SUPPLIMENTARY MATERIAL

Enhanced Thermoelectric Performance, Inter-Layer Coupling Effects and Reduced Lattice Thermal Conductivity in Transition Metal Oxide Two-Dimensional Compounds:

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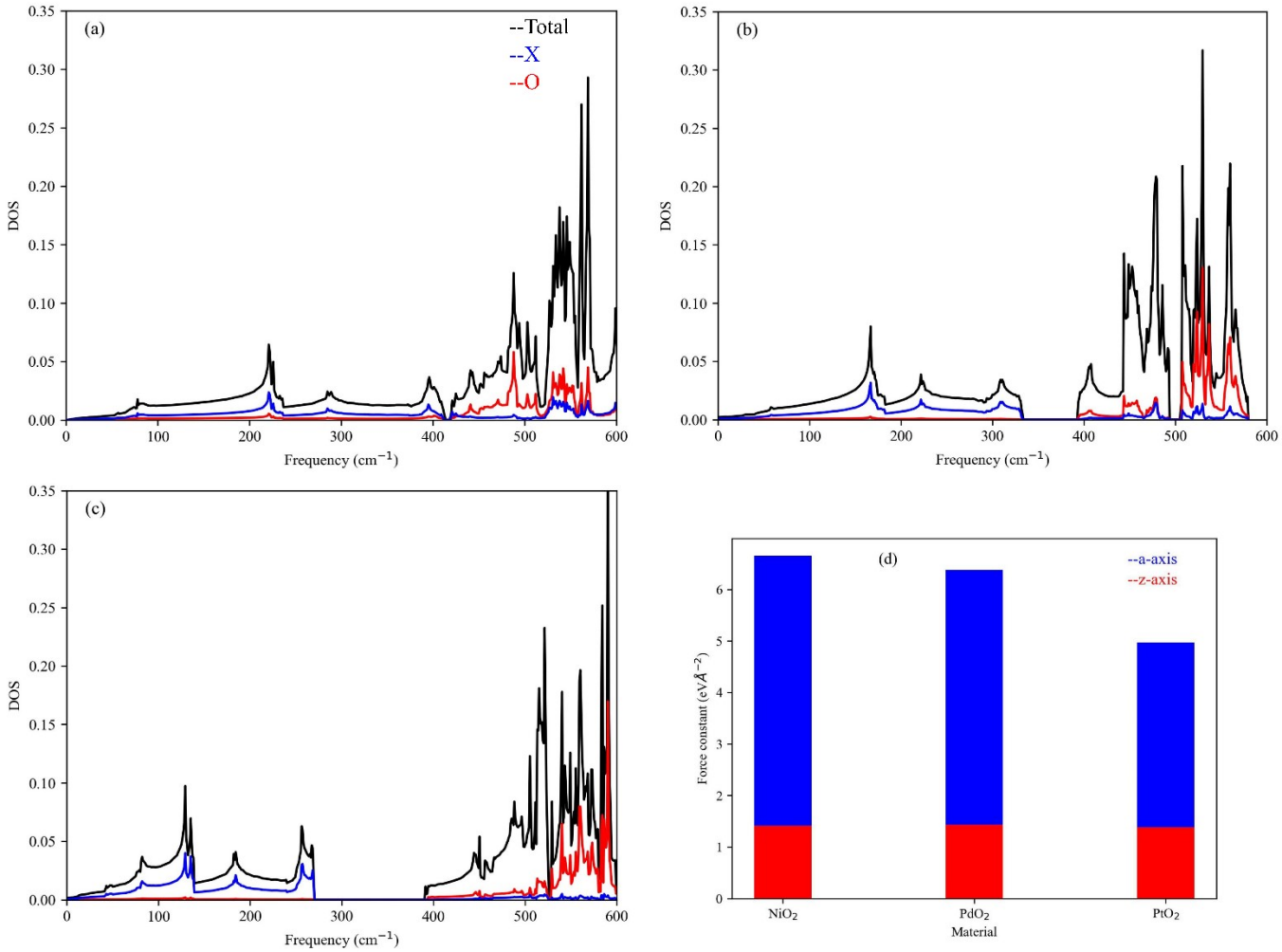

Figure S1. Atom-projected phonon density of states (PDOS) for (a) NiO_2 (b) PdO_2, (c) PtO_2 bilayers, respectively. (d) Harmonic force constants for the nearest-neighbor atom pairs for XO_2 bilayers along a and z-directions.

