

Abstract Submitted
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Group-IV Impurity Defect Levels in beta-Gallium Oxide STEFAN BADESCU, Wyle Aerospace/US AFRL — Beta-Gallium Oxide (β -Ga₂O₃) is a wide-bandgap semiconductor with a significant potential as a native substrate for electronic devices. One avenue for tuning its carrier concentration and electronic properties is doping with group-IV impurity atoms. This work presents a first-principles understanding of the effects of C, Si, Ge and Sn dopants at Ga sites. C is found to act like a bistable center whereas the other dopants preserve the symmetry of the Ga site. Hybrid functionals are used to describe accurately the effects that occur mainly in the conduction band. A Brillouin zone unfolding is used that enables a direct comparison to possible spectroscopy experiments. We delineate the effects on bandgap modulation induced by charge density on the one hand, and by conduction band resonances and effective masses on the other hand.

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