Electronic Supplemental Information (ESI):

SnO as a Potential Oxide Thermoelectric Candidate

Samuel A. Miller,[†] Prashun Gorai,[‡] Umut Aydemir,[†] Thomas O. Mason,[†] Vladan Stevanović,[‡] Eric S. Toberer,[‡] and G. Jeffrey Snyder[*,†]

†*Northwestern University, Evanston, IL 60208, USA*

‡*National Renewable Energy Laboratory, Golden, CO 80401, USA*

¶*Colorado School of Mines, Golden, CO 80401 USA*

E-mail: jeff.snyder@northwestern.edu

The synthesized SnO was determined to be phase-pure after the precipitation reaction procedure using X-ray diffraction (Fig. S1). SnO was stable in air, vacuum, and inert atmosphere (argon) up to ∼300°C for one week. However, increasing the annealing temperature to 325 °C caused the decomposition of SnO to begin, as SnO_2 impurities were observed after 12 hours. Figure S2 shows the diffraction pattern of unannealed SnO as well as SnO sealed in fused silica tubes evacuated to 10^{-5} mbar and annealed. Additionally, it was found that ball milling for more than a few minutes produced increasing amounts of SnO_2 impurity, as did attempts to dope SnO with Sb (Fig. S3). SnO showed no impurities after pressing pellets, and annealing them at 275°C for up to one week did not lead to any further densification. The optical band gap was determined to be 0.68 eV using diffuse reflectance measurements and the Kubelka-Munk method (Fig. S4) and is in good agreement with previous reports.

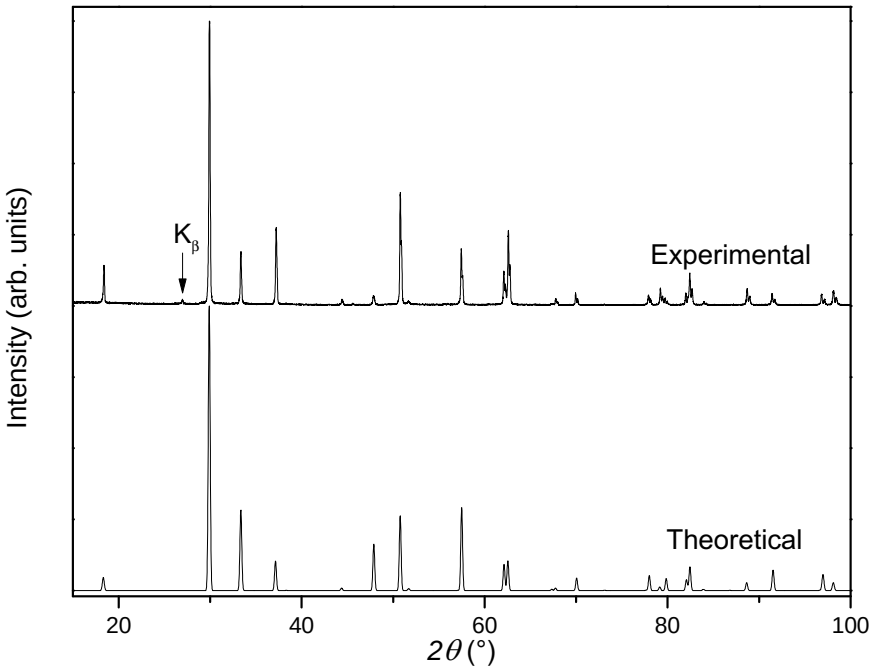

Figure S1: The theoretical pattern for SnO (space group 129) as well as the diffraction pattern for phase-pure SnO synthesized using the precipitation reaction synthesis.

