

Abstract

This thesis, entitled “**Solar Cells and Sensors: Simulation, Fabrication and Characterization,**” explores the development of advanced nano-engineered photovoltaic and sensing devices through a combination of simulation, fabrication, and experimental characterization. The work addresses the growing demand for sustainable energy harvesting and intelligent sensing technologies by investigating novel materials, device architectures, and optimization strategies.

The first part of the research focuses on an axially graded $\text{Si}_{(1-x)}\text{Ge}_x$ nanowire solar cell analyzed using Monte Carlo simulation. The influence of germanium composition on photovoltaic performance is systematically studied, demonstrating that the Ge– $\text{Si}_{0.5}\text{Ge}_{0.5}$ –Si axial configuration achieves the highest efficiency due to improved light absorption, carrier transport, and reduced recombination losses. The second study presents the fabrication and characterization of a TiO_2 quantum-dot-based solar cell for ultraviolet light utilization in tandem photovoltaic structures. Structural, optical, and electrical analyses confirm the suitability of TiO_2 quantum dots as environmentally friendly UV absorbers, achieving a power conversion efficiency of 4.68%.

The sensing component of the thesis includes the development of a crossbar architecture-based hydrogen gas sensing platform using palladium-functionalized silicon structures. Device-level and network-level simulations reveal the effects of interconnect resistance, array size, and work-function variation on sensor sensitivity and scalability. Furthermore, a graded SiGe channel dielectric-modulated tunnel field-effect transistor (TFET) biosensor is proposed and analyzed. Comparative studies demonstrate that the graded SiGe architecture offers superior tunneling efficiency, enhanced sensitivity, improved selectivity, and reduced defect formation compared with conventional channel configurations.

Overall, the research demonstrates that nanostructured materials, quantum confinement effects, graded semiconductor architectures, and advanced simulation methodologies can significantly improve the performance of next-generation solar cells and sensors. The outcomes provide valuable design guidelines for the development of efficient, scalable, and environmentally sustainable energy harvesting and sensing technologies for future electronic, healthcare, environmental monitoring, and IoT applications.