Datasets and Benchmarks for Nanophotonic Structure and Parametric Design Simulations

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Contributions

- Development of a **generic simulation scheme and pipeline for nanophotonic structures in Python**, based on the open-source software, Meep, and licensed under the MIT license
- Creation of datasets of a myriad of nanophotonic structures for **electromagnetic interference shielding, anti-reflection, and solar cells**
- Investigation into the **effects of altering grid sizes** in electrodynamic simulations, providing insights into tradeoffs between time and accuracy
- Introduction of benchmarks designed for the **optimization of parametric structures**

Real-World Applications

- **Electromagnetic Inference Shielding**

As the usage of electronic devices has grown, there is a growing demand for strategies to shield these devices from external electromagnetic waves and interference.

- **Anti-Reflective Coatings**

Light traveling from air to glass partially reflects due to the disparity in index of refraction. Better anti-reflective structures can achieve broad-spectrum and wide-angle anti-reflection.

- **Solar Cells**

Nanomaterials are revolutionizing solar cell technology, promising significantly enhanced efficiency and reduced costs.

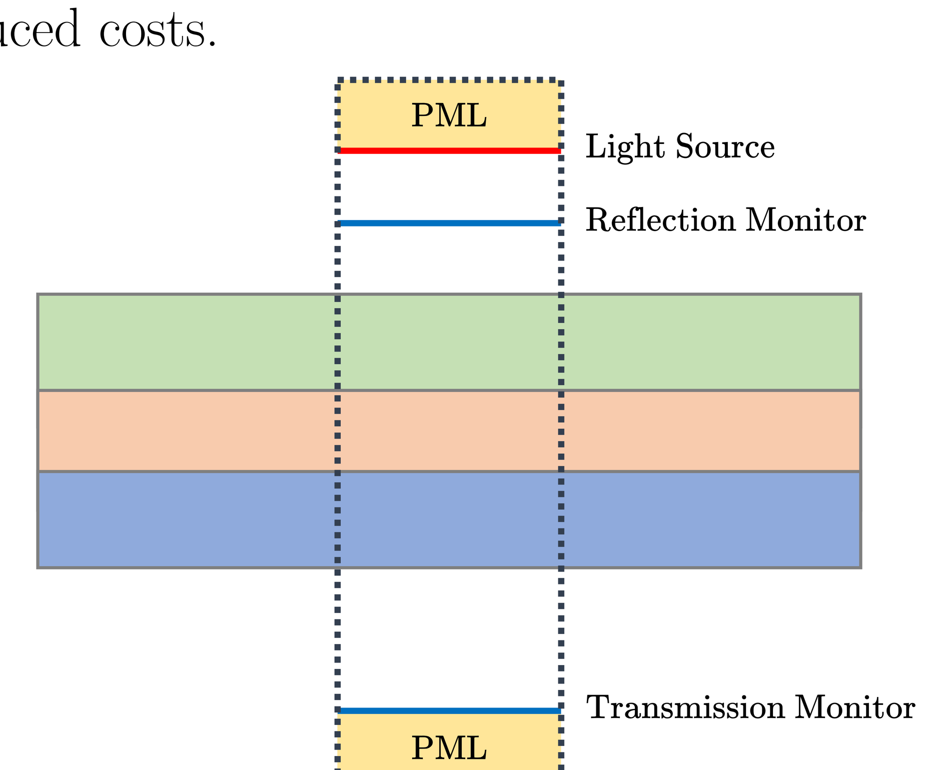
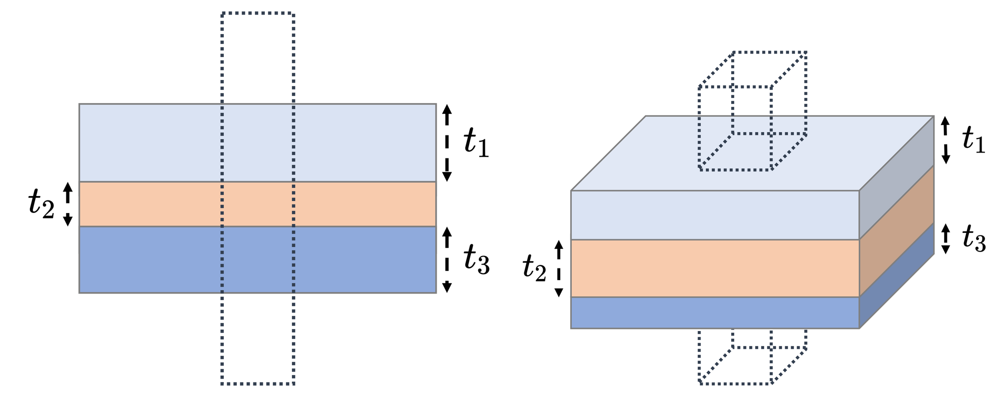
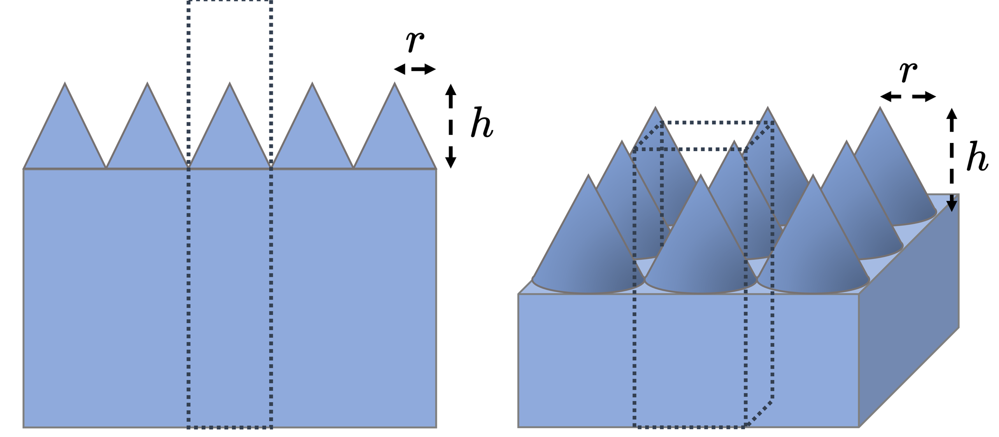