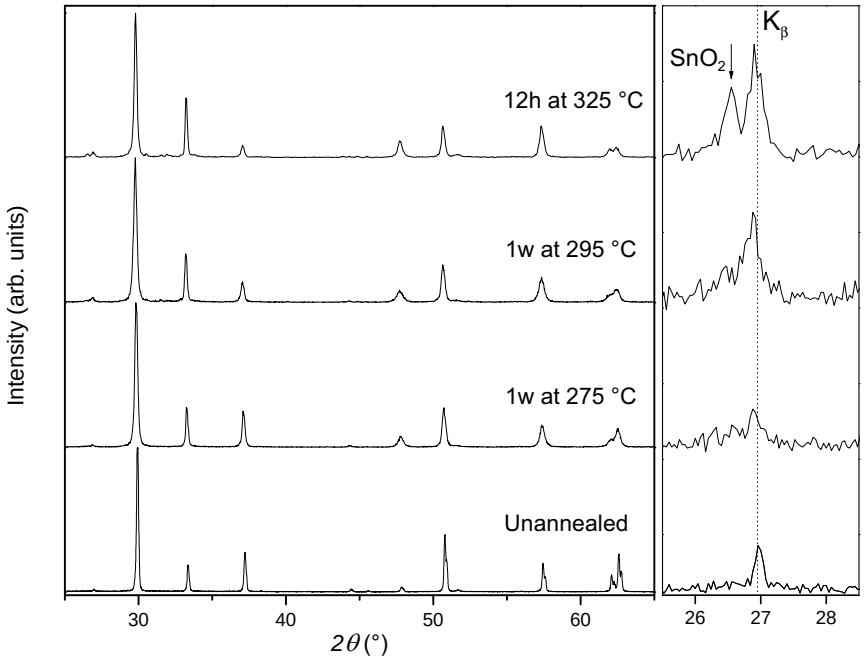

Figure S2: The diffraction pattern for the unannealed SnO as well as SnO sealed, evacuated, and then annealed at various times and temperatures. The K_β peak for the main SnO peak is labeled and apparent in all diffraction patterns and the main SnO_2 peak is indicated with an asterisk for the anneal at 325 °C

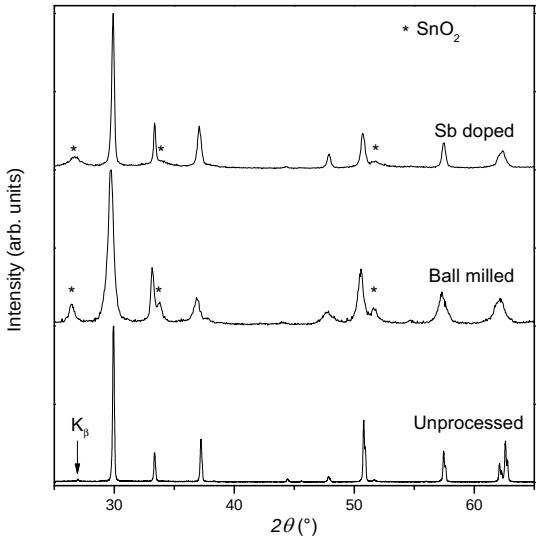

Figure S3: The diffraction pattern for the as-synthesized SnO, SnO ball milled for 10 minutes in an argon atmosphere, and SnO doped with Sb during the precipitation reaction. Both the ball milled and Sb doped samples show SnO_2 impurity with the main peaks indicated with an asterisk.

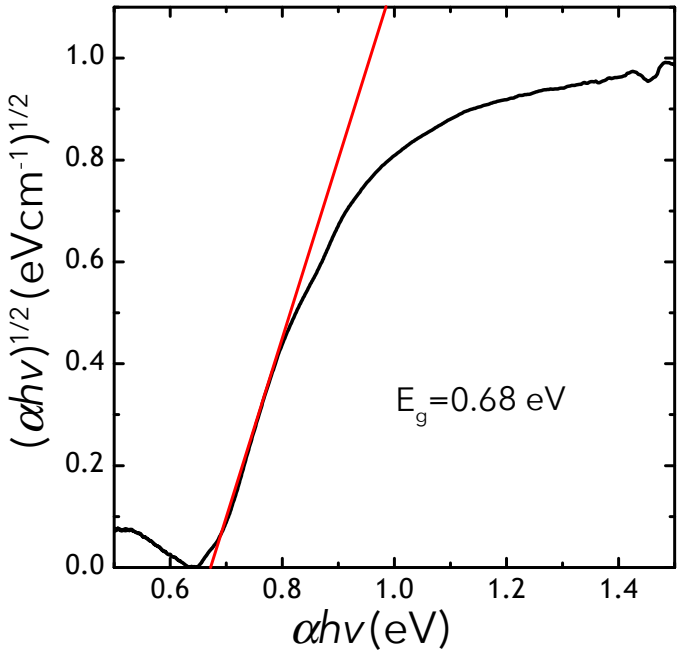

Figure S4: The normalized absorption vs. energy spectra for bulk SnO powder calculated using the Kubelka-Munk method. The indirect gap estimated from diffuse reflectance measurements is approximately 0.68 eV.