

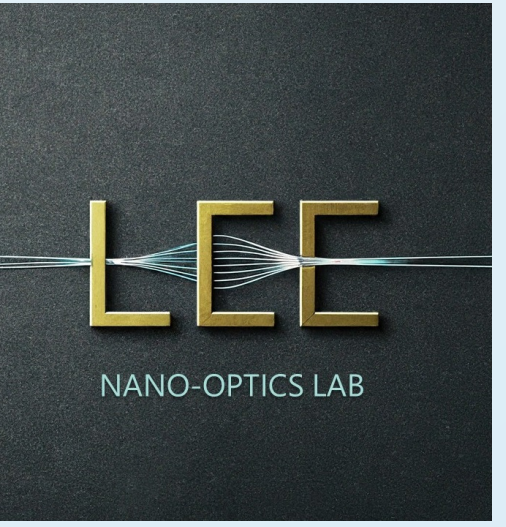
Physics-Validated Generative AI for Freeform Optical Metasurface Design

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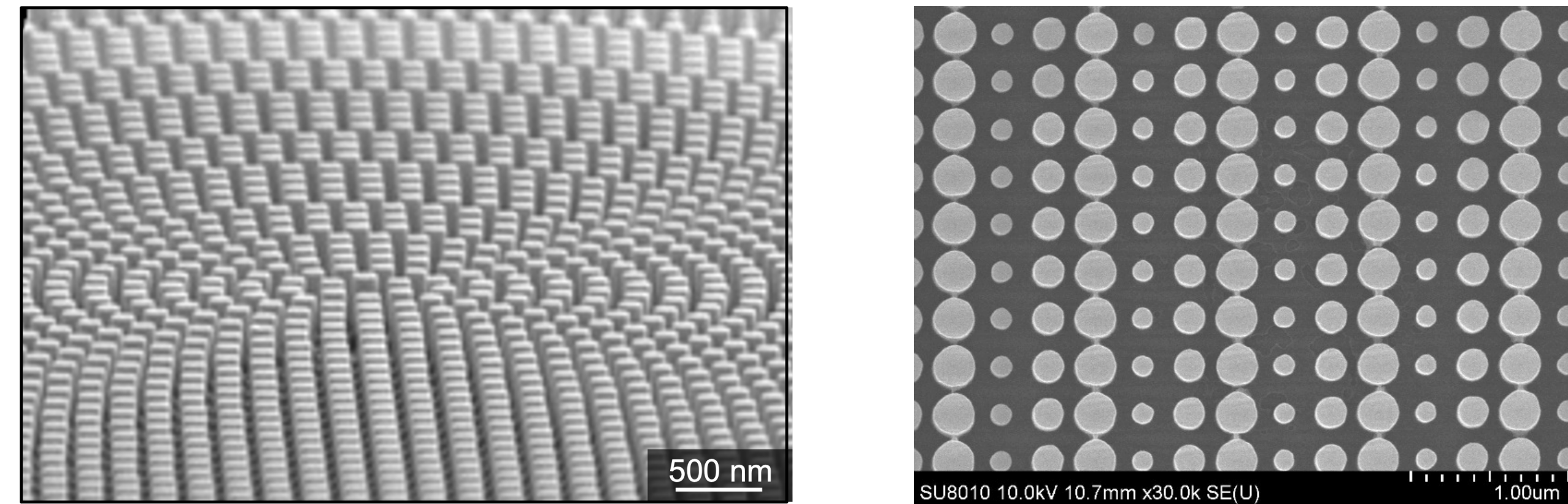
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Background & Motivation

A metasurface is an ultrathin layer of nanoscale patterns that steers or focuses light [1]. Our simulated TiO_2 layer is just 200 nm (0.2 micrometers) thick.



Scanning electron micrographs (SEM) of nanopillars and nanofins for shaping light. Images supplied by H. Lee.

