Radiative and Auger Recombination in Indium Nitride from First-Principles

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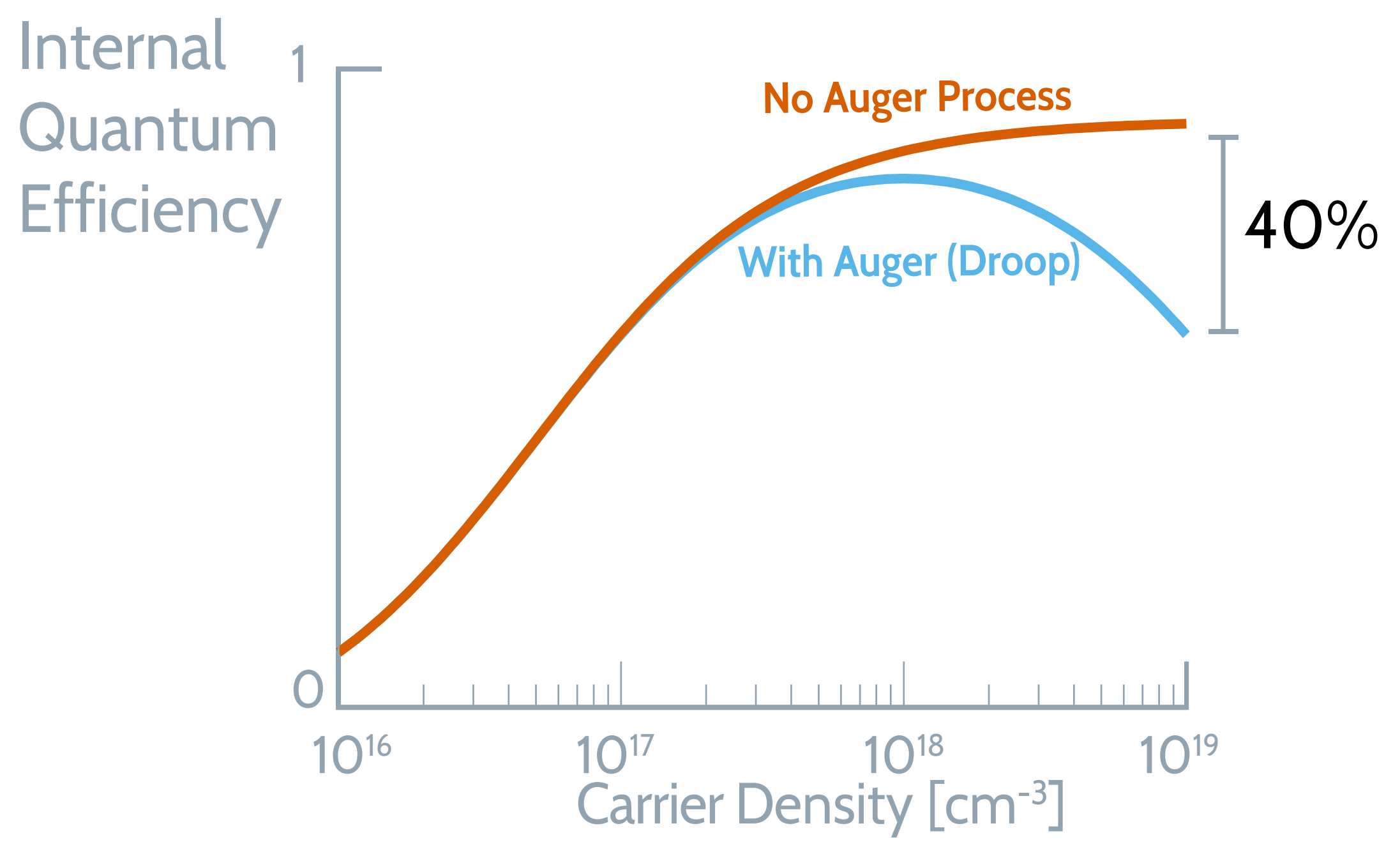
Why Indium Nitride?

The group-III nitrides (AlN, GaN, and InN and alloys) have revolutionized the lighting industry. With gaps ranging from the deep-UV to the infrared, these devices can be tuned to many different emission wavelengths. The center of excitement has been the middle of this range: GaN and Ga-rich InGaN. These materials have allowed the creation of efficient blue light-emitting diodes (LEDs), which efficiently create white light through phosphor down-conversion. But the infrared end of the alloy spectrum could help another industry. InN has a very small gap (0.7 eV) which is near the primary telecommunications wavelength of 1550 nm (0.8 eV). In-rich InGaN could be tuned to this wave length, and the material has other properties for telecomm applications (Winden, JJAP, 2013).

