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Supporting Information

$YCuTe_2$: A Member of A New Class of Thermoelectric Materials with $CuTe_4$-Based Layered Structure

Umut Aydemir,[a,b*] Jan-Hendrik Pöhls,[c] Hong Zhu,[d,e] Geoffroy Hautier,[f] Saurabh Bajaj,[a] Zachary M. Gibbs,[a] Wei Chen,[g] Guodong Li,[a,b] Saneyuki Ohno,[a,b] Danny Broberg,[h] Stephen Dongmin Kang,[a,b] Mark Asta,[h] Gerbrand Ceder,[d,g,h] Mary Anne White,[c] Kristin Persson,[g,h] Anubhav Jain,[g] and G. Jeffrey Snyder[a,b*]

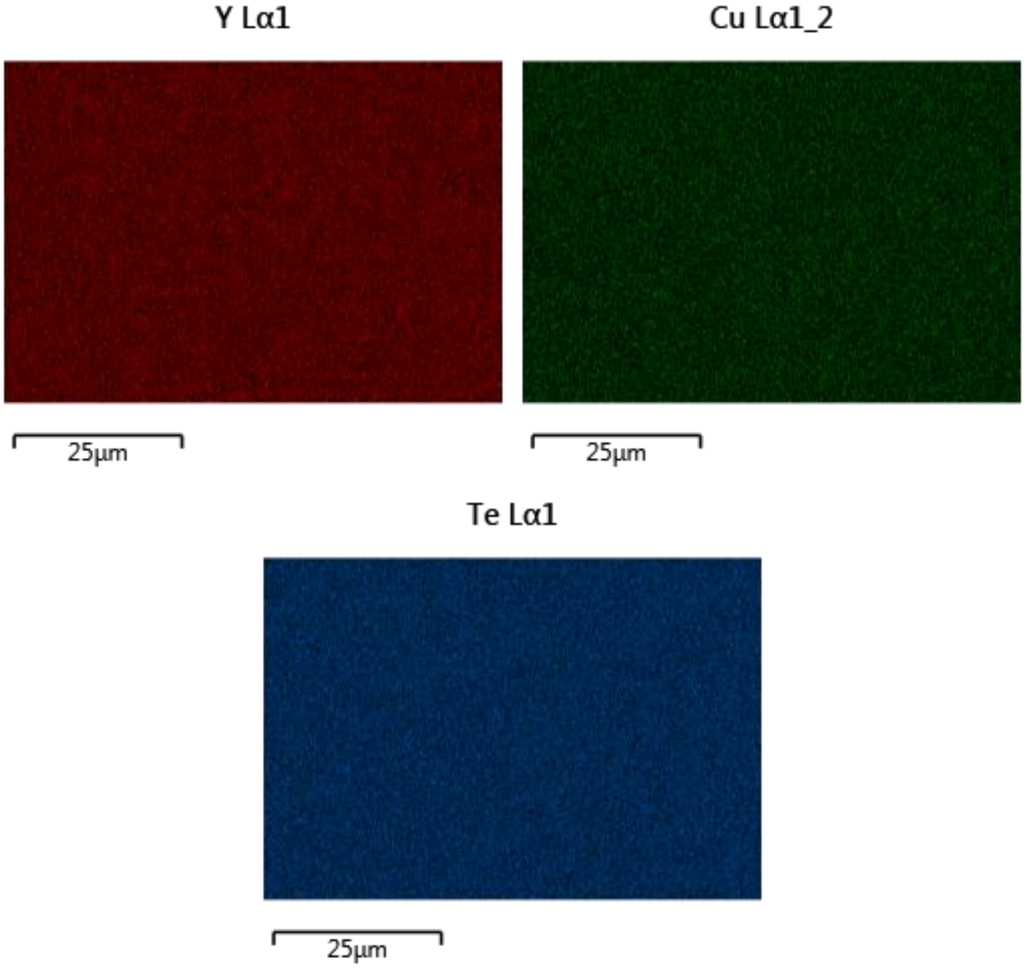

Figure S1: EDS mapping of a $YCuTe_2$ sample (the target phase) showing homogenously distributed Y, Cu and Te atoms.

