

**Overview:** This project aims to advance the theoretical understanding and computational exploration of semiconductor quantum dots as qubits for quantum computing. Semiconductor quantum dots possess properties ideal for implementing qubits, but their successful application requires addressing numerous challenges, including the design of quantum dot arrays, the development of optimal qubit control techniques, and strategies for mitigating decoherence. This research will employ quantum simulations to optimize gate fidelities and overall quantum circuit performance, with a focus on contributing to the emerging field of quantum computing.

**Intellectual Merit:**

- **Electronic Structure Methods:** Theoretical investigations into the electronic structure of semiconductor quantum dots are essential to understand their qubit behavior. This project will delve into the electronic properties of quantum dots, utilizing advanced electronic structure methods such as density functional theory (DFT) and tight-binding models.
- **Nanostructures:** Quantum dots are nanoscale structures, and their design, fabrication, and manipulation fall under the purview of nanostructures. This project will explore the design of quantum dot arrays, including the determination of optimal geometries, dimensions, and material choices for achieving stable and coherent qubits.
- **Quantum Coherence:** Maintaining coherence in quantum dots is crucial for quantum computing. The research will focus on theoretical models to enhance and manipulate quantum coherence, including control over spin states and coherence time, making quantum dots suitable for qubit applications.
- **Soft Condensed Matter:** Quantum dots in semiconductor materials can be viewed as part of the realm of soft condensed matter. Their interactions with the surrounding environment, encapsulation, and the study of their behavior in mesoscopic systems are essential for achieving practical qubits.

**Tools and Simulations:** This project will employ a combination of theoretical and computational methods. Quantum simulations will be carried out using state-of-the-art quantum computing simulators and tools like IBM Qiskit, Rigetti Forest, and Google Cirq. Classical simulations will utilize advanced computational packages for quantum dynamics and materials modeling, such as Quantum ESPRESSO and VASP, to optimize quantum gate operations and assess their performance in realistic environments.

**Broader Impacts:** This research contributes to the broader scientific community by advancing our understanding of semiconductor quantum dots as viable qubit candidates for quantum computing. Additionally, the project has broader societal implications as quantum computing holds the potential to revolutionize fields ranging from cryptography to materials discovery. The research team will actively engage in educational outreach, supporting the training of students and fostering public awareness of quantum technologies. This project aligns with the goals of the CMMT program by combining electronic structure methods, nanostructures, quantum coherence, and soft condensed matter research to enable groundbreaking advancements in quantum computing using semiconductor quantum dots. The ultimate aim is to design robust qubits that can be integrated into quantum computing platforms, enabling transformative applications in science and technology.