Supporting Information

Evaluating Thermoelectric Properties of $BaTiS_3$ by Density Functional Theory

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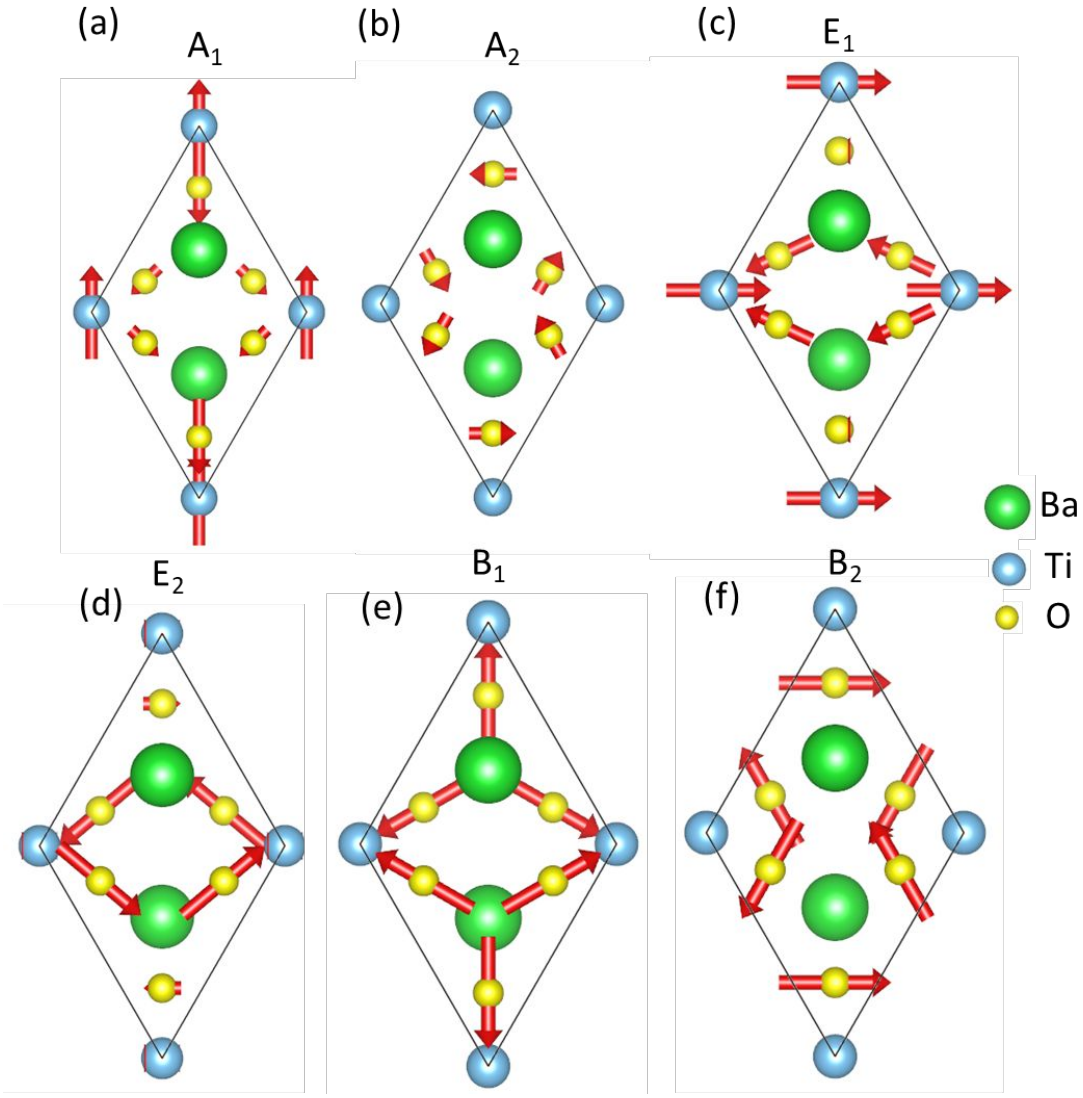

Figure S1. Symmetry resolved phonon modes corresponding to A_1(a), A_2(b), E_1(c), E_2(d), B_1(e) and B_2(f).