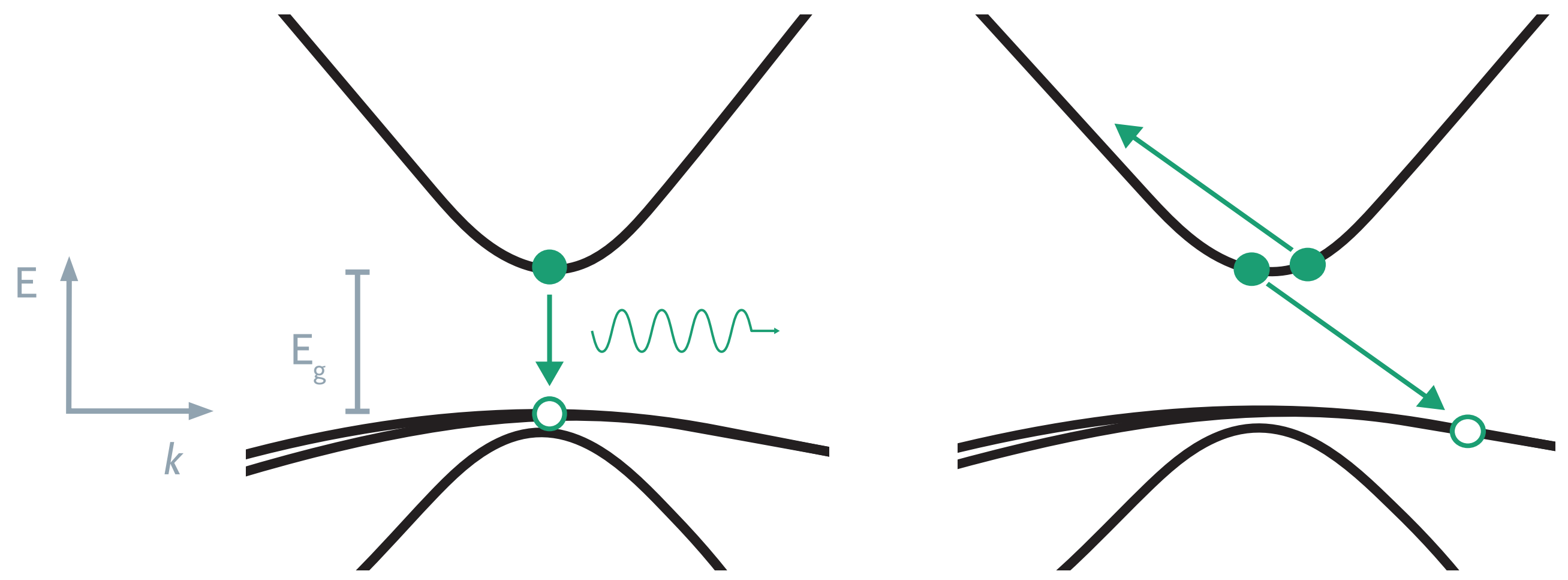
The Problem: Efficiency Drop-off or "Droop"