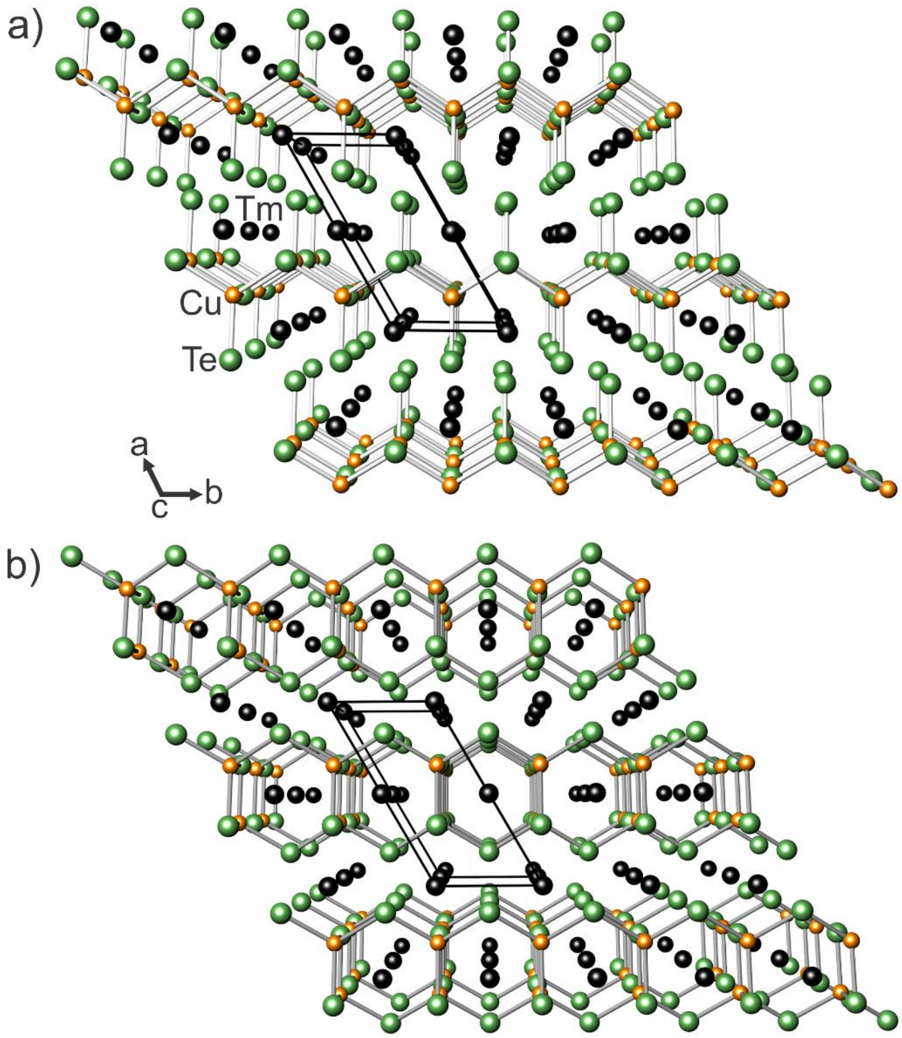

Figure S2: The low (**a**) and high (**b**) energy configuration of the low-temperature $YCuTe_2$ phase based on the total energy calculations. The configurations were constructed based on 2 × 1 × 1 supercell.

