Supporting information

Ideal Strength and Deformation Mechanism in High-Efficiency Thermoelectric SnSe

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Figure S1. (a) The intact atomic positions for shear loads along the (100)/<001> slip system, (b) The Sn3–Se1–Se5 bond angle and the $c$-axis lattice parameter with the increasing shear strain along the (100)/<001> slip system. The red dashed line in Figure S1(b) represents the strain 0.081 corresponding to the minimum length of the Se1–Sn3 bond as shown in Figure 3 in the manuscript.