As carrier density increases, efficiency goes down

What we **want:** Radiative Recombination

What we also **get:** Auger Recombination

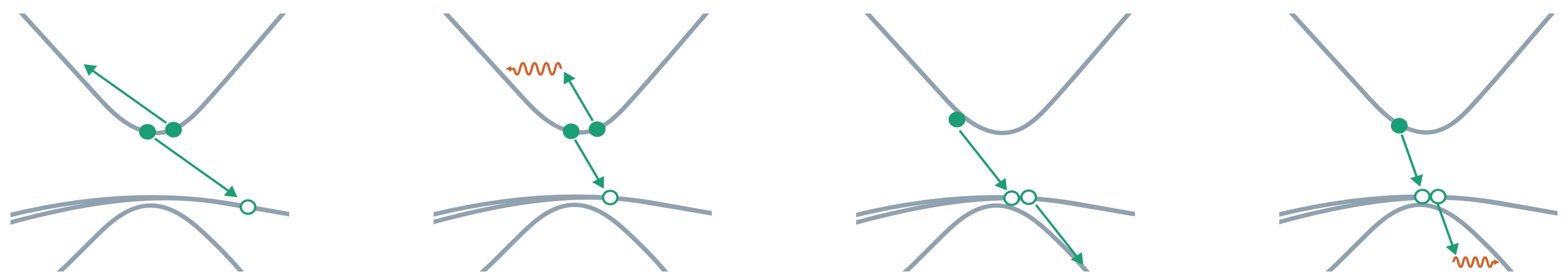


Auger is expected to *increase* as the band gap of a material decreases, making InN more likely to suffer from the Auger process. Because of the non-radiative nature of the process, it is difficult to observe experimentally. The magnitude of its influence on InN is not known with certainty; experimental estimates place the C coefficient between 10^{-28} to 10^{-} cm^{6}s^{-1} (Cho, APL, 2013; Jang, APL, 2008; Tsai, APL 2007).

Our First-Principles Workflow

DFT+U → G_0W_0 → Wannier → Auger + Radiative

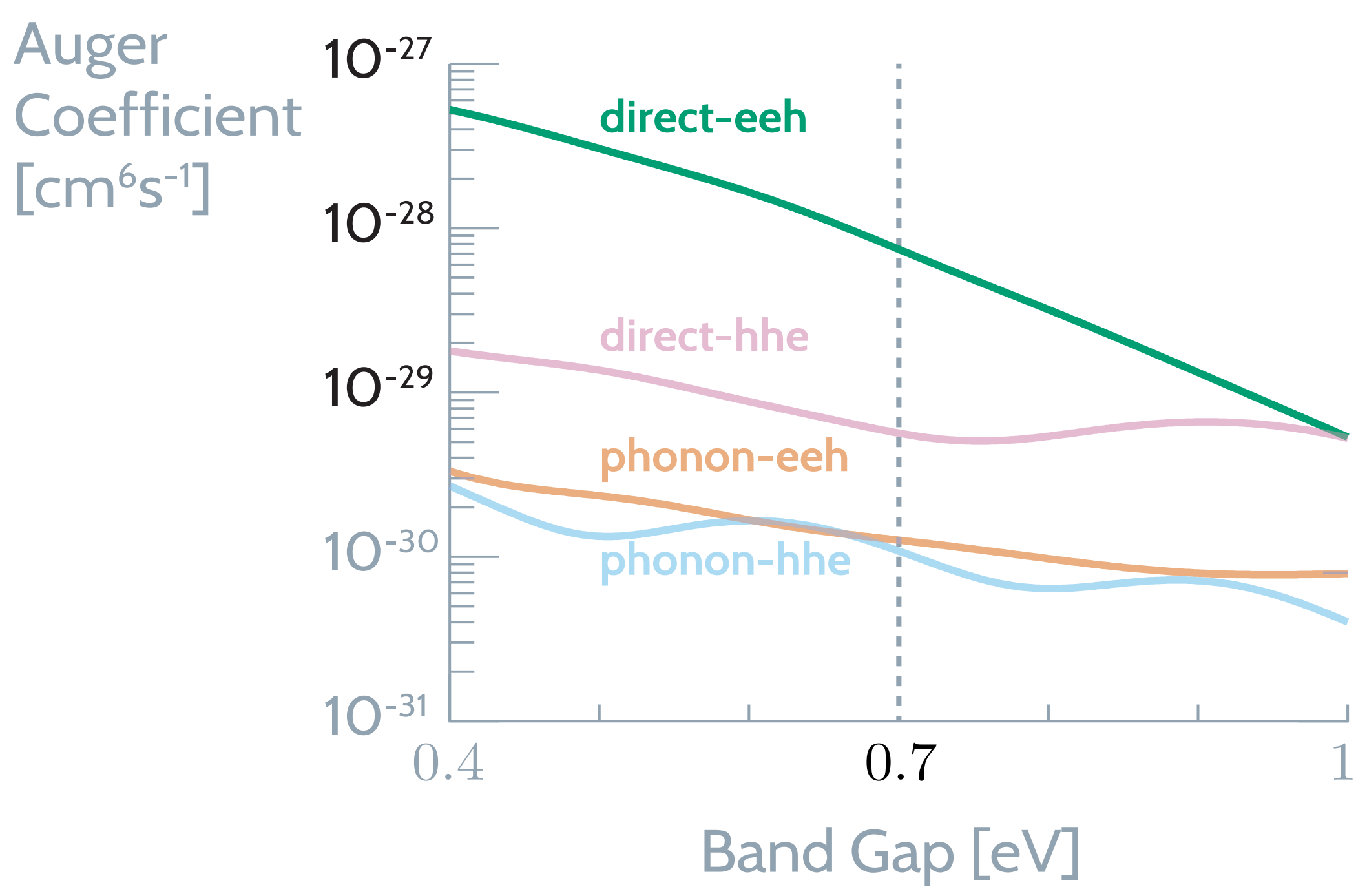
Which Auger Process is Most Important?



