

Electronic Supplementary Information

Stress/Pressure-Stabilized Cubic Polymorph of Li_3Sb with Improved Thermoelectric Performance

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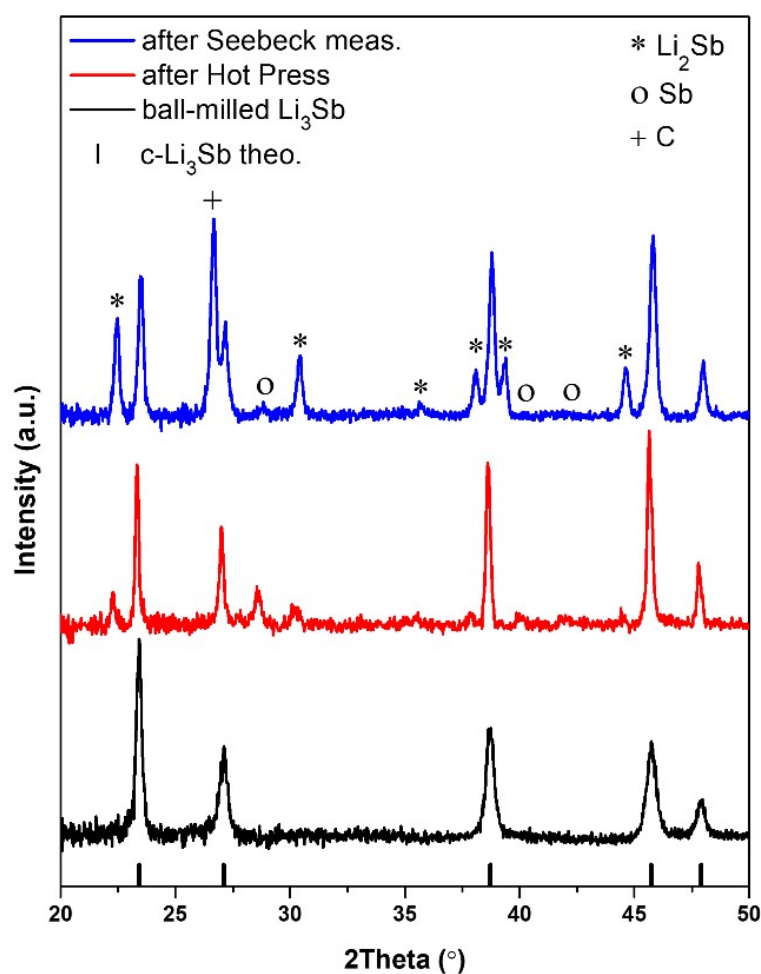


Figure S1. Experimental XRD patterns (Cu $\text{K}\alpha$) of as synthesized (ball milled) powder (black) and hot pressed (red) Li_3Sb samples along with the data after Seebeck measurement (blue). Ticks mark the calculated reflection positions of the c- Li_3Sb .

