AI-Enabled Multi-Objective Inverse Design of Chiral Metasurfaces for Biosensing via Moth-Eye Template Nanofabrication

Xiaoyang Zheng

Research Motivation and Background

Detecting biomolecular chirality is essential for drug discovery and diagnostics, yet traditional circular dichroism (CD) spectroscopy requires expensive instrumentation and large sample volumes [1]. Professor Mana Toma's group has pioneered plasmonic metasurface biosensors leveraging collective plasmon modes for label-free colorimetric detection using silver nanodome arrays [2, 3, 4], enabling practical spectrometer-free biosensing through industrially scalable moth-eye nanoimprint lithography [5].

I aim to extend this platform to chiral sensing, where superchiral electromagnetic fields achieve ultrasensitive detection of molecular handedness [6]. Current AI-driven metasurface design methods cannot efficiently generate manufacturable chiral structures optimized for both signal enhancement and biosensing performance [7], creating urgent need for an AI framework generating moth-eye-compatible designs with multi-objective optimization.

Research Objectives

I propose developing a conditional Generative Adversarial Network (cGAN) framework tailored to Professor Toma's moth-eye fabrication platform for rapid generation of optimized chiral plasmonic metasurface biosensor designs [8, 9]:

1. **Define parametric design space:** Mathematical model describing achievable 3D chiral nanostructures within moth-eye constraints, inspired by Professor Toma's silver nanodome architectures.
2. **Generate training dataset:** High-quality dataset ($>$10,000 designs) via automated FDTD simulations evaluating CD enhancement and LSPR wavelength shifts.
3. **Develop cGAN architecture:** PyTorch-based cGAN with dual performance targets (chiroptical response + colorimetric sensitivity) as inputs and manufacturable parameters as outputs.
4. **Experimental validation:** Fabricate top designs using moth-eye templates and characterize via Professor Toma's protocols (CD spectroscopy, colorimetric immunoassays).

Methodology

Phase 1 (Months 1–8): Develop automated Python-FDTD pipeline sampling moth-eye parameter space (silver thickness, template depth, asymmetry), generating paired geometric and performance data (CD enhancement, refractive index sensitivity).

Phase 2 (Months 9–16): Train forward-predicting surrogate network for rapid evaluation, then train cGAN with multi-objective loss (adversarial learning, dual-target reconstruction, physics constraints), validated via FDTD and comparison with Professor Toma's published designs.

Phase 3 (Months 17–24): Fabricate selected designs using Professor Toma's moth-eye process with silver deposition. Characterize via SEM, CD spectroscopy, and label-free binding assays with model biomolecules (chiral amino acids, IgG) [4, 10].

Expected Outcomes and Impact

Deliverables: (1) validated cGAN tool for rapid chiral biosensor customization without re-training, (2) design library demonstrating chiroptical-colorimetric trade-offs, and (3) proof-of-concept devices with $<$10% prediction-experiment deviation. This directly advances Professor Toma's mission of democratizing biosensing [11] by combining her scalable moth-eye platform with AI-driven multi-objective design for pharmaceutical quality control and point-of-care diagnostics.

References

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