Excess energy to electron: EEH Process

Excess energy to hole: HHE Process

Auger recombination comes in different forms. For large gap materials like GaN, assisted processes are dominant (Kioupakis, APL, 2011). However, for a small-gap material we expect to find that *direct Auger* is dominant.



Direct EEH Auger is dominant in indium nitride

Recombination with degenerate carriers

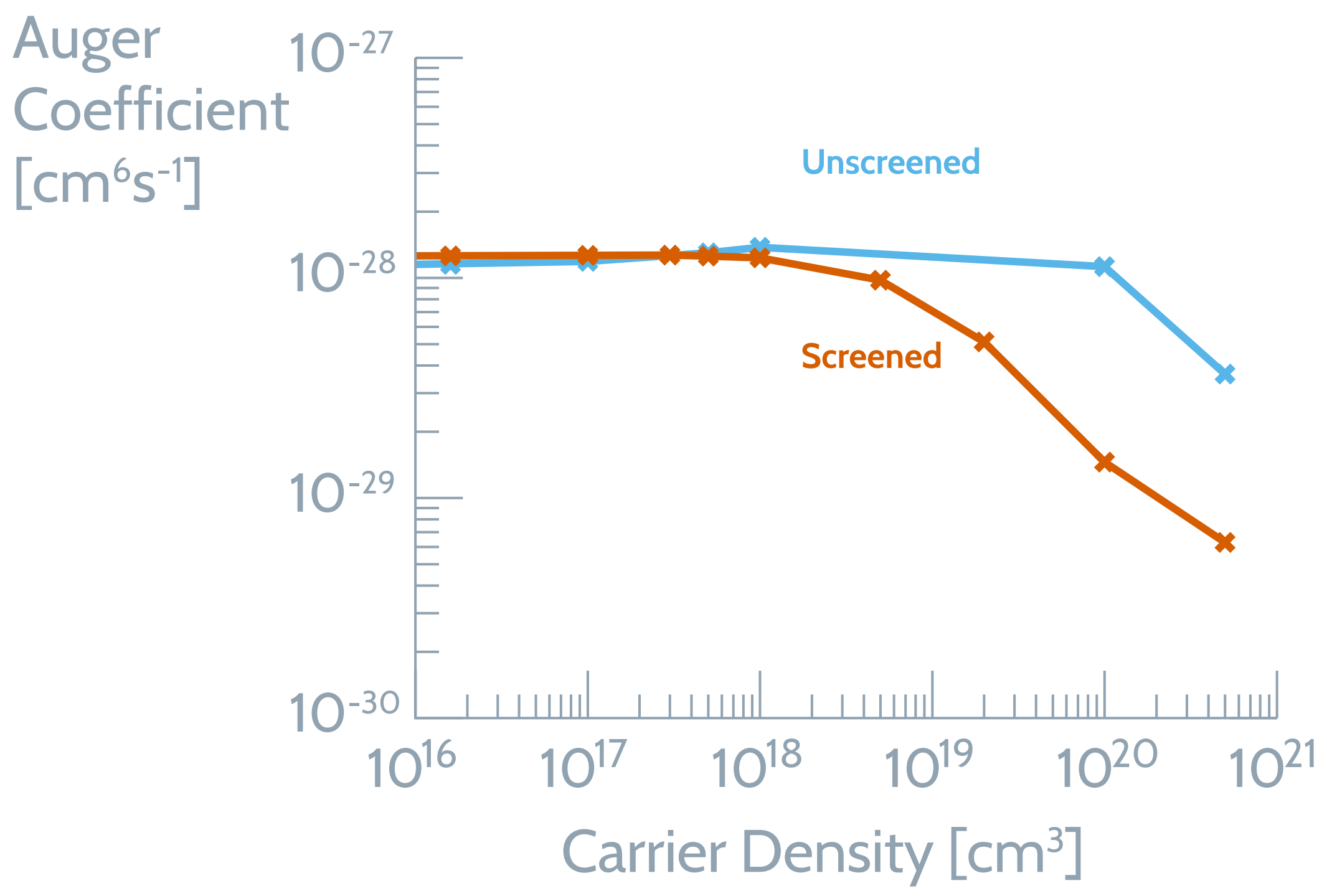
Recombination in semiconductors is typically modeled using the *ABC Model*. At higher carrier densities the model must be modified.

