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Extreme quantum confinement in nitrides for improved LED efficiency.

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Nitride materials are indispensable for LEDs in the ultraviolet and the short-wavelength part of the visible spectrum (2014 Nobel Prize in Physics). However, their efficiency is reduced at high power (efficiency droop) and longer wavelengths (green-gap problem). In this talk, I will discuss how first-principles calculations provide insights into the efficiency-limiting mechanisms in nitride LEDs. We identified the origin of the efficiency problems to be nonradiative Auger recombination and its interplay with the intrinsic polarization fields and alloy composition fluctuations of InGaN quantum wells. Our predictive calculations also suggest engineering solutions to improve the LED efficiency. I will discuss how extreme quantum confinement in atomically thin binary nitrides (GaN and InN) is a promising method to stabilize excitons at room temperature and realize efficient LEDs in the deep-ultraviolet and green part of the spectrum. I will also present our results for the design of BInGaN alloys that are lattice-matched to GaN for visible-light emission. This work was supported by the NSF CAREER (1254314) and DMREF (1534221) programs. Computational resources were provided by the DOE NERSC facility (DE-AC02-05CH11231) and by XSEDE, supported by NSF grant ACI-1053575.