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Theoretical Study of native defects in $CdGeAs_2$[1] TULA R. PAUDEL, Department of Physics, Case Western Reserve University, WALTER R.L. LAMBRECHT, Department of Physics Case Western Reserve University — First-principles results are presented for various native defects *viz* : V_{Cd}, V_{Ge}, V_{As}, Cd_{Ge}, Ge_{Cd}, Ge_{As} and As_{Ge} in $CdGeAs_2$ under different growth conditions. The defects were calculated by constructing a 64 atom supercell in the full potential linearized muffin-tin orbital implementation of the density functional theory under the local density approximation (LDA). Calculations of the energy of formation show that antisites should be the most abundant type of defect. The LDA band gap is adjusted to experimental band gap by introducing a non-local orbital dependent constant potential shift to the *s*-orbitals of Cd and Ge and *d*-orbitals of Cd within the LSDA+U approach. The defect transition levels for different charge states are calculated. The calculations support the earlier suggestion that Ge_{As} is a shallow acceptor. The calculated transition levels are found to be significantly different form corresponding defects levels of $ZnGeP_2$. The defect levels are interpreted in a simple molecular-orbital theory and compared with the available experimental data.

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