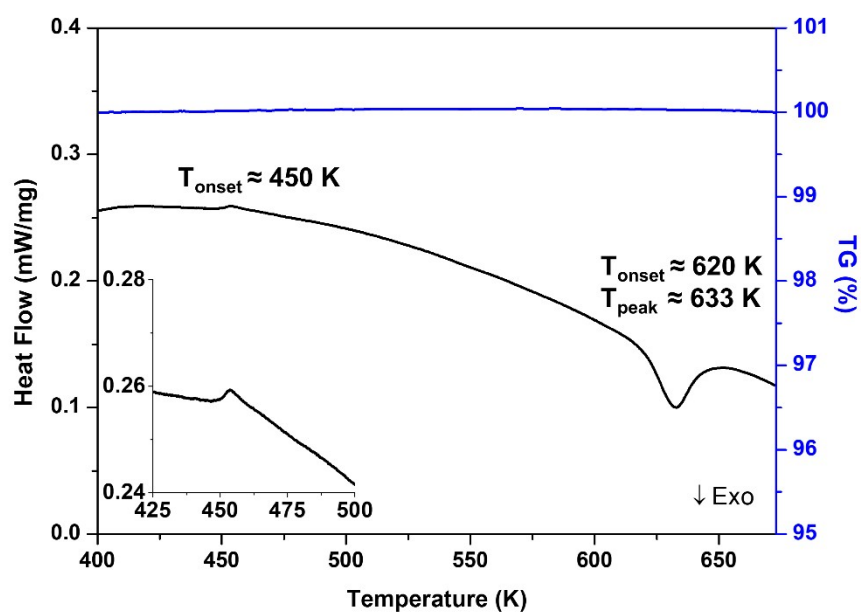


Figure S2. DSC/TG diagrams of c-Li₃Sb (scanning rate 10 K min⁻¹) showing an endothermic peak at $T_{\text{onset}} \approx 450$ K and an exothermic peak at $T_{\text{onset}} \approx 620$ K and $T_{\text{peak}} \approx 633$ K.

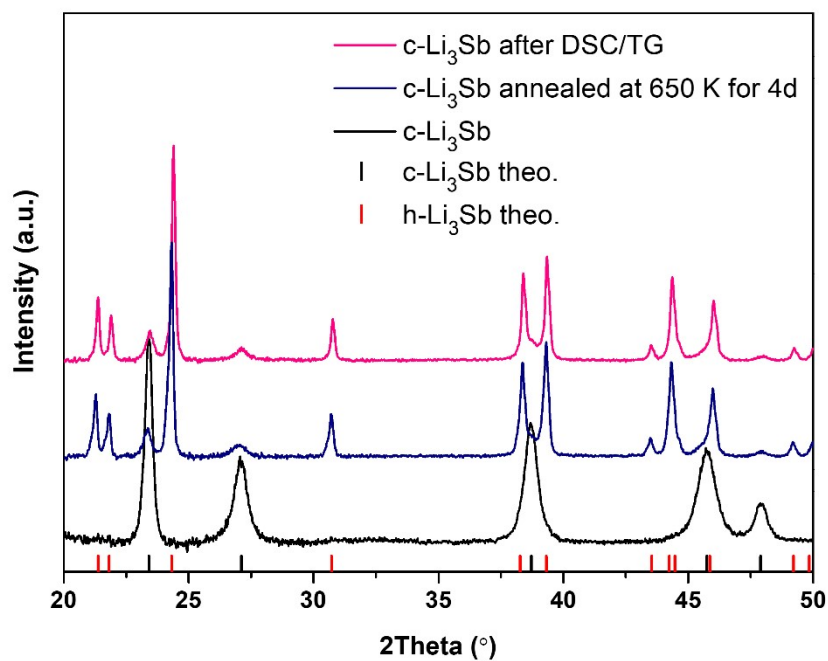


Figure S3. Experimental XRD patterns (Cu K α) of as synthesized c-Li₃Sb powder (black), c-Li₃Sb annealed at 650 K for 4d (blue), and c-Li₃Sb after the DSC/TG measurement. Black and red ticks mark the calculated reflection positions of the c-Li₃Sb and h-Li₃Sb, respectively.

