

Abstract Submitted
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Comparing deep level transient spectroscopy with first-principles calculations¹ CHRIS VAN DE WALLE, DARSHANA WICKRAMARATNE, Univ of California - Santa Barbara , CYRUS DREYER , Rutgers University, JIMMY-XUAN SHEN, Univ of California - Santa Barbara , JOHN LYONS, Naval Research Laboratory, AUDRIUS ALKAUSKAS , Center for Physical Sciences and Technology, Vilnius, Lithuania — Deep level transient spectroscopy (DLTS) has been used extensively to determine the ionization energy and capture cross sections of defects in semiconductors. We examine the standard formulation used to analyze DLTS measurements, and perform first-principles calculations of ionization energies and nonradiative capture coefficients using density functional theory with a hybrid functional. A critical evaluation highlights discrepancies that can arise in the analysis of DLTS measurements. We apply our analysis to gallium vacancy complexes and impurities in GaN. The ionization energy extracted from a DLTS measurement includes a barrier for nonradiative capture. Our calculations show this barrier is unique to each defect and can be as large as 0.6 eV. The barrier can also have a strong temperature dependence. We comment on the consequences of failing to account for this barrier when interpreting activation energies extracted from DLTS measurements.

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Chris Van de Walle
Univ of California - Santa Barbara

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