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Remarkable Thermoelectric Efficiency of Cubic Antiperovskites Rb_3X(Se & Te)I with Strong Anharmonicity

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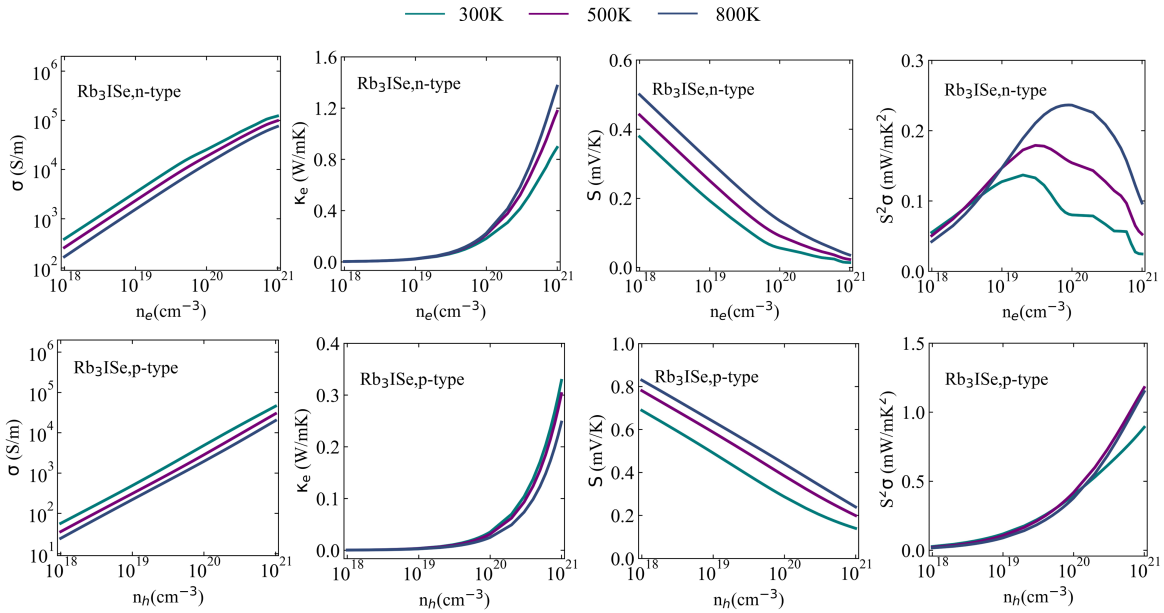

FIG. S1. The calculated electron conductivities σ, electronic thermal conductivity κ_e, Seebeck coefficient S, and power factor (PF), for n-type and p-type doping levels ranging from 1.0×10^{18} to 1.0×10^{21}cm^{-3}, at 300 K, 500 K and 800 K for Rb_3SeI.