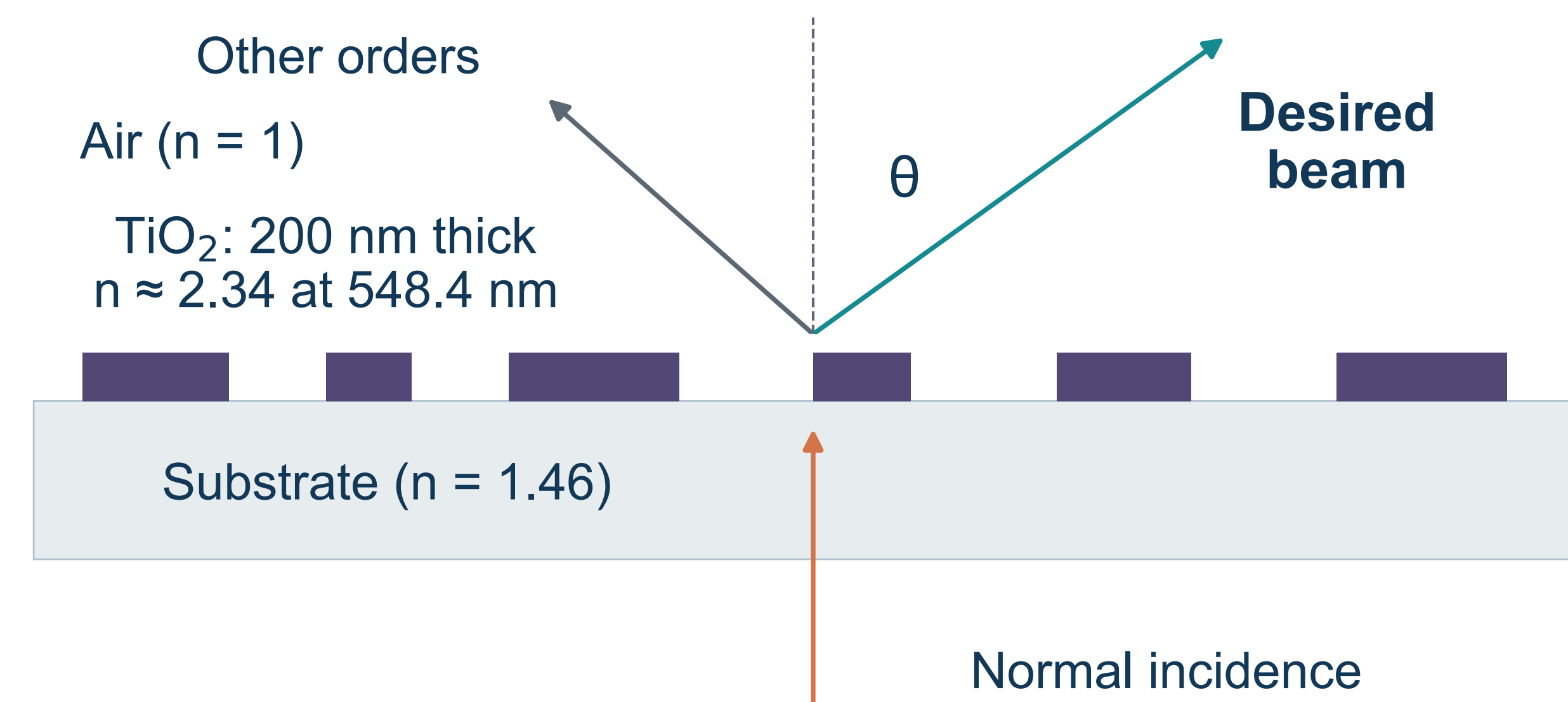
Why freeform? Simple shapes offer fewer design choices; freeform patterns provide more flexibility to control light. Topology optimization searches these patterns to improve steering efficiency [2].

Limitations of topology optimization:

- **Vast search space:** many geometric variables to explore.
- **Slow iteration:** repeated simulations can take hours per device.
- **Local optima:** starting geometry can limit the final efficiency.

Goal: Efficient Optics, Faster Design

Our solution: generative AI. Learn from optimized designs to rapidly propose patterns for a chosen wavelength and angle, targeting high beam-steering efficiency [2,3,6].