Figure: Schematic of nanophotonic structure simulations.

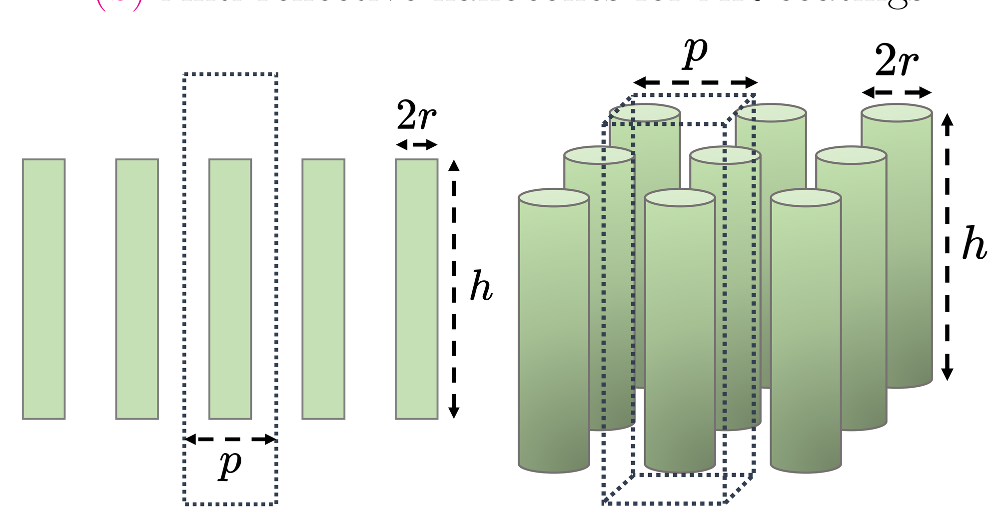
Nanophotonic Structures



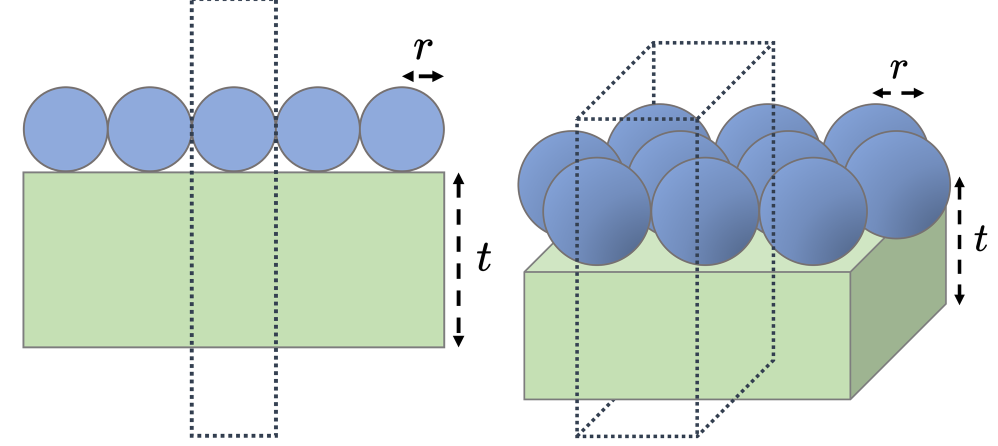
(a) Three-layer film for EMI shielding



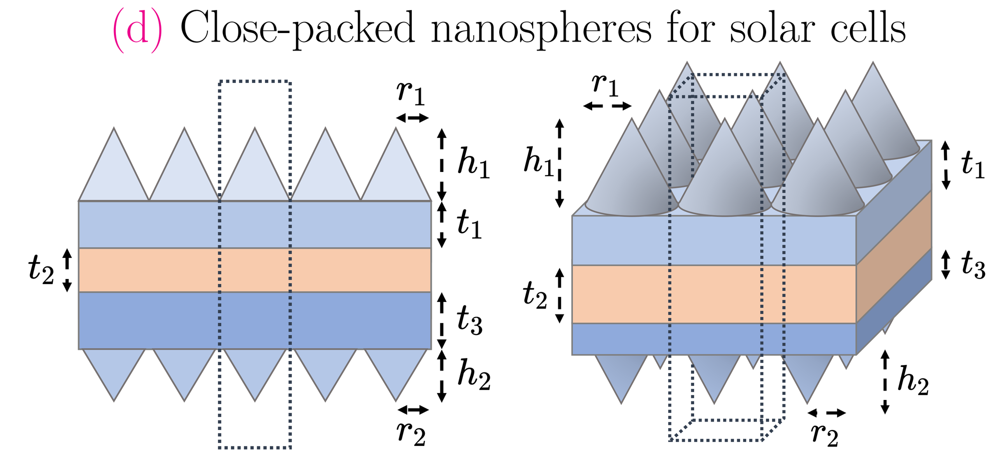
