“Atomistic insights on nitrides with first-principles calculations: Addressing the high-power, green, and deep UV emission challenges”

Group III nitrides find numerous applications for visible and UV optoelectronics and for power electronics. However, several open research questions remain about the efficiency of nitride optoelectronic devices at high power and for wavelengths approaching the green and the deep UV part of the spectrum.

In this talk I will present insights obtained from first-principles calculations about the atomistic properties of nitrides for high-power, green, and UV light emitters. I will discuss the atomistic details of nonradiative Auger recombination in InGaN alloys, and how it leads to the efficiency droop problem at high power. I will also discuss how the interplay of Auger recombination with polarization fields further reduces the high-power efficiency of devices operating at longer wavelengths (green-gap problem). To further understand Auger recombination in compound semiconductors, I will also present results for GaAs and InN. On a separate topic, ultrathin InN and GaN nanostructures (quantum wells, nanowires, quantum dots) are alternatives to nitride alloys for visible and deep UV emission, respectively. I will present results on the electronic, optical, and excitonic properties of atomically thin InN and GaN quantum wells and nanowires, with a thickness of one to four atomic monolayers (< 1 nm). Atomically thin InN wells and nanowires yield visible light emission, while atomically thin GaN have potential applications for deep UV LEDs and lasers. Excitons in atomically thin GaN are predicted to be stable at room temperature, with exciton binding energies comparable to two-dimensional materials. I will also discuss the thermoelectric coefficients of bulk nitrides and short-period nitride superlattices for applications in cooling of optoelectronic and power devices.

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