Non-degenerate Degenerate

$$\frac{dn}{dt} = R = \underbrace{An}_{\text{Defect}} + \underbrace{Bn^2}_{\text{Radiative}} + \underbrace{Cn^3}_{\text{Auger}} \Rightarrow R' = An + B'n + C'n^2$$

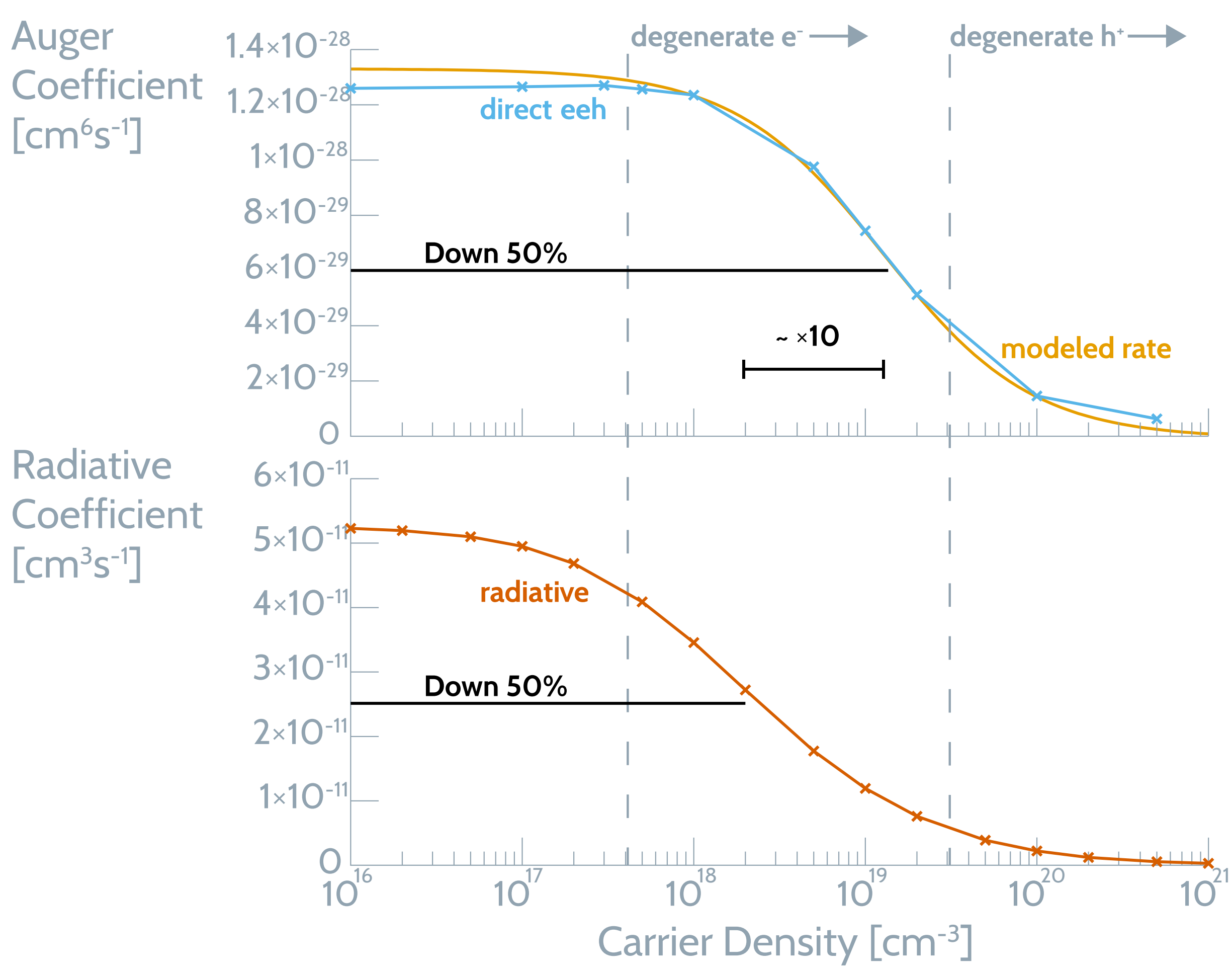
Phase Space Filling: Transitions forbidden by occupied states
Carrier Screening: Carriers not feeling effects of all carriers

Which affects Auger More?