(b) Anti-reflective nanocones for AR coatings



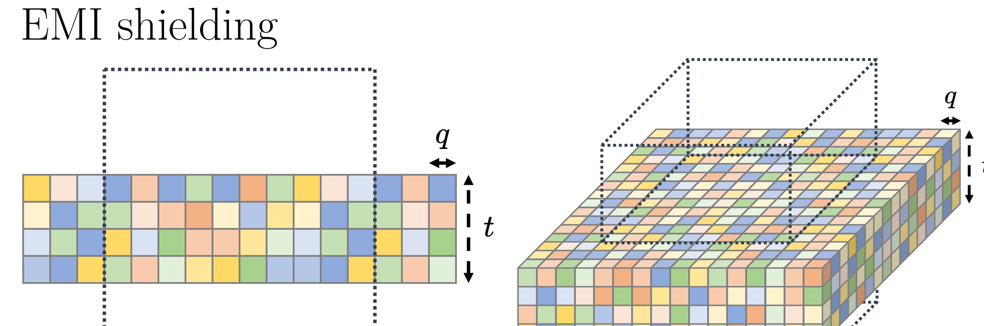
(c) Vertical nanowires for solar cells



(d) Close-packed nanospheres for solar cells



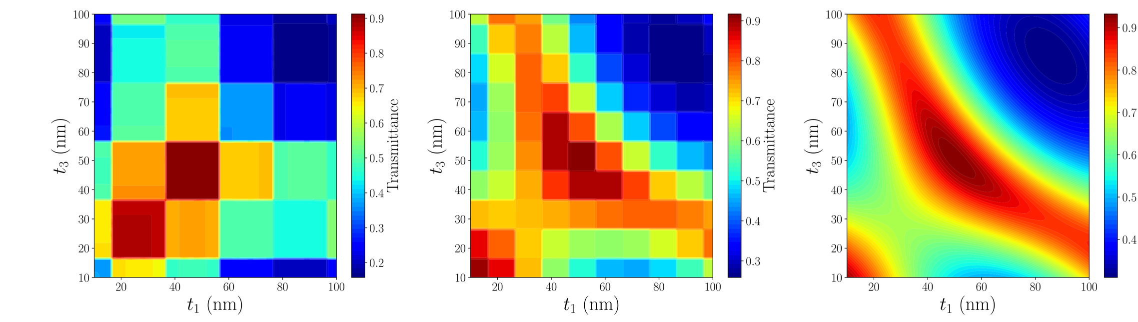
(e) Three-layer film with double-sided nanocones for EMI shielding



