

Supporting Information

YCuTe₂: A Member of A New Class of Thermoelectric Materials with CuTe₄-Based Layered Structure

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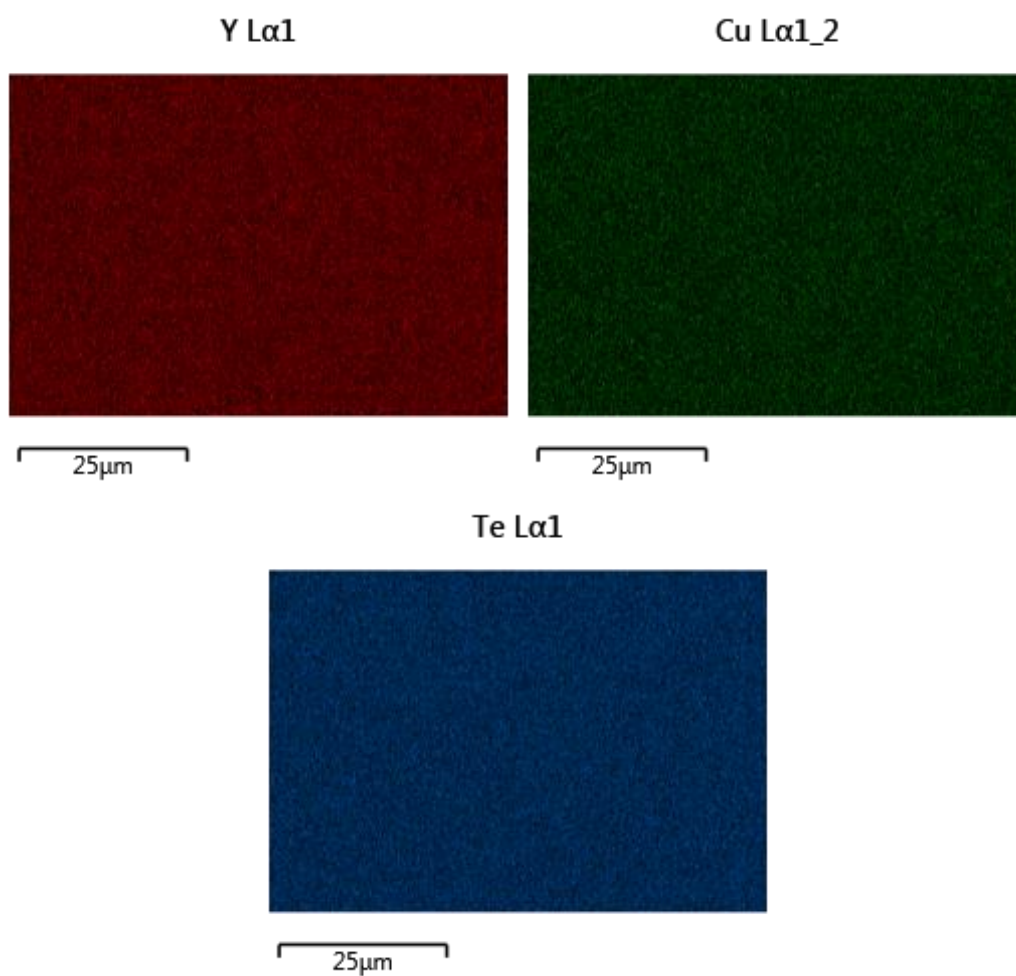


Figure S1: EDS mapping of a YCuTe₂ sample (the target phase) showing homogeneously distributed Y, Cu and Te atoms.