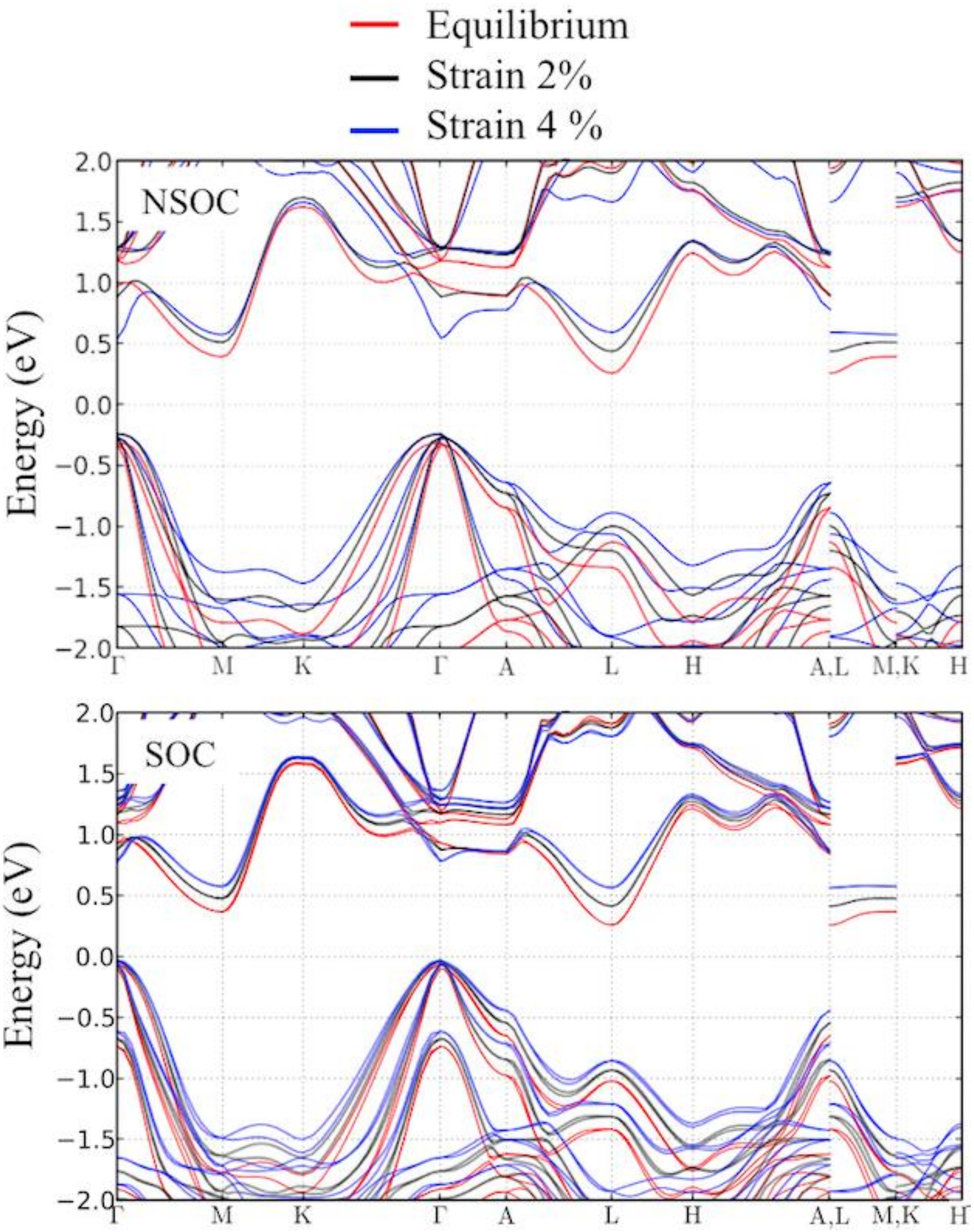

Figure S3: The electronic band structure for the high-temperature phase of $YCuTe_2$ with the equilibrium lattice parameter (shown in red) and at 2% (black) and 4 % (blue) extensive lattice strain computed with (lower) and without (upper) consideration of spin-orbit coupling (SOC).