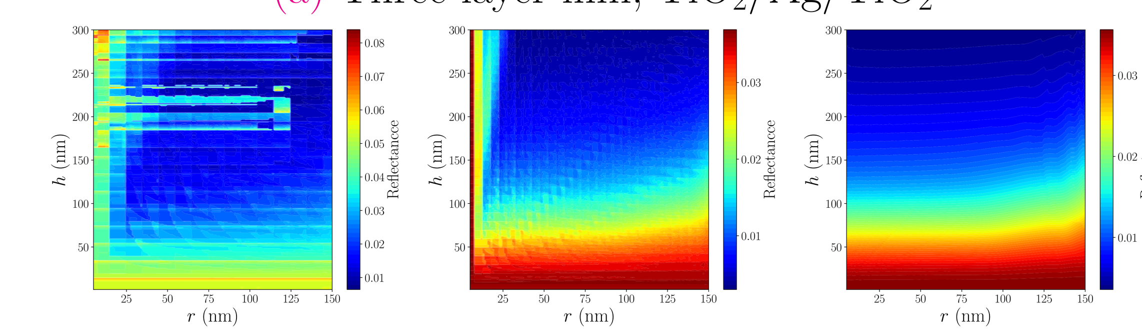
(f) Combinatorial system with material blocks for versatile applications

Figure: Two- and three-dimensional nanophotonic structures.