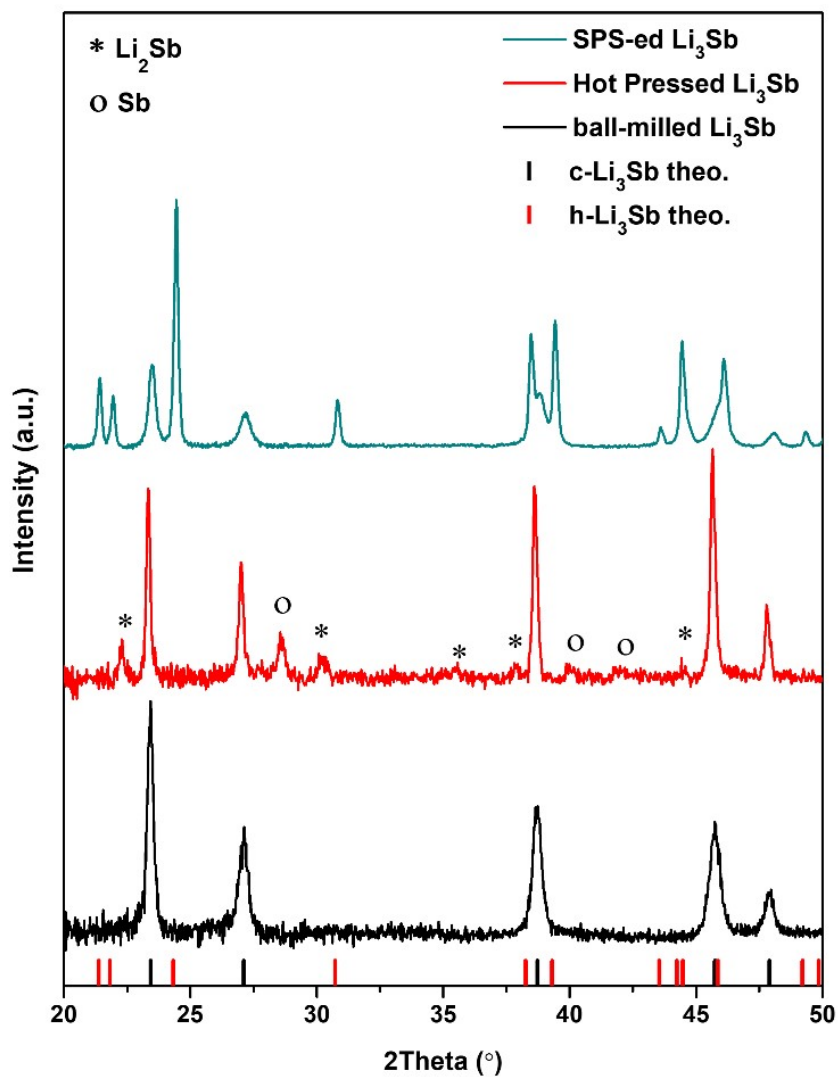


Figure S4. Experimental XRD patterns (Cu $\text{K}\alpha$) of as synthesized powder (black), hot pressed (red), and SPS-ed (green) Li_3Sb samples. Black and red ticks mark the calculated reflection positions of the c- Li_3Sb and h- Li_3Sb , respectively.

