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The role of electron-phonon coupling in carrier capture at defects[1]

CYRUS E. DREYER, Rutgers University

Understanding capture of charge carriers by point defects is crucial to improving the performance of electronic and opto-electonic devices. For example, the process of Shockley-Read-Hall (SRH) recombination, which limits the efficiency of light emitters and photovoltaics, involves the sequential capture of an electron and hole at a defect. Capture processes can occur radiatively, through the emission of a photon, or nonradiatively, mediated by phonons. In both cases, understanding the coupling of the carrier to the vibronic structure of the defect is crucial to calculating the rate of the process. I will outline our recently-developed methodology to calculate radiative and nonradiative capture rates. Then I will demonstrate how this quantitative understanding allows us to predict defects that will result in SRH in optoelectronic devices. The material system that we explore is InGaN alloys, which are key materials for high-efficiency light emitting diodes across the visible spectrum. We find that gallium vacancies complexed with hydrogen and/or oxygen have SRH rates that will be detrimental to devices emitting at yellow and green wavelengths.[2] For wider-band-gap InGaN alloys, we demonstrate that a novel mechanism involving the excited electronic states of defects is required to explain experimentally observed SRH rates.[3,4]

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