# Mechanism of Ultra-Low Thermal Conductivity and Insulating-to-Semiconducting Transition Driven by Configurational Entropy

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**Abstract:** Thermoelectric materials have garnered interest as a clean energy technology for their ability to convert waste heat into electricity, however the current best thermoelectrics are neither efficient nor cost effective enough for general industrial use. To further improve thermoelectric efficiency, new classes of materials with lower thermal conductivity and more cost-effective synthesis are required. We report a method for driving insulating transition metal oxides into a semiconducting state with ultra-low thermal conductivity $\left(\kappa < 1 \frac{W}{m\,K}\right)$ by introducing configurational entropy which substantially increases phonon-defect scattering. Further, we report that the transition from insulating to semiconducting relies on the combination and interplay of 3 novel mechanisms. This new understanding illuminates a new method for thermoelectric material design, driving an insulating system into a semiconducting state with ultra-low thermal conductivity via the introduction of configurational entropy, that illuminates an exciting new avenue for the design of thermoelectrics.