

Abstract Submitted
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Role of excited states in Shockley-Read-Hall recombination in wide band-gap semiconductors AUDRIUS ALKAUSKAS, Center for Physical Sciences and Technology, Lithuania, CYRUS E. DREYER, JOHN L. LYONS, CHRIS G. VAN DE WALLE, University of California Santa Barbara — Defect-assisted recombination is an important limitation on efficiency of optoelectronic devices. However, since nonradiative capture rates decrease exponentially with energy of the transition, the mechanisms by which such recombination can take place in wide-band-gap materials are unclear. We investigate the role of electronic excited states in the recombination process, focusing on group-III nitrides, for which accumulating experimental evidence indicates that defect-assisted recombination is an important limiting factor in efficiency. Based on first-principles electronic structure calculations, we show that excited states of gallium vacancy complexes make these defects very efficient recombination centers. Our work provides new insights into the physics of nonradiative recombination. The mechanism discussed in this work is suggested to be very critical and ubiquitous in wide-band-gap semiconductors. This work was supported by DOE and the European Union.

Audrius Alkauskas
Center for Physical Sciences and Technology, Lithuania

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