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Theoretical Study of native defects in CdGeAs₂¹ TULA

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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 calcu-
lated 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 for-
mation 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 ac-
ceptor. The calculated transition levels are found to be significantly
different from 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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