

AI-Assisted Materials Discovery for Integrated Quantum Photonic Devices

1. Introduction

Quantum photonics explores the generation, manipulation, and detection of individual photons — the fundamental particles of light — in regimes where quantum mechanical effects dominate [1]. Historically, quantum photonics has enabled crucial demonstrations of quantum phenomena, such as the Einstein-Podolsky-Rosen paradox and Bell test experiments [2,3]. Today, it is a cornerstone technology for the future of quantum computing, quantum communication, quantum sensing, and quantum metrology [4].

Photons offer exceptional advantages as carriers of quantum information, including low decoherence, high-speed transmission, and easy manipulation. However, traditional quantum optics relied heavily on bulk optical components, limiting scalability and stability. The shift towards Integrated Quantum Photonics [4]— fabricating large-scale photonic circuits on semiconductor chips [5]— addresses these challenges. Integrated devices offer:

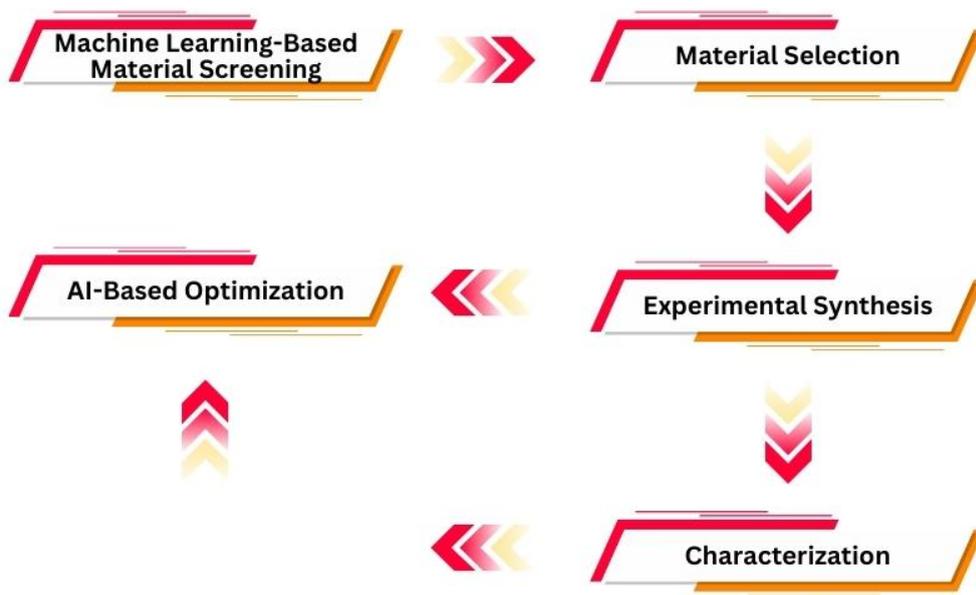
- Miniaturization—Smaller system footprints dramatically reduce the size, weight, and power consumption of quantum photonic systems.
- Stability - Miniaturized components, produced using advanced lithographic techniques, create waveguides and optical elements that are inherently phase-stable (coherent) and do not require frequent optical realignment.
- Experiment size - Many optical components can be integrated into a compact chip measuring just a few square centimeters, enabling more complex experiments and devices within a much smaller footprint.
- Scalability and Manufacturability - Devices based on integrated photonic circuits can be produced in large volumes at substantially lower cost using existing semiconductor fabrication techniques.

Parallely, machine learning (ML) [6] and artificial intelligence (AI) [7] have revolutionized material discovery by predicting properties beyond traditional trial-and-error methods. The integration of AI with quantum materials research can significantly accelerate the development of new quantum photonic devices.

Recent breakthroughs in nanoscience and quantum control have further expanded the horizon: engineered quantum materials are now being developed to address major challenges in quantum-limited sensing and quantum/classical information processing. In particular, atomically thin semiconductors and insulators provide a promising platform for the atomic-scale control of quantum emitters and the exploration of many-body quantum effects, such as magnetism, spin liquids, and superconductivity [11].

At Kalasalingam Academy of Research and Education, the Quantum Photonics Laboratory collaborates across disciplines to tackle these frontiers using tools from first-principles theory, quantum optics, spectroscopy, quantum information science, and device engineering. These low-dimensional quantum materials are perhaps the most likely candidates to “close the loop” on materials design, achieving both atomic precision and quantum coherence in functional devices.

This research aligns closely with the long-envisioned idea of exploring the “plenty of room at the bottom,” a concept championed by Feynman and rooted in the ancient atomic theory of Democritus — now realized in the engineering of quantum systems, one atom at a time.



2. Objectives

The major goals of the proposed research are:

1. **Material Discovery using ML:**

Develop machine learning [6] models to identify 2D and low-dimensional materials with desirable quantum photonic properties (e.g., efficient single-photon emission, strong nonlinearity, low loss).

2. **Experimental Material Synthesis and Characterization:**

Synthesize selected materials and validate their physical and optical properties using advanced experimental techniques.