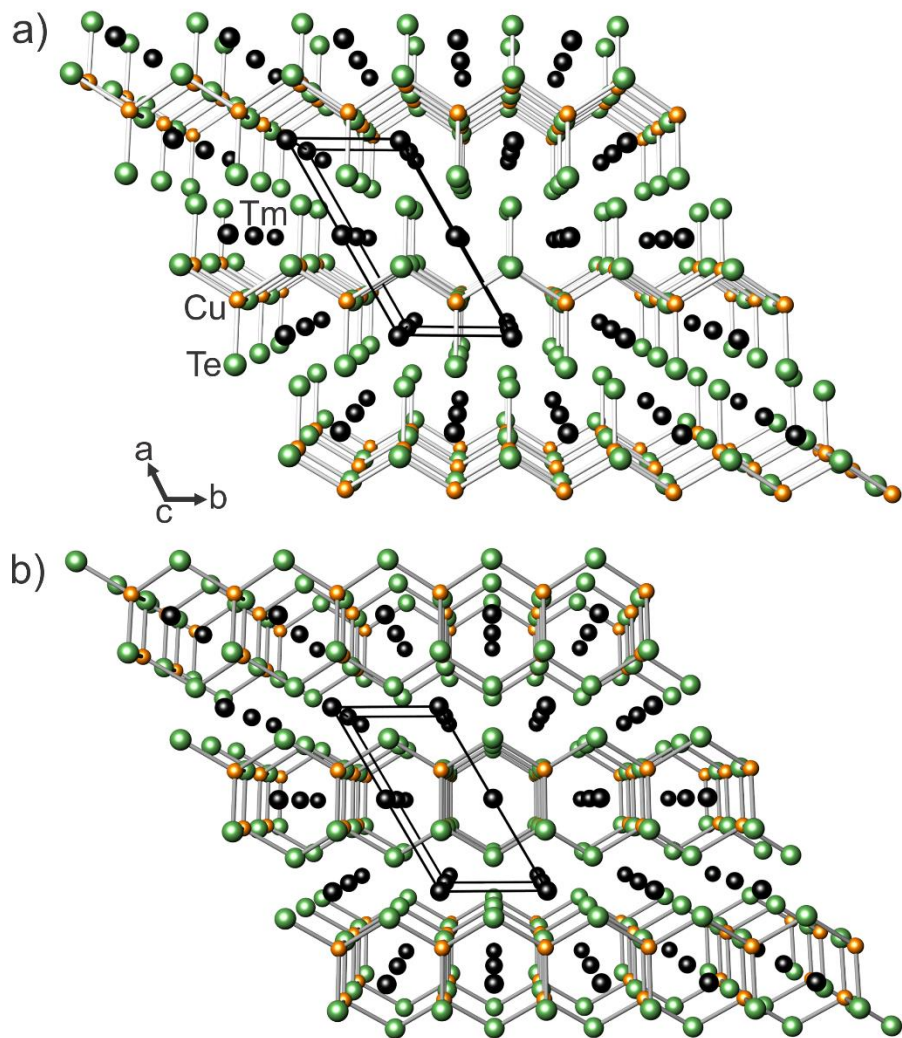


Figure S2: The low (a) and high (b) energy configuration of the low-temperature YCuTe₂ phase based on the total energy calculations. The configurations were constructed based on $2 \times 1 \times 1$ supercell.

