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Disorder in $ZnSnN_2$: Characterization and Band Structure Effects N. FELDBERG, SUNY University at Buffalo, W.M. LINHART, T.D. VEAL, University of Liverpool, P.A. STAMPE, R.J. KENNEDY, Florida A&M University, D.O. SCANLON, University College London, L.F.J. PIPER, Binghamton University, Y. YANG, R. CLARKE, University of Michigan, R.J. REEVES, University of Canterbury, S.M. DURBIN, Western Michigan University — $ZnSnN_2$ represents a critical member of the Zn-IV-N_2 family of materials proposed as alternatives to conventional III-V semiconductors for use in optoelectronic devices. Importantly, it consists of what are known as "earth abundant" elements. This compound is predicted to exhibit a tetragonal ordering and to crystallize in an orthorhombic lattice structure. In contrast with density functional theory calculations, films grown by molecular beam epitaxy appear to have a monoclinic structure with γ>118°, possibly due to the disordering of the Zn-Sn sublattice. Similar effects having been seen in other members of the family. We show that increasing cation sublattice disorder is predicted to cause a decrease in the band gap, theoretically by a full 0.9 eV and may be useful for device engineering. Hall Effect shows a degenerate carrier concentration in all samples to date, likely due to disorder and/or deviations from stoichiometry. The onset of optical absorption occurs at higher energy in samples with lower carrier concentrations and ranges from 2-2.4 eV. We see evidence for this in hard x-ray photoelectron spectroscopy, along with signs of band filling. Increasing cation sublattice disorder may be competing with Moss-Burstein band filling.

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