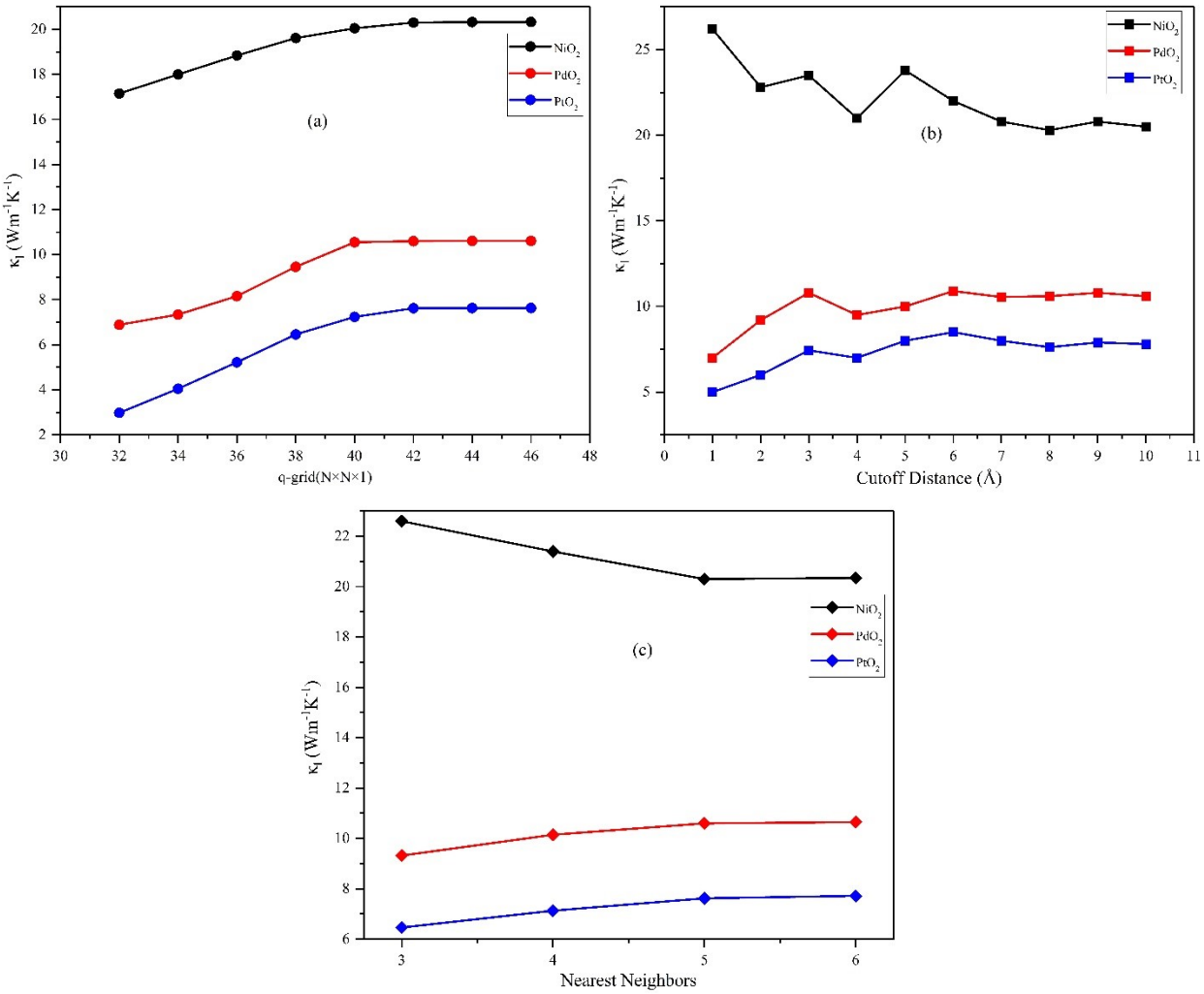

Figure S2. Convergence of lattice thermal conductivity with respect to (a) q-grid, (b) cutoff distance and (c) nearest neighbors of XO_2 (X=Ni, Pd, Pt) bilayers.