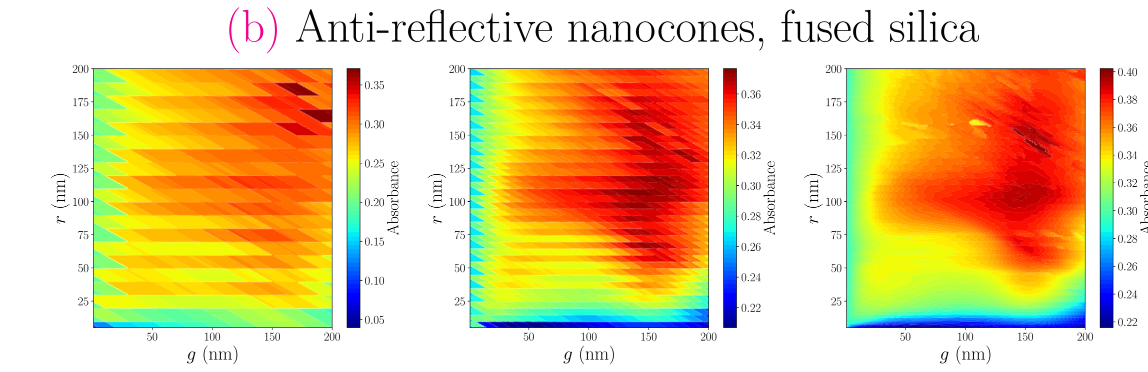
Visualization



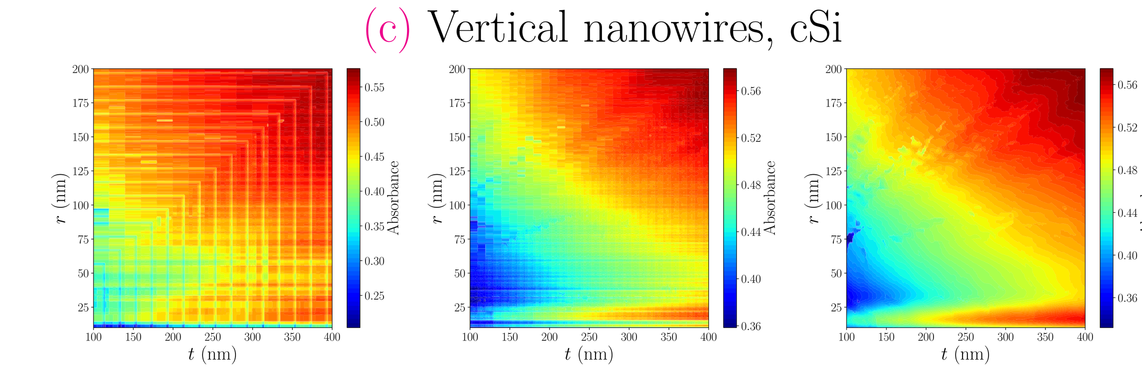
(a) Three-layer film, $TiO_2/Ag/TiO_2$



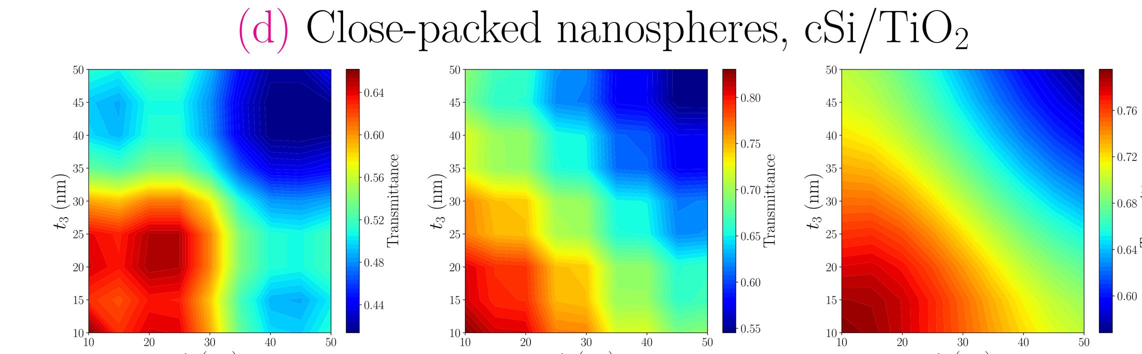
(b) Anti-reflective nanocones, fused silica



(c) Vertical nanowires, cSi



(d) Close-packed nanospheres, cSi/TiO_2



(e) Three-layer film with double-sided nanocones

Figure: Visualization of target properties over parameters. The last structure is made of $TiO_2/Ag/TiO_2/TiO_2/TiO_2$.