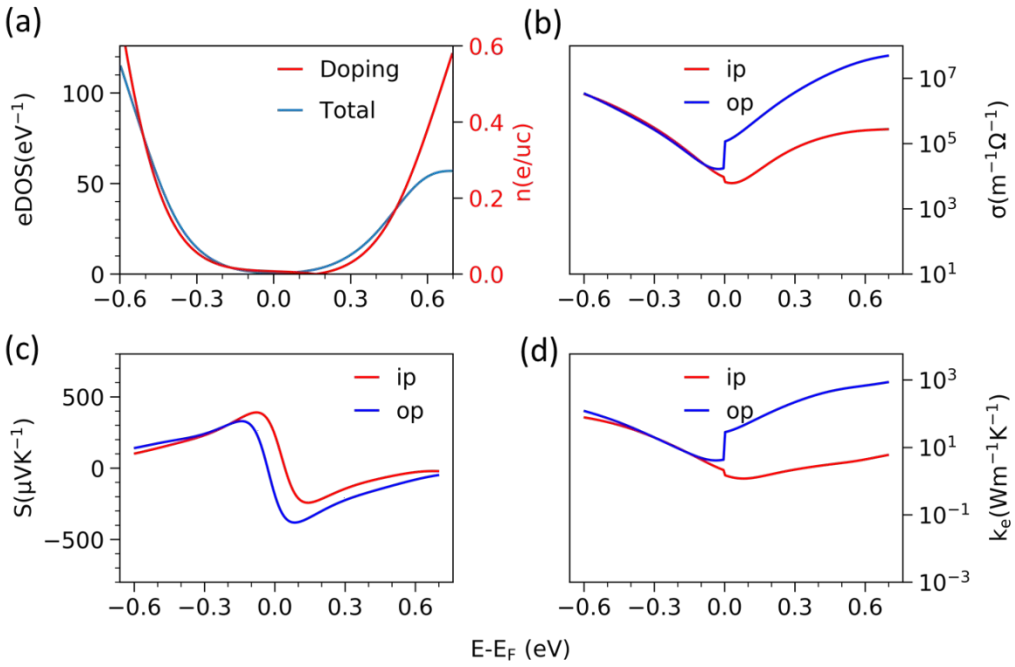

Figure S2. Calculated total electronic density of states, DOS, (in blue color) and doping concentration (in red color) (a) in-plane, ip, (red color) and out-of-plane, op, (blue color) components of transport coefficients: electronic conductivities, σ (b), Seebeck coefficients, S (c), electronic part of thermal conductivities, κ_e (d) at elevated temperature, 800K, plotted as a function of chemical potentials, $\mu_c = E - E_F$.

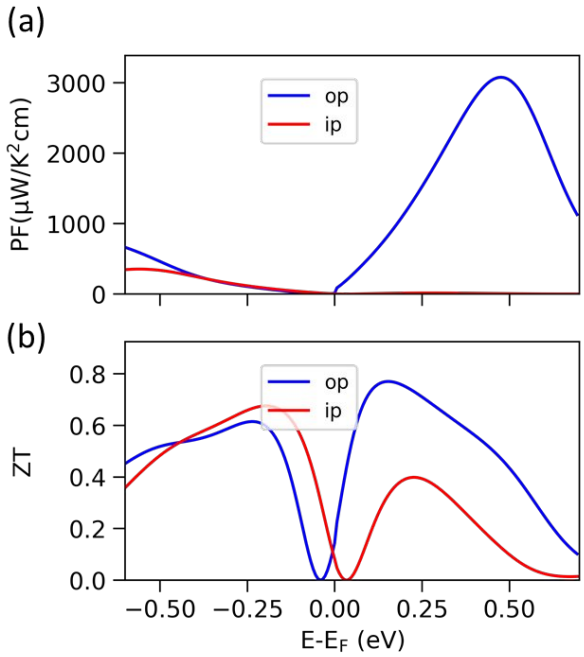

Figure S3. In-plane, ip, (red color) and out-of-plane, op, (Blue color) components of calculated power factor, PF, (a) and thermoelectric figure of merit, ZT, (b) at elevated temperature, 800K, as a function of the chemical potentials, $\mu_c = E - E_F$.

