Abstract Submitted
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Doping and defects by design: Ga2O3[1] STEPHAN LANY, NREL — Density functional supercell calculations are widely employed to describe the defect physics in semiconductors and insulators. Due to a variety of challenges such as finite size effects for charged defects and the band gap error of DFT, results were often controversial in the past. With developments over the past decade, defect theory should hopefully be truly predictive, and be able to guide experimental efforts. The present work on n-type doping in Ga2O3 compares different potential doping routes via anion-site doping with F, and cation site doping with group IV elements (C, Si, Ge, Sn). The study addresses dopant solubility, electrical activity, and compensation by native defects, including non-equilibrium effects due to supersaturated dopant concentrations and the mechanism of dopant-defect pair formation.

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