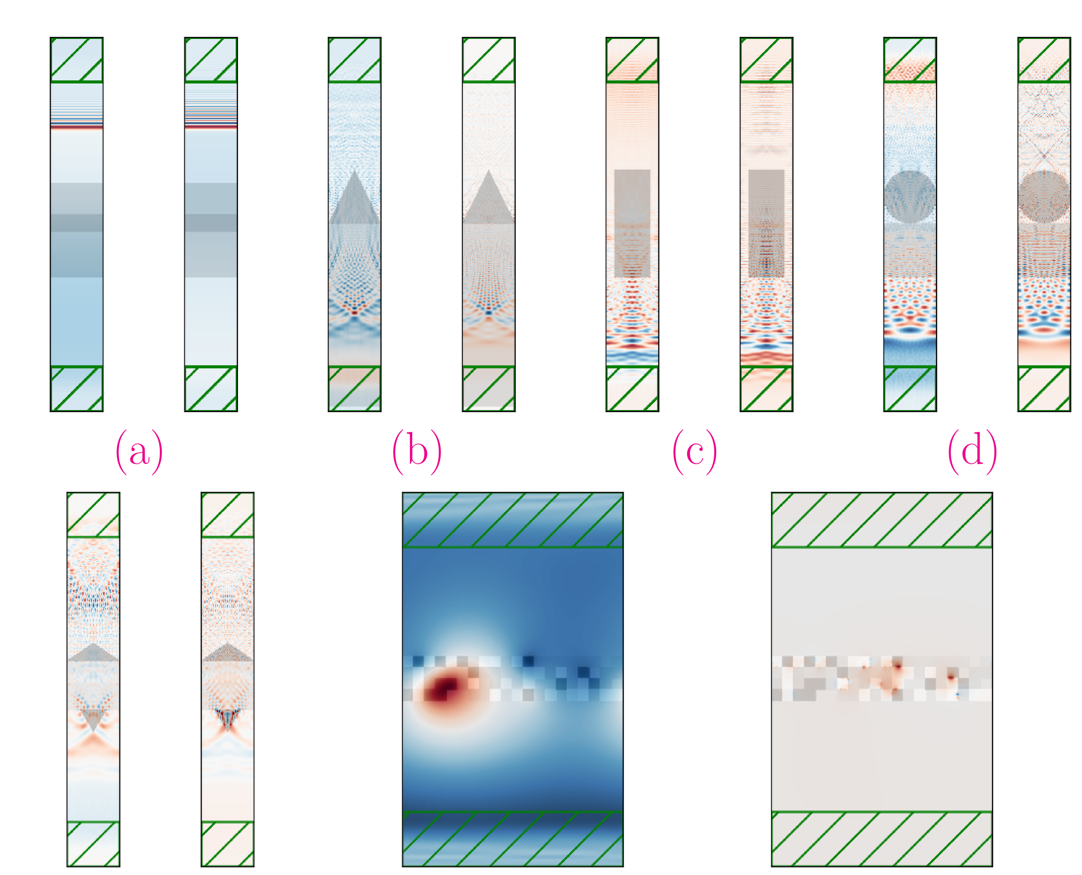


Figure: Examples of E-fields (left of each panel) and H-fields (right of each panel) out of plane for the structures studied.

Optimization Modes

Our benchmarks support two modes for fast prototyping of optimization methods as follows.

- **Discretized Search Space Mode**

A search space is discretized with the increment specified. At each configuration a simulation is run and the outcome of the simulation is recorded.

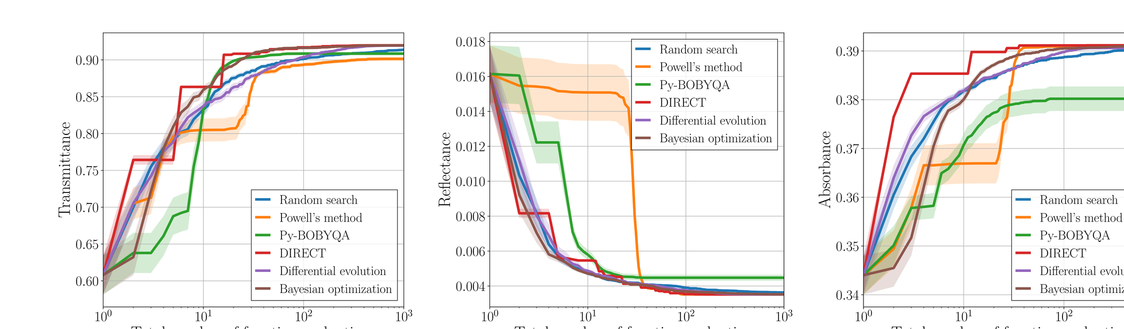
- **Surrogate Model Mode**

Based on the dataset collected from the discretized search space, we fit a surrogate model. This allows us to evaluate any structural configuration in the search space using the trained surrogate model.

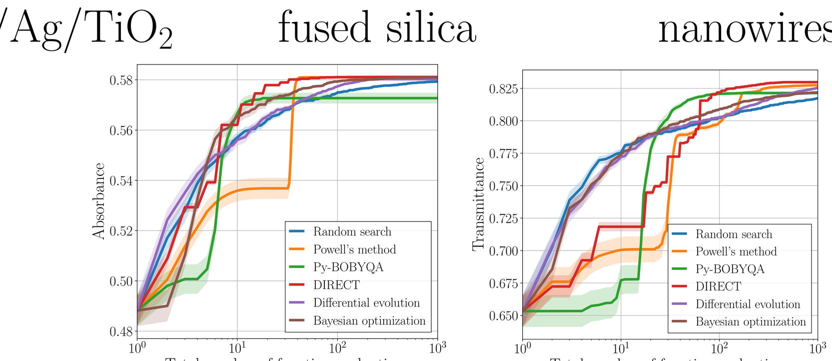
- **Simulation Mode**

Users can directly run these simulations using our frameworks and perform an optimization algorithm by conducting a simulation at every iteration.

Experiments with the Surrogate Model Mode



(a) TL film, $TiO_2/Ag/TiO_2$ (b) AR nanocones, fused silica (c) Vertical nanowires, cSi



(d) Nanospheres, cSi/TiO_2 (e) DS nanocones, $TiO_2/Ag/TiO_2/TiO_2/TiO_2$

Figure: Results on nanophotonic structure optimization.

Project Page **arXiv**