Screening affects Auger rate before Phase-Space Filling

Degeneracy affects the radiative and Auger rates differently



Auger declines closer to degenerate hole densities

Radiative declines closer to degenerate electron densities

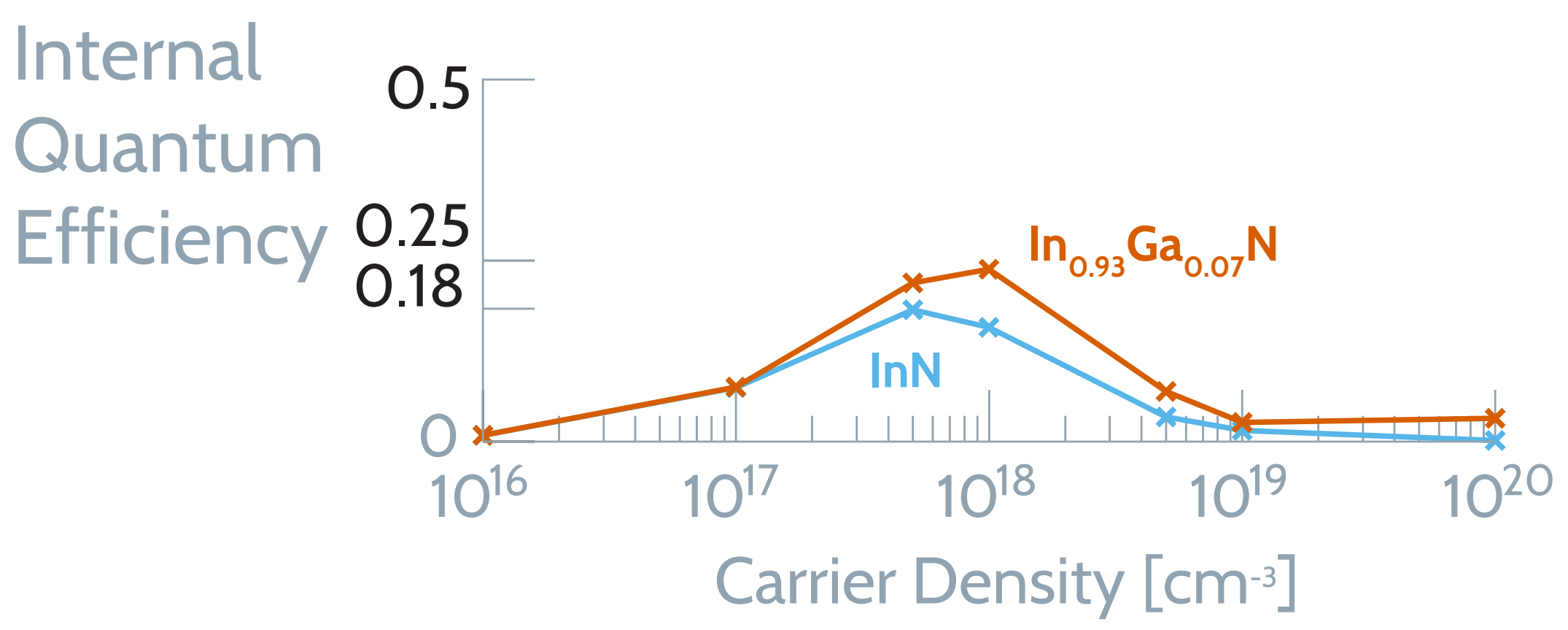
We also modeled the Auger rate as a function of carrier density using:

$$f(x) = \frac{C_0}{1 + \left(\frac{n}{n_0}\right)^b}$$

Low Density Limit
Transition and Density Dependence

At high densities, Auger is n^2

Improvement of efficiency by alloying with GaN



Adding Ga can help reduce Auger

Because the Auger and radiative processes begin to decline at different carrier densities it becomes a major hurdle to create efficient pure InN devices. But by only changing the gap slightly or reducing the background carrier density, we can create more efficient In-rich InGaN devices with gaps at 0.8 eV. These devices would emit in the main telecommunications range (~1550 nm).

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