Intrinsic *n*-type Conductivity in InAs: First-Principles Study of Native Defects

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InAs, III-V semiconductor with a narrow direct band gap (0.43 eV), intrinsically exhibits high *n*-type conductivity (~10^{16} cm^{-3}), however, the underlying defect mechanisms for this carrier concentration remain unclear.[1] This lack of understanding is compounded by the limitations of first-principles methods, which severely underestimate the band gap, making defect analysis difficult.[2] Here, using hybrid exchange-correlation functional calculations, we achieved the InAs band gap in agreement with the experimental value, then we identified that In_i and As_{In} are dominant donor defects under In-rich and As-rich conditions, respectively, while V_{In} acts as the unique acceptor. Notably, by correctly treating exact exchange energy via hybrid functionals, we obtained the increased formation energy of V_{In}, leading to a carrier density (~10^{16} cm^{-3}) consistent with experimental observations. Our findings will provide quantitative insight into defect behavior in InAs, explaining its intrinsic *n*-type conductivity, and contribute to the design of more efficient field-effect transistors and infrared photodetectors.

References

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