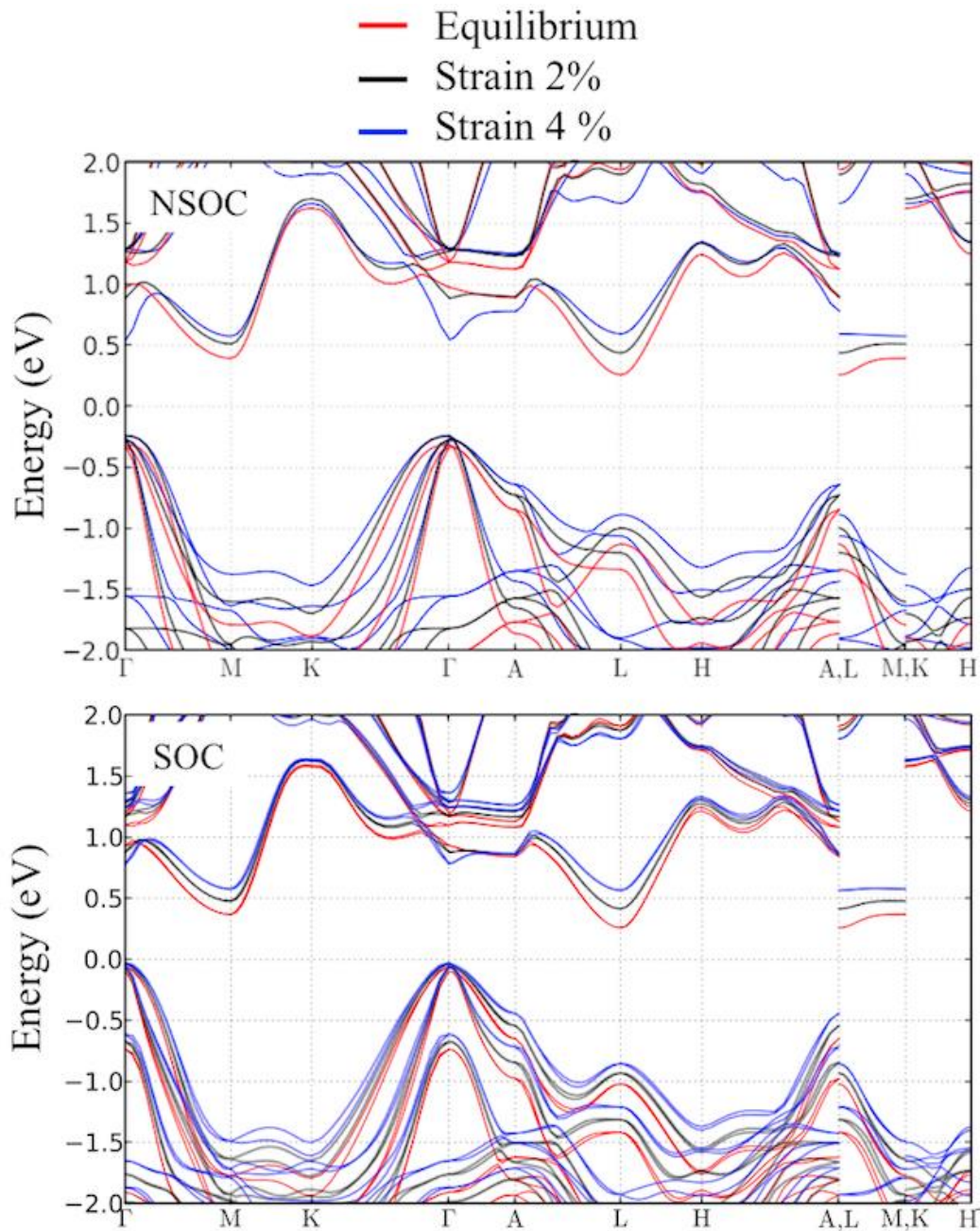


Figure S3: The electronic band structure for the high-temperature phase of YCuTe₂ with the equilibrium lattice parameter (shown in red) and at 2% (black) and 4 % (blue) extensive lattice strain computed with (lower) and without (upper) consideration of spin-orbit coupling (SOC).