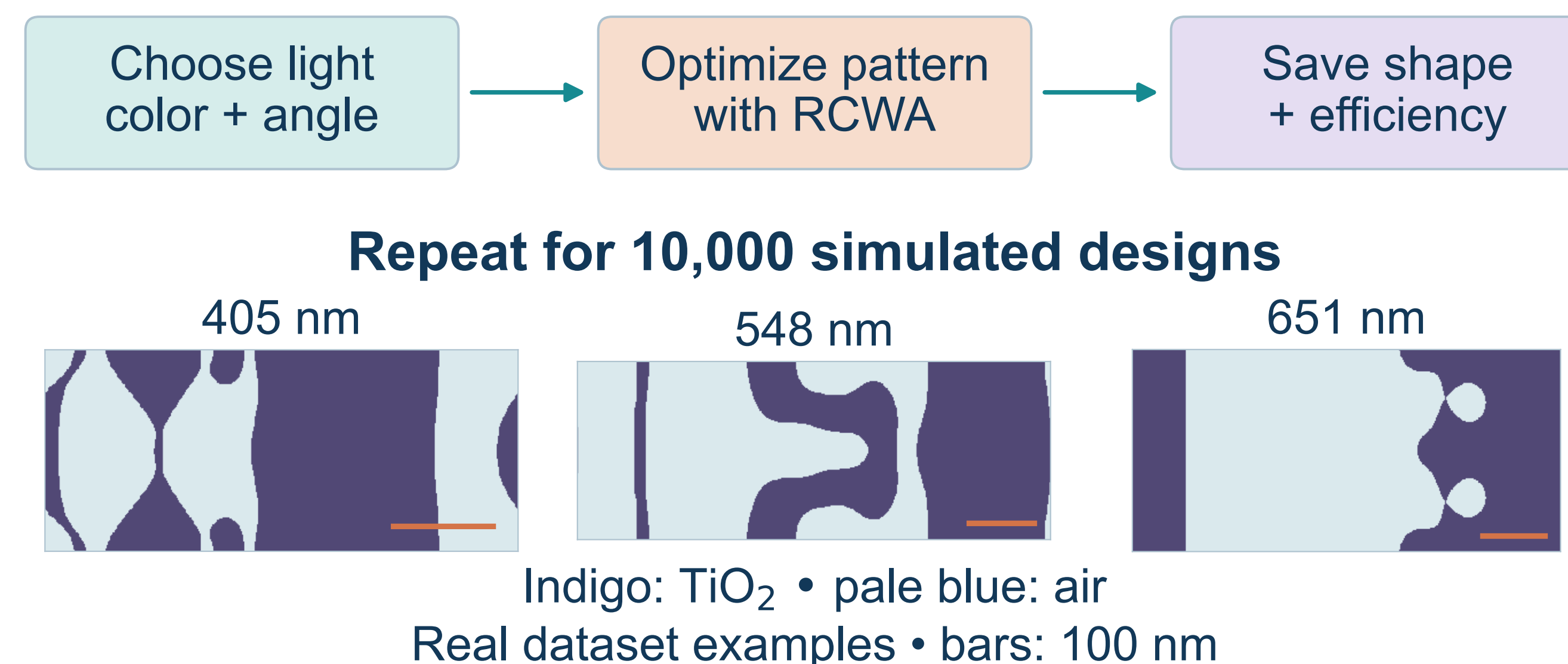
Schematic cross-section; TiO_2 index varies with wavelength. Target order (+1,0): first order along x, zero along y.

Efficiency = target-beam power / incoming power. We average the efficiencies for two input polarizations.

Physics check: RCWA (rigorous coupled-wave analysis) calculates the power in the desired beam, other transmitted beams, and reflected light. We use it to check each AI-generated design against the optical target [4].

Build a Library of Designs

Build training examples with optical simulations. At each sampled wavelength and angle, we optimize a pattern using RCWA, then save its shape, conditions and efficiency.

