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Identification of nonradiative recombination centers in GaN[1]

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Defect-assisted recombination limits the efficiency of solid-state devices. Since nonradiative capture rates decrease exponentially with the energy of the transition, the mechanisms by which recombination take place in wide-band-gap materials are unclear. We will discuss the methodology we have developed to address nonradiative recombination rates from first principles [1], and illustrate its application with the important case of Fe in GaN [2]. Research on Fe has been motivated by the use of Fe to achieve semi-insulating GaN substrates and room-temperature ferromagnetism in GaN. Iron can also be introduced unintentionally into GaN during growth. In traditional semiconductors such as silicon, transition metal impurities are known to act as efficient Shockley-Read-Hall centers by introducing midgap defect levels. Iron impurities in GaN do not follow this pattern: their defect level is close to the conduction band, and hence iron is not expected to act as a strong nonradiative recombination center. We use first-principles calculations based on density functional theory with a hybrid functional to uncover the electronic properties of Fe in GaN. We demonstrate that its high efficiency as a nonradiative center is due to a recombination cycle involving excited states. Unintentional incorporation of iron impurities at modest concentrations leads to nanosecond nonradiative recombination lifetimes. These calculations provide insight into the mechanisms that govern efficient nonradiative recombination in wide-band-gap semiconductors, which is essential for engineering improved materials to be adopted in efficient devices. This work was performed in collaboration with J.-X. Shen, C. E. Dreyer, G. Kresse, S. Marcinkevicius, A. Alkauskas, and C. G. Van de Walle. [1] C. E. Dreyer et al., Appl. Phys. Lett. 108, 141101 (2016). [2] D. Wickramaratne et al., Appl. Phys. Lett. 109, 162107 (2016).

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