Abstract Submitted
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Optical spectroscopy and band gap analysis of hybrid improper ferroelectric Ca3Ti2O7[1] JANICE MUSFELDT, JUDY CHERIAN, University of Tennessee, TURAN BIROL, Rutgers University, NATHAN HARMS, University of Tennessee, BIN GAO, SANG CHEONG, DAVID VANDERBILT, Rutgers University — We bring together optical absorption spectroscopy, photoconductivity, and first principles calculations to reveal the electronic structure of the room temperature ferroelectric Ca3Ti2O7. The 3.94 eV direct gap in Ca3Ti2O7 is charge transfer in nature and noticeably higher than that in CaTiO3 (3.4 eV), a finding that we attribute to dimensional confinement in the n = 2 member of the Ruddlesden-Popper series. While Sr substitution introduces disorder and broadens the gap edge slightly, oxygen deficiency reduces the gap to 3.7 eV and gives rise to a broad tail that persists to much lower energies.

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Janice Musfeldt
University of Tennessee

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