Abstract Submitted
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Electronic Structures of Zn(Te,O)[1] BYOUNGHAK LEE, Texas State University, LIN-WANG WANG, Lawrence Berkeley National Laboratory — It was recently observed that highly mismatched semiconductor alloys display multiple band gaps of solar spectra, opening a possibility of higher efficiency photovoltaic materials in bulk systems [1]. The highest solar radiation conversion efficiency in these materials is expected to reach 56%, almost twice as high as the best existing single crystal material. The existing empirical model explains observed band structures [2], but it lacks details of atomic level information and cannot explain the constituent atomic composition dependence. We present a theoretical study of Zn(Te,O) using newly developed Linear Scaling 3-Dimensional Fragment method [3] to answer technologically important questions, such as existence of nonradiative recombination centers, charge transfer, and wavefunction localization. [1] K. M. Yu, W. Walukiewicz, J. Wu, W. Shan, J. W. Beeman, M. A. Scarpulla, O. D. Dubon, and P. Becla, Phys. Rev. Lett. 91, 246403 (2003). [2] W. Shan et al. Phys. Rev. Lett. 82, 1221 (1999). [3] L.-W. Wang, Z. Zhao, and J. Mexa, Phys. Rev. B 77, 165113 (2008).

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