

# Modeling and simulation of type-II superlattice absorbers: from semi-classical to quantum

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In the realm of material science, the high costs of fabrication necessitate the use of advanced modeling and simulation techniques. These methods provide a precise framework for examining material capabilities and other critical properties, significantly reducing experimental expenses. This talk will explore the evolution from conventional semi-classical approaches to sophisticated quantum transport models utilizing Non-Equilibrium Green's Function (NEGF) method. Additionally, we will delve into industry-oriented techniques, with a particular emphasis on TCAD based simulations. By integrating these methodologies, we aim to offer a comprehensive understanding of both theoretical and practical aspects of material analysis, ultimately bridging the gap between research on photodetectors and industrial applications.

In the first part of my talk, I will present an overview of advanced modeling and simulation techniques essential for understanding carrier transport in high-performance next-generation optoelectronic devices. I will discuss several key methods, including the **k.p** approach for band structure calculations, the semi-classical Boltzmann transport equation (BTE) within the relaxation time approximation (RTA) for analysing carrier dynamics, and the NEGF formalism for elucidating miniband formation in type-II superlattices. Our recent work has focused on developing simulation modules to calculate various carrier transport and optoelectronic parameters, such as mobility, conductivity, and absorption spectra in infrared photodetectors. In this context, I will highlight the significance of elastic and inelastic scattering mechanisms, particularly the impact of interface roughness and polar optical phonon scattering. We advance the Rode's method for the BTE, integrating it with the **k.p** band structure and the envelope function approximation, to capture these effects accurately [1]. Moreover, I will present our evaluations of structure-specific Hall mobility and Hall scattering factors in III-V type-II superlattices. Through our in-depth analysis, we provide a comprehensive microscopic understanding of carrier dynamics in these technologically relevant superlattices. The models developed offer highly accurate and precise transport parameters, surpassing the conventional RTA, particularly for mid-wavelength infrared (MWIR) photodetectors. This talk aims to provide a clear picture of the state-of-the-art simulation techniques and their applications, demonstrating how these models can lead to significant advancements in the performance and understanding of optoelectronic devices.

In the second half of my talk, I will delve into the design and modeling of various infrared detector structures, including nBn, M-superlattice, T2SL, p-i-n, and pBn, to evaluate and enhance their performance. Our goal is to identify and address the bottlenecks in designing MWIR, long-wavelength infrared (LWIR), and very long-wavelength infrared (VLWIR) photodetectors. We not only calculate the critical parameters such as absorption, responsivity, and efficiency, but also explore strategies to enhance photocurrent by reducing the dark current component in these structures. I will discuss the various components of dark current analysed using Synopsys TCAD, providing insights into minimizing these unwanted contributions. Our extended models for determining TE- and TM-polarized optical absorption reveal significant findings. Specifically, TE-polarized absorption shows a substantial influence near the conduction-heavy hole band transition energy, which diminishes due to the dominant TM-contribution from the conduction-light hole band transition [2]. These insights are crucial to understand the modeling of superlattice absorber regions to improve detector performance. We offer guidelines for optimizing infrared photodetectors by refining the modeling and design of superlattice absorbers, ultimately leading to significant advancements in their efficiency and functionality.

In conclusion, I will highlight our recent efforts on developing an optically gated double-gate tunnel field-effect transistor (TFET) photosensor, utilizing a monolayer of TMDCs as the channel material [3]. This design targets the visible wavelength range of 300 nm to 1100 nm, achieving detection at low intensities of 0.5 W/cm<sup>2</sup>. We calculate the photosensitivity and responsivity of the device, observing superior quantum efficiency at a wavelength of 700 nm. Additionally, I will discuss the influence of dielectric materials on the performance of photosensor, along with the impact of the dimensions and positioning of the illumination window. These factors play a crucial role in optimizing the sensitivity and efficiency of the device. This section aims to provide

insights into cutting-edge TFET photosensor designs, showcasing how advanced material choices and structural optimizations can lead to significant improvements in photodetection capabilities.

### References:

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- [3] J. Talukdar and B. Muralidharan, "Performance analysis of optically gated MoS2 photosensor for visible light detection," in *IEEE Sensors Journal*, 24, 23810, (2024).