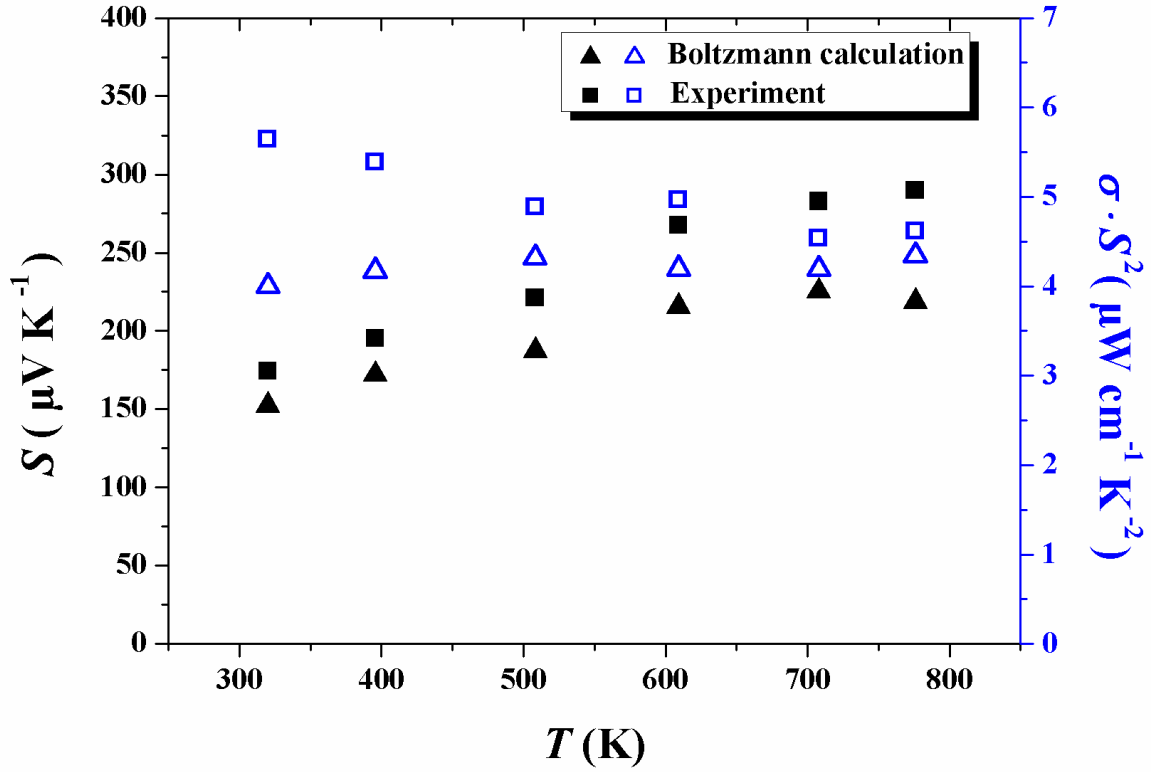


Figure S4: Experimental Seebeck coefficient (■) and power factor (□) of YCuTe₂ compared to the calculated data using Boltzmann transport equations (Seebeck: ▲; power factor: Δ), with temperature-dependent relaxation time as described in the main text. Seebeck coefficient is underestimated at high temperatures due to increasing effective mass.

Table S1: Atomic coordinates, displacement parameters (in Å²) and site occupancy factor (*SOF*) of LT-YCu_{1.04}Te₂ in *P*-3*m*1 (*R*_i = 0.06; *R*_p = 0.19, *R*_{wp} = 0.21). Standard deviations are provided in parentheses.

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}	<i>SOF</i>
Y1	2 <i>c</i>	0	0	0.2369(7)	0.018(3)	1
Y2	6 <i>i</i>	0.4987(5)	1- <i>x</i>	0.2555(6)	0.0213(11)	1
Cu1	2 <i>d</i>	1/3	2/3	0.4309(7)	0.019(6)	1
Cu2	6 <i>i</i>	0.162(1)	1- <i>x</i>	0.0681(5)	0.035(4)	0.656(7)
Cu3	6 <i>i</i>	0.838(1)	1- <i>x</i>	0.4232(6)	0.036(7)	0.516(7)
Te1	2 <i>d</i>	1/3	2/3	0.1178(4)	0.014(2)	1
Te2	2 <i>d</i>	1/3	2/3	0.6230(4)	0.010(2)	1
Te3	6 <i>i</i>	0.8257(3)	1- <i>x</i>	0.1209(2)	0.0109(7)	1
Te4	6 <i>i</i>	0.1664(3)	1- <i>x</i>	0.3816(2)	0.0105(7)	1

Table S2: Atomic coordinates, displacement parameters (in Å²) and site occupancy factor (*SOF*) of HT-YCu_{1.04}Te₂ in *P*-3 (*R*_i = 0.05; *R*_p = 0.16, *R*_{wp} = 0.20). Standard deviations are provided in parentheses.

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}	<i>SOF</i>
Y1	1 <i>a</i>	0	0	0	0.014(2)	1
Cu1	2 <i>d</i>	1/3	2/3	0.6322(7)	0.016(3)	0.670(6)
Te1	2 <i>d</i>	1/3	2/3	0.2525(3)	0.009(2)	1

Table S3: Selected interatomic distances for LT-YCu_{1.04}Te₂ in *P*-3*m*1 with their multiplicity (*n*).

Atoms	<i>n</i>	<i>d</i> (Å)
Y1 -Te3	3×	3.056(5)
-Te4	3×	3.189(6)
Y2 -Te2	1×	3.016(6)
-Te4	2×	3.031(6)
-Te3	2×	3.071(6)
-Te1	1×	3.117(6)
Cu1 -Te4	3×	2.582(4)
-Te2	1×	2.657(11)
Cu2 -Te3	2×	2.619(9)
-Te3	1×	2.612(7)
-Te1	1×	2.644(9)
Cu3 -Te4	2×	2.518(11)
-Te2	1×	2.634(11)
-Te4	1×	2.698(8)

Table S4: Selected interatomic distances for HT-YCu_{1.04}Te₂ in *P*-3 with their multiplicity (*n*).

Atoms	<i>n</i>	<i>d</i> (Å)
Y1 -Te1	6×	3.053(1)
Cu1 -Te1	3×	2.624(2)
	1×	2.635(5)