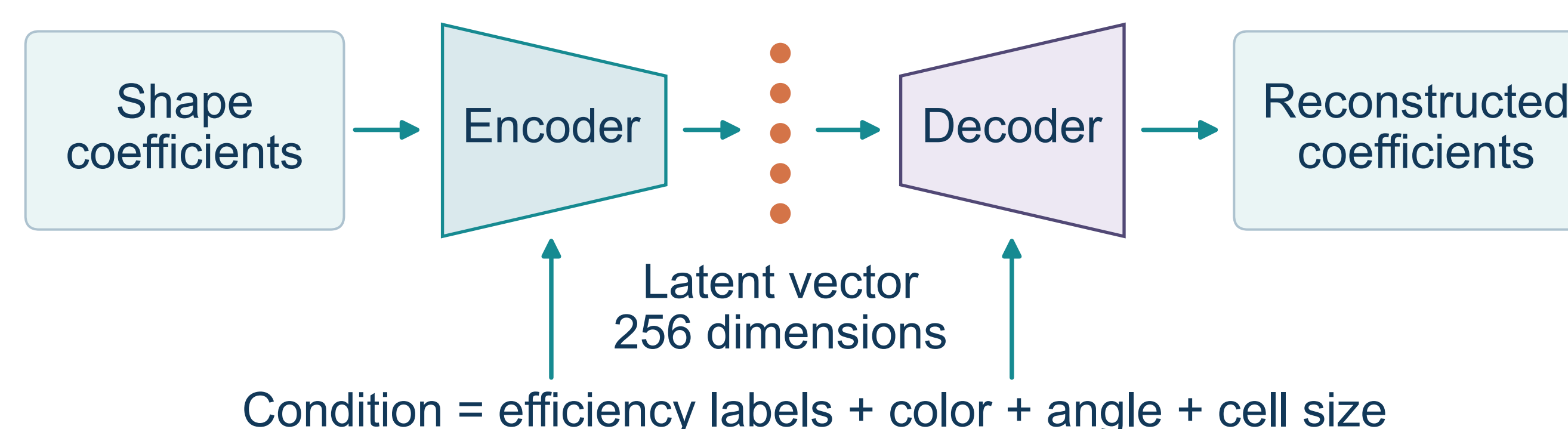


10,000 simulated designs: 380–750 nm, 25–75 degrees.
9,000 training / 1,000 validation examples.

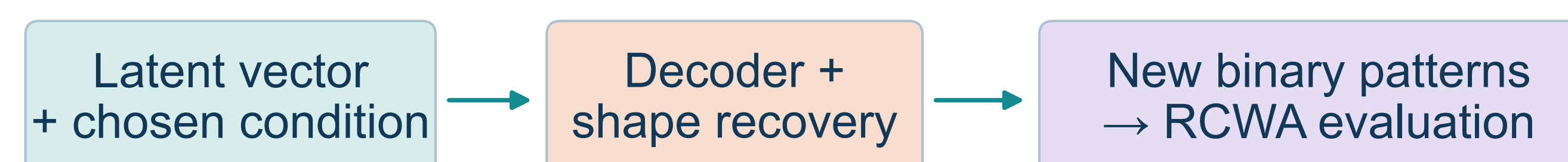
AI Proposes New Designs

One condition, many designs. Our conditional variational autoencoder (cVAE) accepts wavelength and angle within 380–750 nm and 25–75 degrees. Sampling latent vectors produces different candidate patterns [5].

TRAIN: compress and reconstruct example shapes



GENERATE: sample latent vectors for new shapes



Learning the shapes. The model reconstructs 160×64 discrete cosine transform (DCT) coefficients from a 256-dimensional latent vector.

Fine-tuning. Simulated binary-pattern efficiency provides feedback for further training.

Checking the designs. Efficiency labels guide generation; RCWA then measures each recovered binary pattern's optical efficiency.

Results: Does AI Improve the Designs?