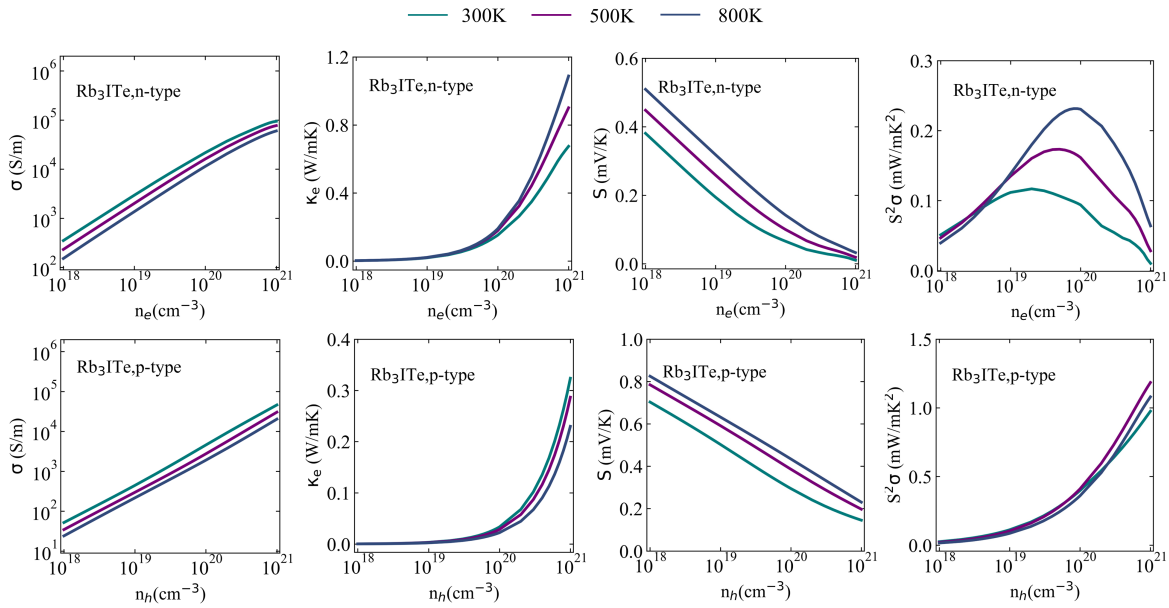

FIG. S2. The calculated electron conductivities σ, electronic thermal conductivity κ_e, Seebeck coefficient S, and power factor (PF), for n-type and p-type doping levels ranging from 1.0×10^{18} to 1.0×10^{21}cm^{-3}, at 300 K, 500 K and 800 K for Rb_3TeI.

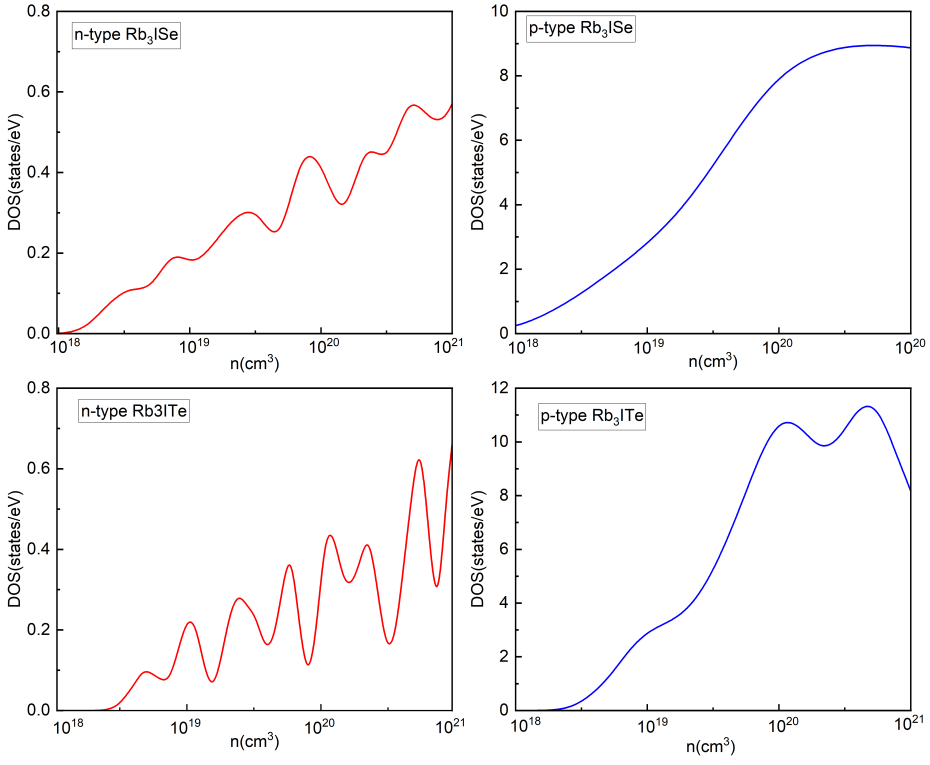

FIG. S3. The DOS values for various doping concentrations at 300 K.