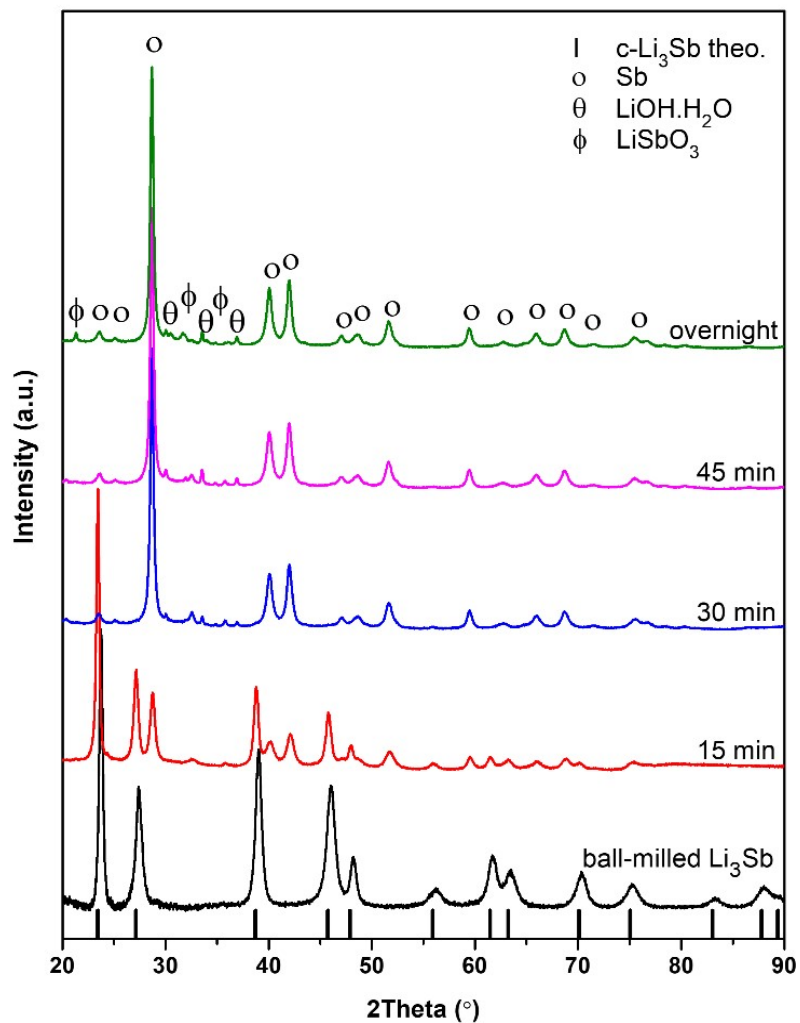


Figure S5. Experimental XRD patterns (Cu $K\alpha$) of as synthesized powder (with Kapton foil) and air exposed Li_3Sb samples. Each scan corresponds to about 15 minutes of exposure (red, blue, and pink) and an overnight exposure (green). Ticks mark the calculated reflection positions of the c- Li_3Sb .

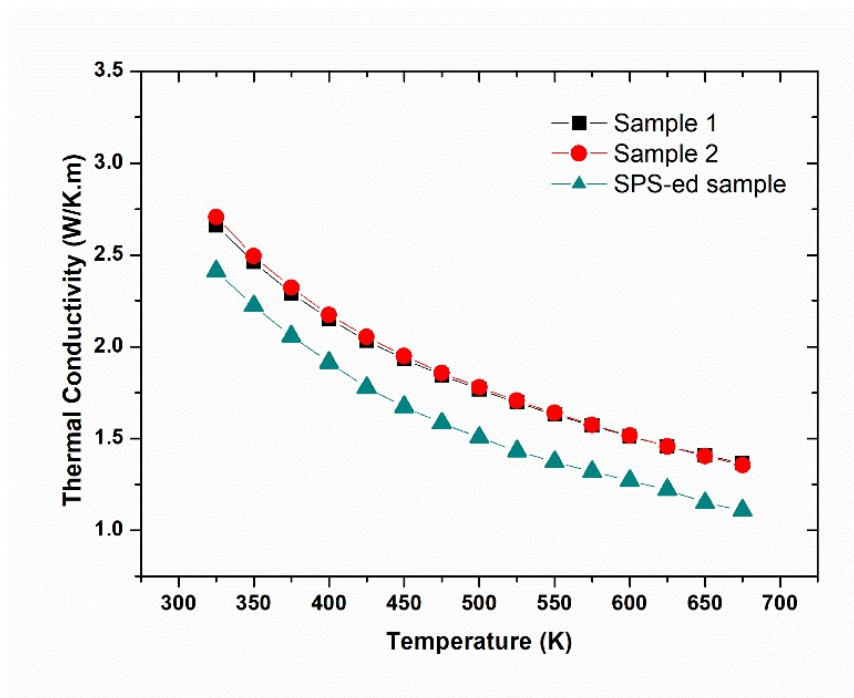


Figure S6. Temperature dependence of the total thermal conductivity of hot pressed (sample 1 and sample 2) and SPS treated (green) Li_3Sb samples.