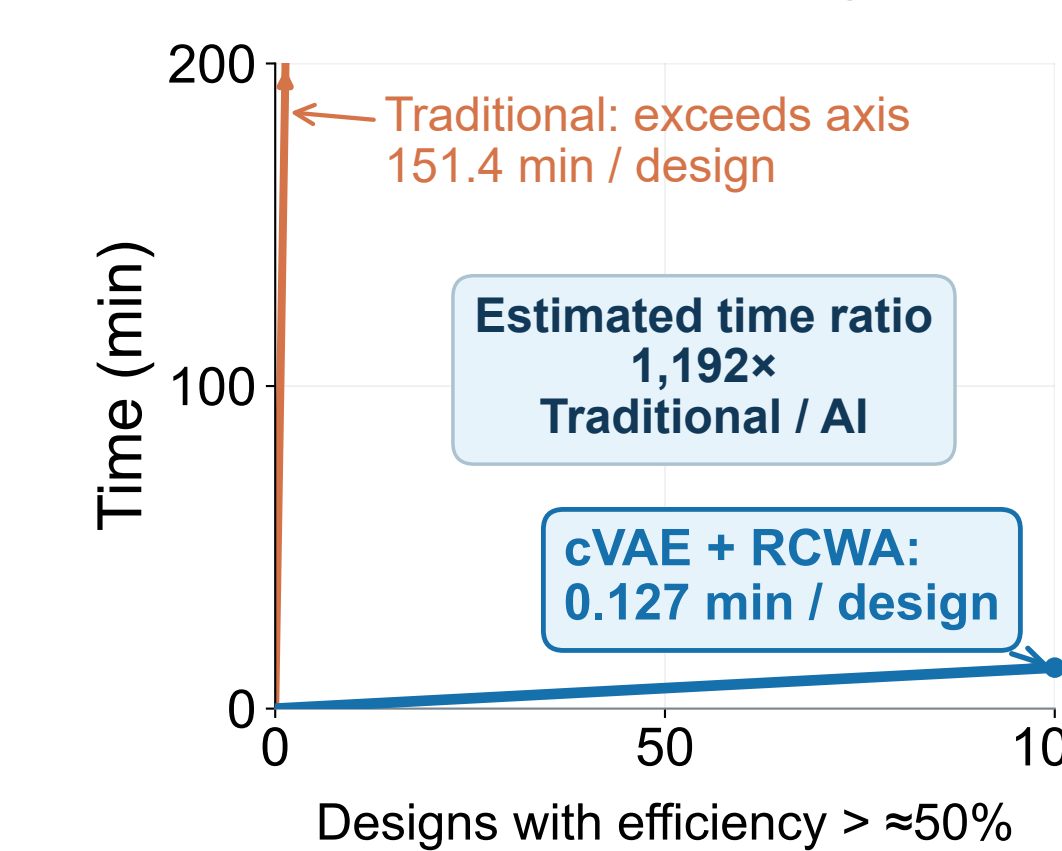
≈3 s / 1,000 candidates

Decoder only, A100; screening extra.

Estimated curve: targets, hardware and RCWA settings differ.

