Abstract Submitted
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Atomic-resolution study of charge transfer and structural disorder in thermoelectric $Ca_3Co_4O_9$ ROBERT KLIE, University of Illinois at Chicago — Thermoelectric oxides have attracted increasing attention due to their high thermal power and temperature stability. In particular, $Ca_3Co_4O_9$, a misfit layered structure consisting of single layer hole-doped CoO_2 sandwiched between insulating Ca_2CoO_3 rocksalt layers, exhibits figure of merit (ZT) of >1 at 1000 K.[1]It was suggested that the Seebeck-coefficient can be further increased by controlling the spin- and valence-state of the Co-ions in the CoO_2 layers. This study combines aberration-corrected scanning transmission electron microscopy with electron energy loss spectroscopy (EELS) to examine the atomic and electronic structures of $Ca_3Co_4O_9$. Using annular dark and bright field imaging, it will be demonstrated that the CoO_2 layers are ordered, while the CoO columns in the Ca_2CoO_3 layer exhibit a modulation along (010). Atomic-column resolved EELS reveals that the Ca_2CoO_3 layers act as charge reservoirs providing mobile holes to the CoO_2 layers; the structural disorder in Ca_2CoO_3 is responsible for the low in-plane thermal conductivity. The temperature dependence of the Co-ion spin-state as the origin for the unusually high Seebeck coefficient of $Ca_3O_4O_9$ will be examined.[2] [1] K. Fujita, et al., *Jpn. J. Appl. Phys.* **40** (2001), 4644–47 [2] Funded by: NSF CAREER Award DMR-0846748

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