3. **Integrated Quantum Photonics Device Fabrication:**

Engineer and test quantum photonic circuits incorporating these materials.

4. **Exploration of Quantum Effects:**

Study many-body quantum phenomena like superconductivity, magnetism, or spin liquids in engineered materials for advanced applications.

5. **AI-Enhanced Experimental Control:**

Implement reinforcement learning or optimization algorithms to fine-tune experimental conditions for material growth and device fabrication [7].

3. Origin and Motivation of the Proposal

Recent advances in nanofabrication, quantum control, and AI open up new possibilities for functional quantum systems. However, bottlenecks remain:

- Discovery of materials with suitable quantum-optical properties is slow.
- Integration of quantum emitters with photonic chips is still maturing.
- Many-body quantum interactions remain poorly understood at the nanoscale.

4. State of the Arts

Modern quantum photonics involves:

- Integrated photonic chips with hundreds of elements [8]
- Electrically driven quantum emitters, such as quantum dots, rare-earth ions, or defects in SiC [9]
- Nanophotonic enhancement techniques (Purcell effect, Bragg mirrors) for improving emission and coupling efficiency

AI, especially quantum machine learning (QML), is being used to:

- Predict properties of quantum materials using large databases
- Discover exotic phases like superconductors or topological states [8]
- Guide autonomous laboratories with active learning and decision-making frameworks like QMLMaterial [10]

5. National and International Research Status

International:

- MIT, Stanford, and the University of Maryland lead in hybrid quantum photonics.
- Research groups in Germany and Japan are developing on-chip quantum light sources and nanophotonic cavities.
- Platforms like QMLMaterial are used in automated material discovery [10].

National:

- India's National Mission on Quantum Technologies aims to build indigenous quantum infrastructure.
- Indian institutions like IISc and IITs are initiating research in quantum photonics and ML-based material design.

6. Research Methodology

A. Machine Learning-Based Material Prediction

- **Dataset Preparation:**

Curate databases from sources such as Materials Project, NOMAD Repository, and AFLOW.

- **Model Development:**

Apply supervised learning models (Random Forest, Gradient Boosting, Neural Networks) and unsupervised learning (Clustering, PCA) to predict key properties: bandgaps, defect formation energies, exciton binding energies.

- **First-Principles Calculations:**

Use DFT (Density Functional Theory) simulations for validation of machine-predicted materials.

B. Synthesis of Low-Dimensional Quantum Materials

- **Material Growth Techniques:**

- Chemical Vapor Deposition (CVD)
- Mechanical Exfoliation
- Atomic Layer Deposition (ALD)

- **Characterization Techniques:**

- Raman Spectroscopy
- Atomic Force Microscopy (AFM)
- Transmission Electron Microscopy (TEM)
- Photoluminescence (PL) Spectroscopy
- X-ray Photoelectron Spectroscopy (XPS)

C. Integrated Quantum Photonics Device Fabrication

- **Device Design:**

Create optical circuits — waveguides, cavities, beam splitters — with integrated quantum emitters.

- **Fabrication Techniques:**

- Electron Beam Lithography (EBL)
- Dry/Wet Etching
- Thin-Film Deposition

- **Cryogenic Testing:**

Low-temperature optical measurements to study coherence properties of single photons and quantum emitters.

D. AI-Enhanced Experimental Optimization

- **Reinforcement Learning:**

Develop algorithms to dynamically optimize growth parameters (temperature, pressure, precursor flow) during CVD growth.

- **Bayesian Optimization:**

Apply AI to tune photonic device fabrication parameters for optimal light coupling and emission efficiency.

7. Applications and Impact

Quantum Communication:

- Secure information transmission using quantum key distribution (QKD) exploiting the no-cloning theorem.

Quantum Computing:

- Encoding information in qubits based on photon superposition for faster computations than classical computers (e.g., quantum logic gates, quantum annealing).

Quantum Information Processing:

- Quantum error correction, teleportation, and simulation applications.

Fundamental Science:

- Exploration of many-body quantum physics, emergence of superconductivity and magnetism in engineered 2D systems.

This work could also enable practical quantum networks and contribute to the global race in quantum technology leadership.

8. Expected Outcomes

- Development of a data-driven AI platform for quantum material discovery
- Fabrication of highly coherent, integrated single-photon sources
- Demonstration of quantum photonic devices based on novel materials
- Discovery of new material platforms exhibiting superconductivity or spin liquids
- Publications in high-impact journals and conference proceedings
- Enhanced national capacity in quantum technology through skilled PhD training

9. Research Facilities Required

Computational:

- High-performance computing (for DFT, ML training)
- Software: Quantum ESPRESSO, ORCA, scikit-learn, TensorFlow

Experimental:

- Raman, PL, XPS, AFM, TEM
- Cleanroom with EBL, ALD, CVD
- Cryostats and laser-based optical setups for single-photon measurements

10. Conclusion

This research proposal aims to bridge two cutting-edge areas — AI and quantum photonics — to accelerate the discovery, development, and deployment of novel materials and devices. It aligns perfectly with KARE's vision and the national agenda in quantum science and technology.

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