Estimated design time

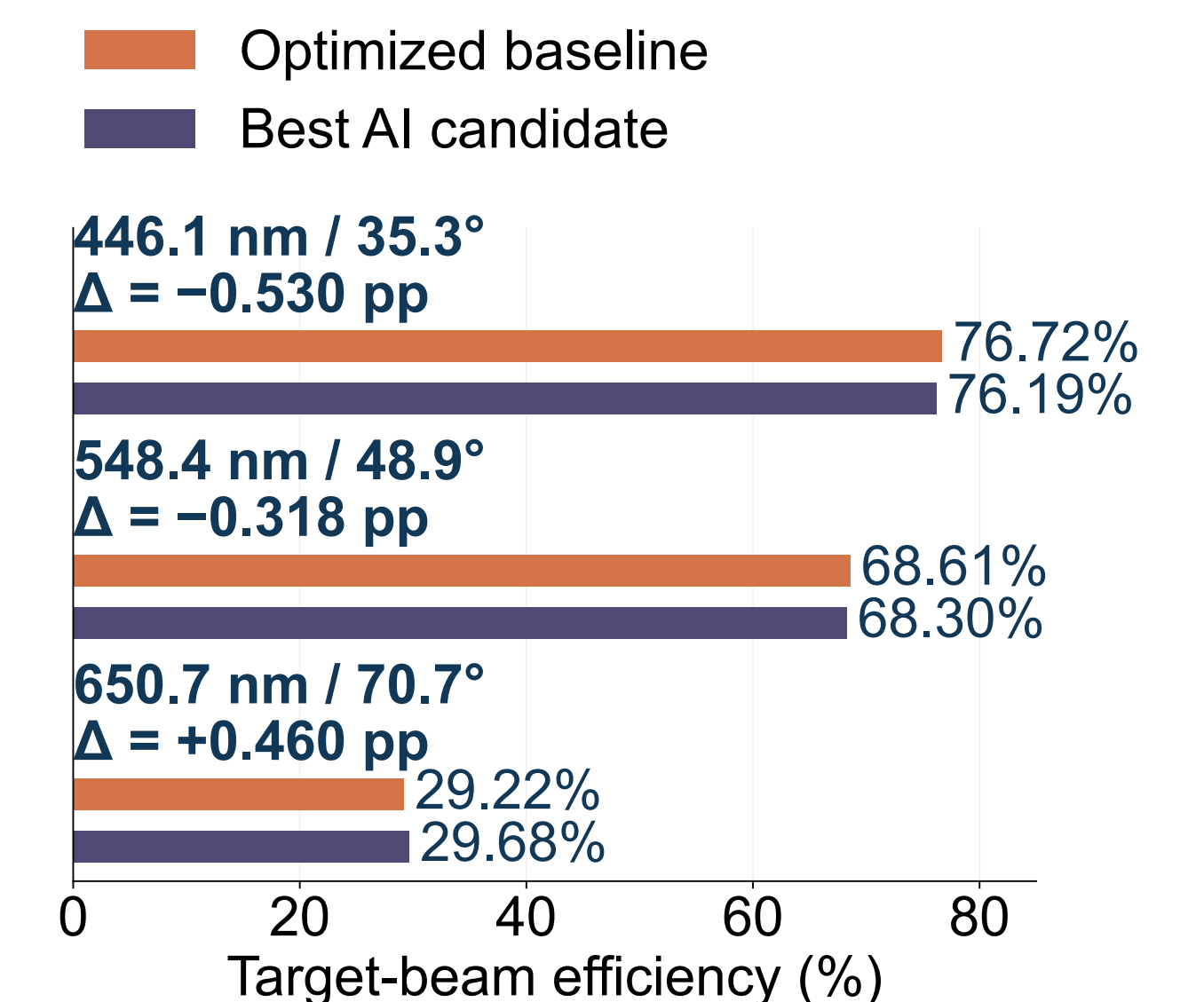
Traditional optimization
cVAE + RCWA screening



