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Carrier-Induced Transient Defect Formation and Nonradiative Recombination in InGaN Light-Emitting Devices: A First-Principles Study[1] JUNHYEOK BANG, Korea Basic Science Institute , YIYANG SUN, Rensselaer Polytechnic Institute, J.-H. SONG, Kongju National University, S. B. ZHANG, Rensselaer Polytechnic Institute — Nonradiative recombination (NNR) of excited carriers is not only one of the fundamental physical processes in materials, but is also crucial to optoelectronics device efficiency. Until now, Shockely-Read-Hall and Auger recombination are the two main nonradiative recombination mechanisms widely discussed. Here, by using first-principles calculations, we propose a new NRR mechanism, where excited carriers recombine via a Frenkel-pair (FP) defect formation and the carrier energy is dissipated to phonon through defect generation and annihilation processes. While in the ground state the FP is high in energy and is unlikely to form, its formation is enabled in the electronic excited states by a strong electron-phonon coupling of the excited carriers. This NRR mechanism is expected to be generally observed in wide-gap semiconductors, rather than being limited to InGaN-based light emitting devices.

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