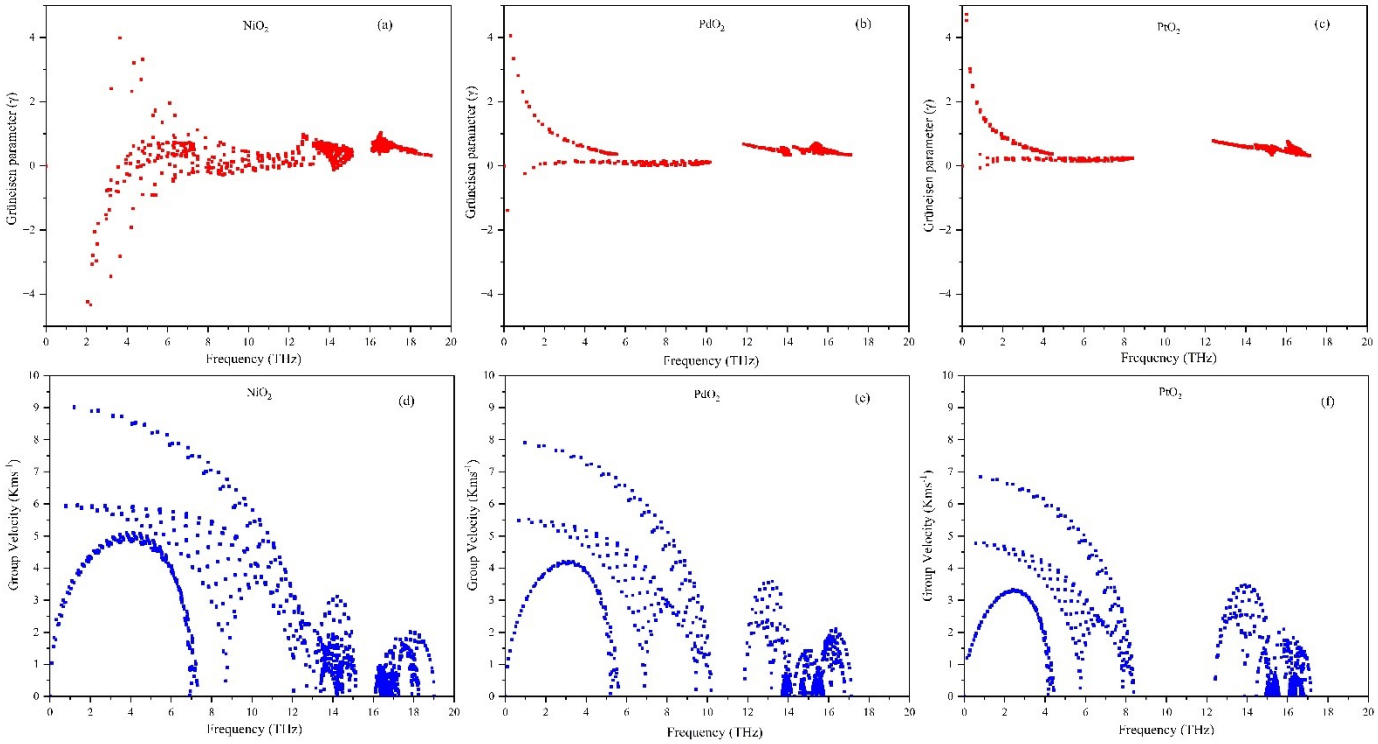

Figure S3. Grüneisen parameter (a, b, c) and group velocity (d, e, f) of NiO_2, PdO_2 and PtO_2 monolayers, respectively, with respect to frequency at room temperature.