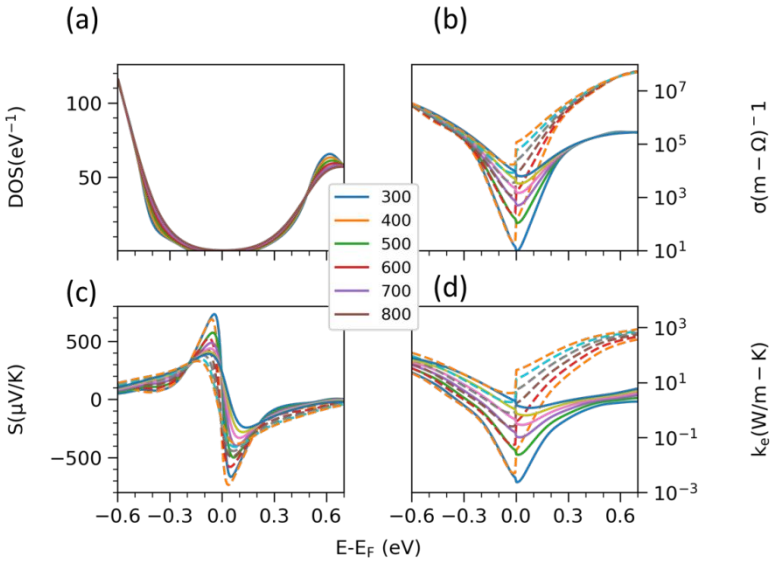

Figure S4. The temperature-dependence of the density of states (DOS) and Inplane (solid line) and out-of-plane (dotted line) (a), electrical conductivity (b), Seebeck Coefficient (c) and electronic part of thermal conductivity (d) plotted as a function of the chemical potentials, $\mu_c = E - E_F$

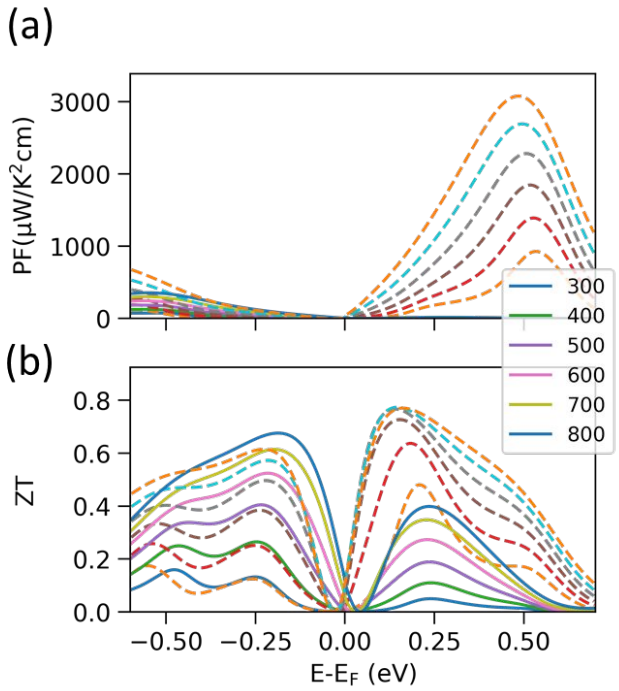

Figure S5. The temperature-dependence of powerfactor (a) and thermoelectric figure of merit (b) plotted as a function of the chemical potentials, $\mu_c = E - E_F$

Table S1. Cell parameters and atomic positions, a part of Quantum Espresso input file.

CELL_PARAMETERS {angstrom}

3.365975391	-5.830040394	0.000000000
3.365975391	5.830040394	0.000000000
0.000000000	0.000000000	5.928950129

ATOMIC_POSITIONS {crystal}

Ba	0.333333330	0.666666670	0.780103593
Ba	0.666666670	0.333333330	0.280103593
S	0.831470924	0.168529076	0.779473251
S	0.662941848	0.831470924	0.279473251
S	0.831470924	0.662941848	0.779473251
S	0.168529076	0.831470924	0.279473251
S	0.337058152	0.168529076	0.779473251
S	0.168529076	0.337058152	0.279473251
Ti	0.000000000	0.000000000	0.529476654
Ti	0.000000000	0.000000000	0.029476654