

Abstract Submitted  
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**Substitutional Defects in CdZnTe using Special Quasirandom Structures** SYLVESTER EKPENUMA, School of Natural Sciences and Mathematics, Claflin University, Orangeburg, SC 29115, YURIY PERSHIN, Department of Physics and Astronomy, University of South Carolina, Columbia, SC 29208 — The special quasirandom structures (SQS) are a type of supercells with constituent atoms occupying lattice sites so as to reproduce the average correlation function of a completely disordered lattice. In this way, SQS represent best periodic supercell approximation for a disordered alloy. An algorithm implemented in the Alloy Theoretic Automated Toolkit (ATAT) has been shown to be computationally efficient in generating supercell approximations to disordered lattices. In this study, we apply first principles density functional theory (DFT) electronic structure calculations to SQS for cadmium zinc telluride (CZT) generated using ATAT. Some initial results of zinc atom site occupations using the SQS approach for the study of defects in CZT will be presented.

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