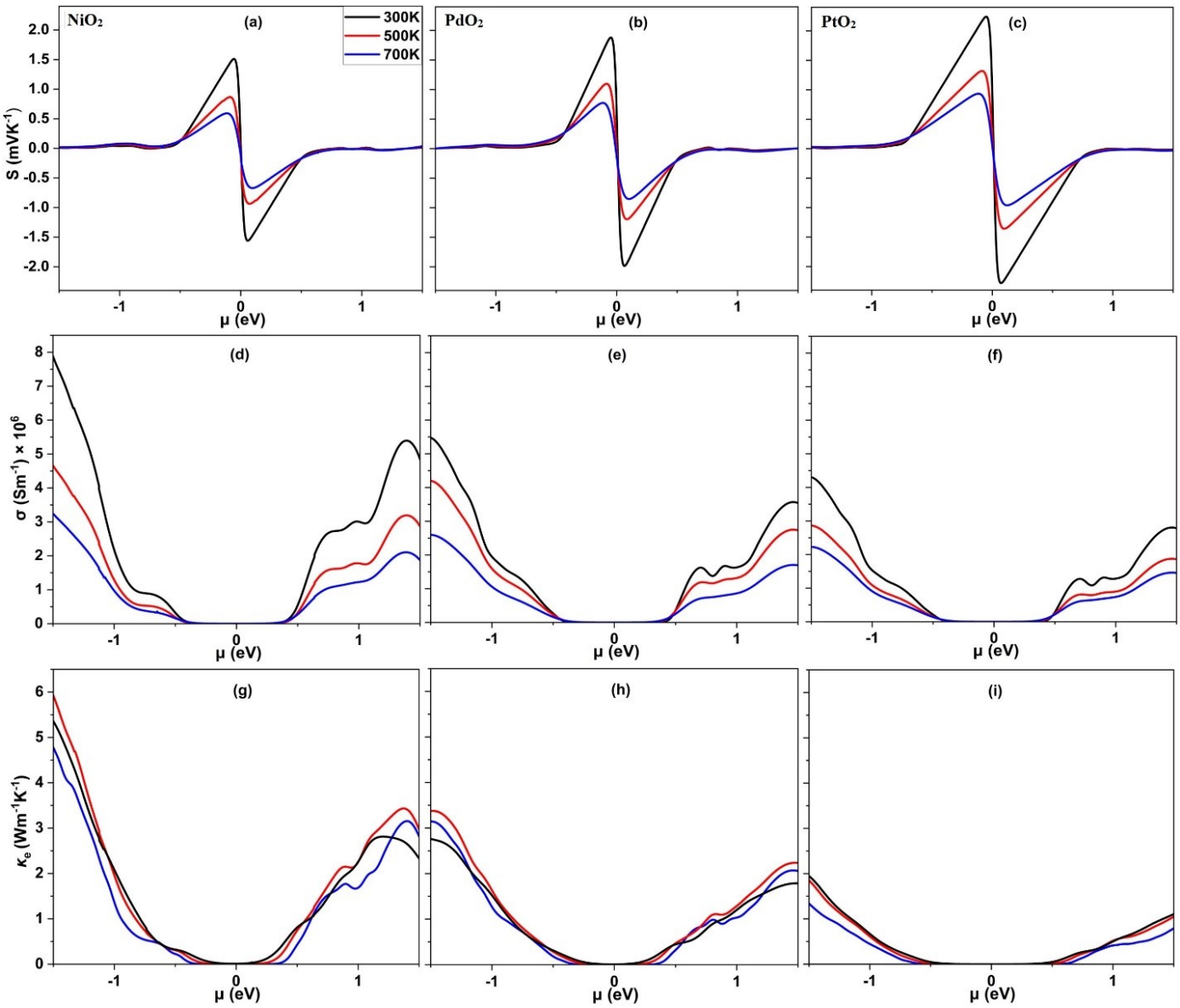

Figure S4. Electronic transport parameters of NiO_2 (left panel), PdO_2 (middle panel) and PtO_2 (right panel) bilayer plotted against chemical potential at various temperatures (300, 500 and 700 K). Seebeck coefficient (S) is shown in a, b, c, electrical conductivity (σ) by d, e, f and electronic thermal conductivity (κ_e) by g, h, i.

