (PF) as a function of carrier concentration for the (a, c) *p*-type and (b, d) *n*-type pentagonal NiX_2 (X = S, Se, and Te) monolayers at 300K.