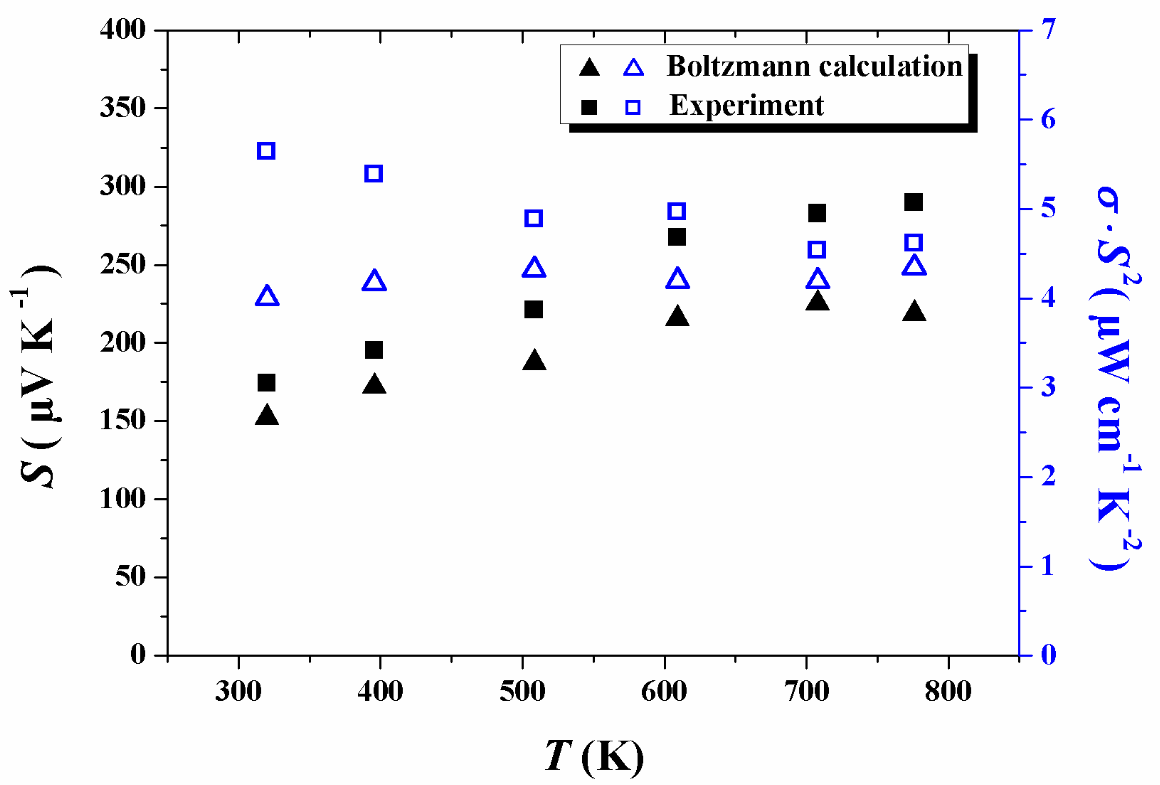

Figure S4: Experimental Seebeck coefficient (■) and power factor (□) of $YCuTe_2$ compared to the calculated data using Boltzmann transport equations (Seebeck: ▲; power factor: Δ), with temperature-dependent relaxation time as described in the main text. Seebeck coefficient is underestimated at high temperatures due to increasing effective mass.

Table S1: Atomic coordinates, displacement parameters (in Å^2) and site occupancy factor (*SOF*) of LT-YCu$_{1.04}$Te$_2$ in P-3m1 (R_i = 0.06; R_p = 0.19, R_wp = 0.21). Standard deviations are provided in parentheses.

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

Table S2: Atomic coordinates, displacement parameters (in Å^2) and site occupancy factor (*SOF*) of HT-YCu$_{1.04}$Te$_2$ in P-3 (R_i = 0.05; R_p = 0.16, R_wp = 0.20). Standard deviations are provided in parentheses.

Atom	**Site**	***x***	***y***	***z***	U_iso	***SOF***
Y1	1*a*	0	0	0	0.014(2)	1
Cu1	2*d*	1/3	2/3	0.6322(7)	0.016(3)	0.670(6)
Te1	2*d*	1/3	2/3	0.2525(3)	0.009(2)	1

Table S3: Selected interatomic distances for LT-YCu$_{1.04}$Te$_2$ in P-3m1 with their multiplicity (*n*).

Atoms	***n***	***d*** **(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-$YCu_{1.04}Te_2$ in *P*-3 with their multiplicity (*n*).

Atoms	***n***	***d* (Å)**
Y1 -Te1	6×	3.053(1)
Cu1 -Te1	3× 1×	2.624(2) 2.635(5)