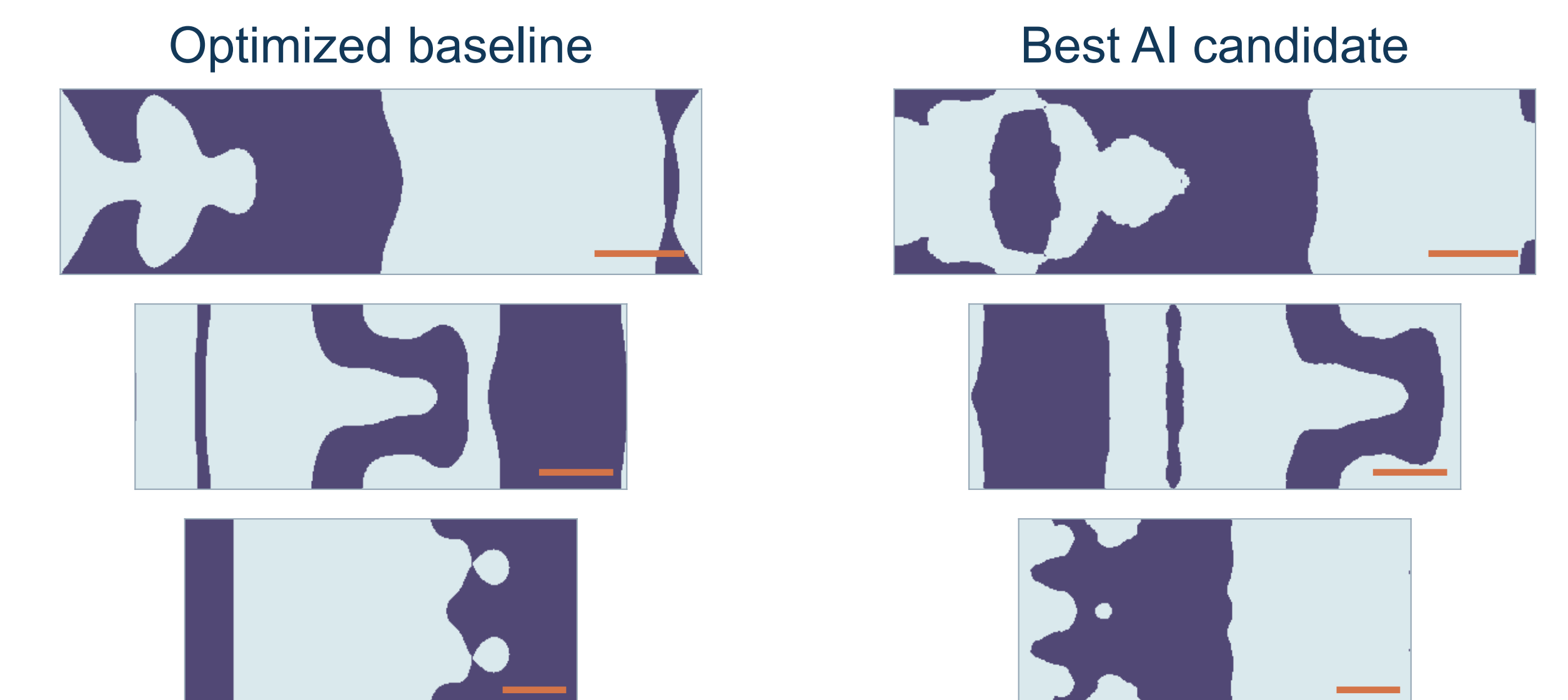
Matched optical targets and RCWA settings.

Best of 1,000 AI candidates versus baseline.

Δ = best minus baseline (pp).



Same optical target, different candidate patterns



Rows match the conditions above. Indigo: TiO_2 ; pale blue: air. Bars: 100 nm. True physical aspect ratios.

Conclusions & Future Goals

AI rapidly proposes freeform designs; optical simulations identify promising candidates.

Mean efficiency: 39.80% → 40.57% with fine-tuning; 20/24 conditions improve (32 matched samples each).

Best-candidate gains are mixed: mean best-of-32, 51.20% → 51.08%. In the three baseline comparisons, two are lower; one gains 0.460 pp.

Future goal: rapid AI design of functional optics for imaging and sensing, with fabrication constraints and matched runtime tests.

Selected References

- [1] Yang et al., Rep. Prog. Phys. 85, 036101 (2022). Metasurface review.
- [2] Jiang et al., ACS Nano 13, 8872–8878 (2019). Generative freeform design.
- [3] Dang et al., J. Mater. Chem. C 11, 12906–12914 (2023). Neural-network optical design.
- [4] Kim & Lee, Comput. Phys. Commun. 282, 108552 (2023). TORCWA.
- [5] Kingma & Welling, Auto-Encoding Variational Bayes, ICLR (2014).
- [6] D. Dang, S. Love et al., Meta-GPT, arXiv:2512.12888 (2025). Preprint.