

Abstract

The continuous scaling of semiconductor devices into the deep-nanometer regime has led to a fundamental shift in the mechanisms governing charge transport, necessitating a departure from classical models and the adoption of semiclassical and fully quantum mechanical approaches. As devices shrink evolve toward low-dimensional material systems, phenomena such as quantum confinement, tunneling, subband formation, and ballistic transport begin to dominate carrier dynamics. These effects profoundly impact not only the electrical behavior of nanoscale transistors but also the performance of emerging sensing technologies—including gas sensors, biosensors, and photodetectors—where surface interactions are strongly coupled with transport physics. The thesis titled “Semi-classical and Quantum Modeling of Low-Dimensional Devices and Sensors” systematically investigates these intertwined effects, developing and applying a suite of transport models across multiple scaled and advanced device architectures and sensor platforms.

Chapter 1 introduces the motivation for the work by highlighting the limitations of classical drift-diffusion and hydrodynamic models in capturing the physics of ultra-scaled devices. The chapter sets the foundation for exploring how these transport paradigms can be systematically applied across different device geometries and material systems for sensing applications.

Chapter 2 provides a framework for understanding the spectrum of transport models ranging from classical to quantum. The limitations of classical drift-diffusion in short-channel, and scaled-dimensional scenarios are outlined, guiding the rationale for semiclassical and quantum extensions. Semiclassical models such as Density Gradient (DG) and Bohm Quantum Potential (BQP) incorporate confinement effects and carrier-density curvature while retaining computational efficiency. In contrast, Non-Equilibrium Green’s Function (NEGF) offers descriptions of tunneling, scattering, and non-equilibrium charge flow—making it essential for devices operating in the quantum-dominated regime. This layered approach to transport modeling forms the backbone of the subsequent device-specific investigations.

Chapter 3 presents a novel p-type MoTe₂ Metal-Oxide-Semiconductor Field-Effect Transistor (MOSFET) hydrogen sensor that utilizes charge-plasma engineering through palladium electrodes to create P⁺ regions in an otherwise undoped MoTe₂ channel. The dual function of palladium—as both a source/drain charge-plasma generator and hydrogen-reactive sensing surface—enhances sensitivity while eliminating the need for physical doping in 2D materials. The NEGF formalism is employed to study quantum transport in the ultra-scaled device (< 10 nm), revealing how quantum confinement and tunneling influence H₂-induced modulation of charge density and current response. The results provide unique insights into the under-explored domain of p-type MOSFET sensors, establishing a pathway for CMOS-compatible hydrogen sensing technologies with quantum-aware design strategies.

Chapter 4 investigates AlGa_xN/GaN Double Channel High Electron Mobility Transistor (DCHEMT) as high-performance biosensors, focusing on the detection of the cancer biomarker C-ERB2. The work emphasizes the role of inter-channel coupling between the upper and lower 2DEG channels formed by polarization-induced charge in the heterostructure. Through Density Gradient (DG)-augmented transport modeling, the study examines how mole-fraction variations in the AlGa_xN barrier modify quantum well depth, sheet charge distribution, carrier confinement, and electrostatic coupling. The results show that increased Al content in the upper channel strengthens coupling and enhances sensitivity, while excessive polarization in the lower channel can degrade performance. This chapter underscores the importance of polarization engineering and quantum corrections in biosensor optimization, addressing challenges such as sensitivity, selectivity, and device stability for biomedical diagnostics.

Chapter 5 combines analytical quantum modeling and BQP-based semiclassical simulation to study SiGe heterojunction Tunnel FET (TFET) biosensors, with device dimensions scaled below 20 nm. The first part of the chapter develops a complete analytical model of a dual-metal double-gate TFET by solving Schrödinger and Poisson equations self-consistently, deriving quantized energy states and using the Landauer formula to compute tunneling current. The second part evaluates the impact of BQP corrections on sensitivity and selectivity across three SiGe-based configurations. The results reveal that quantum

confinement suppresses sensitivity differently depending on material composition and strain distribution. The SiGe-pocket design offers the best balance of classical selectivity and quantum reliability. This chapter highlights how quantum effects modify band-to-band tunneling and illustrates the need for quantum-calibrated models in TFET biosensor design.

Chapter 6 extends the quantum modeling approaches to $\text{In}_{(1-x)}\text{Ga}_x\text{As}_y\text{P}_{(1-y)}/\text{InP}$ multi-quantum-well (MQW) photodetectors, targeting the 1000–2000 nm wavelength range relevant for optical communication and LiFi systems. Using the $k \cdot p$ method, quantum well formalism, and transport simulations, the study evaluates how variation in As mole fraction influences the bandgap, quantum efficiency, dark current, bandwidth, and noise performance. A higher As content widens the bandgap, reducing dark current and low-frequency noise but also lowering photocurrent and narrowing the spectral response. This demonstrates the fundamental trade-off between speed and responsivity in MQW photodetectors and highlights the importance of quantum-engineered band structure tuning for wideband optical sensing and communication applications.

Chapter 7 synthesizes the findings and outlines future directions, emphasizing the need for experimental validation, circuit level simulation/ implementation, physics-based comprehensive analytical models for sensor networks, and progress toward quantum-enhanced sensing platforms.

Overall, the thesis provides a unified, cross-platform exploration of transport phenomena in low-dimensional devices and demonstrates how integrating semiclassical and quantum models with advanced structural engineering can significantly enhance sensing performance. The outcomes contribute new insights and modeling approaches applicable to gas sensors, biosensors, and optoelectronic detectors, marking a meaningful step toward scalable, quantum-enabled sensor technologies for the future.