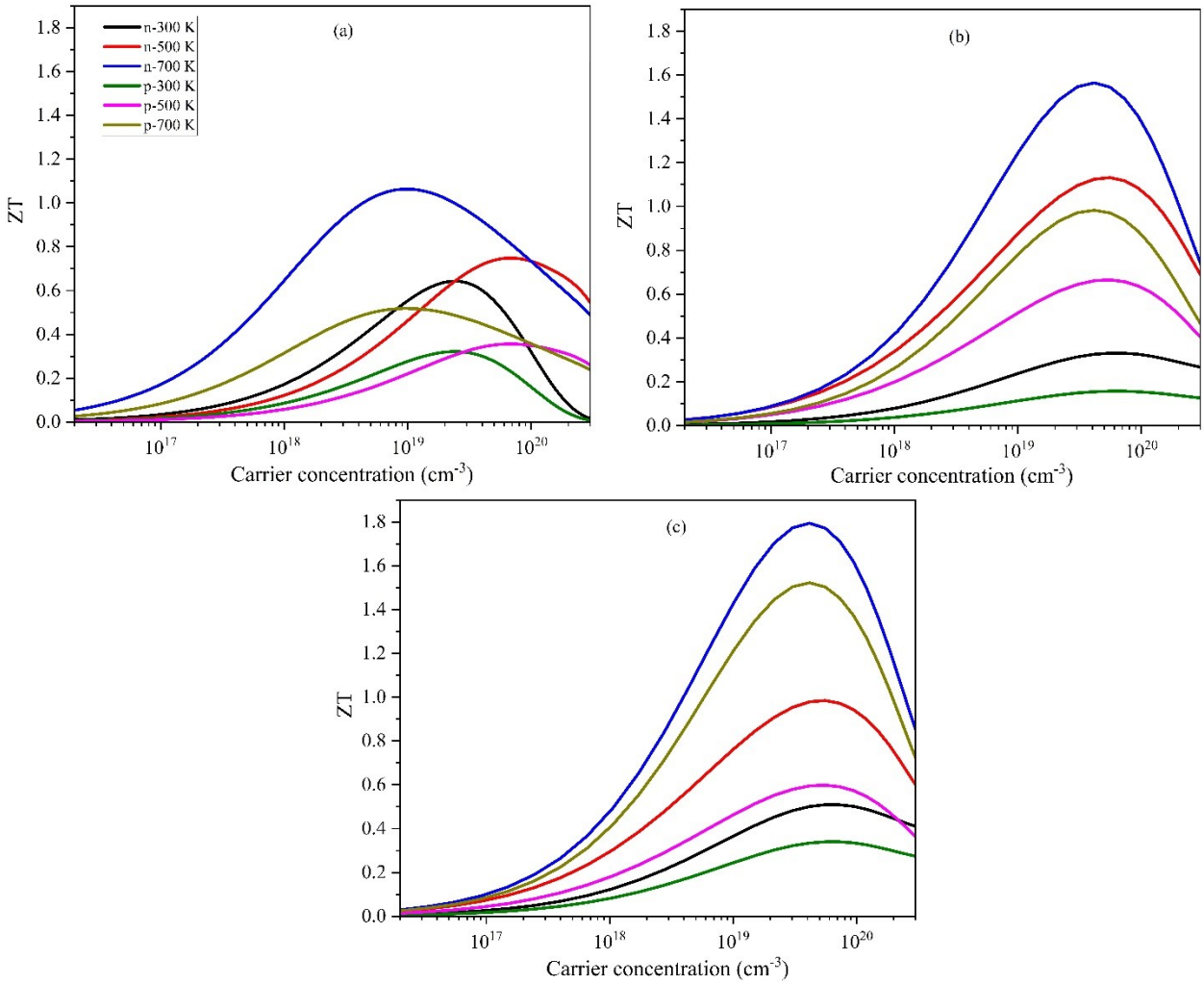

Figure S5. Figure of merit (ZT) as a function of chemical potential at various temperatures. of (a) NiO_2, (b) PdO_2, (c) PtO_2 bilayers.