Surrogate Modeling: Enabling Practical Metalens Design and Simulation

White Paper Version 2.0

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Executive Summary

This white paper describes the **surrogate model** for meta-atom electromagnetic response. The surrogate model replaces on-the-fly RCWA computations with precomputed responses, enabling fast analysis and design support.

Core concepts:

- The surrogate model provides the Jones matrix $\mathbf{M}(\lambda, \theta_x, \theta_y, \boldsymbol{p})$ at inference time.
- **Incident parameter space:** Wavelength λ and local direction (θ_x, θ_y) (or spherical coordinates).
- **Structure parameter space:** Geometry parameters $\boldsymbol{p}$ (e.g., pillar diameter d, nanofin rotation θ_r) with fabrication-defined range and increment $\mathcal{P}_{\text{struct}}$.
- **Forward query:** Given $(\lambda, \theta_x, \theta_y, \boldsymbol{p}, \boldsymbol{J}^{\text{in}}) \rightarrow$ output field $\boldsymbol{J}^{\text{out}}$ and derived quantities include:
  - Amplitudes $|J_x^{\text{out}}|, |J_y^{\text{out}}|$
  - Phases $\arg(J_x^{\text{out}}), \arg(J_y^{\text{out}})$
  - Local common phase $\Psi = \arg(J_x^{\text{out}} + J_y^{\text{out}})$
  - Non-common phases $\arg(J_x^{\text{out}}) - \Psi$, $\arg(J_y^{\text{out}}) - \Psi$
  - Non-common phase variance $\sigma^2(\boldsymbol{J}^{\text{in}}, \boldsymbol{p})$
- **Optimal basis analysis:** Heatmap of $\sigma^2(\boldsymbol{J}^{\text{in}}, \boldsymbol{p})$ with Jones vector $\boldsymbol{J}^{\text{in}}$ over the Poincaré sphere (for one $\boldsymbol{p}$ or averaged over all $\boldsymbol{p}$ as $\Sigma^2(\boldsymbol{J}^{\text{in}})$).
- **Inverse query:** Given desired phase value Ψ^{target}, find $\boldsymbol{p} \in \mathcal{P}_{\text{struct}}$ that best matches.
- **1D/2D scans:** Vary one or two parameters out of $(\lambda, \theta_x, \theta_y, \boldsymbol{p})$ to analyze the output field and the derived quantities.
- **Meta-atom physics:** The queries enable the investigation of the optical characteristics of meta-atoms under multiple circumstances, and by that provide insights into, e.g., their dispersion behavior, aberrations, and polarization sensitivity.

For the theoretical foundation of phase extraction, optimal basis selection, and design strategies, see the Phase Response Paper [1].

The surrogate model is an independent object in VirtualLab Fusion. It is bound to twins which use meta-atoms in their structure definition, with the Metalens twin CS-MPCA01 as a prominent example.

1 Introduction

1.1 What Is a Surrogate Model?

A surrogate model is a computational construct that approximates a high-fidelity simulation. For meta-atom response, the high-fidelity simulation is RCWA (Rigorous Coupled-Wave Analysis), which solves Maxwell's equations for a periodic structure.

Direct RCWA evaluation at simulation time is computationally expensive. The surrogate model precomputes responses over a sampled parameter space and provides efficient inference.

1.2 Scope of This Paper

This paper focuses on the surrogate model as an independent entity. It defines:

- The parameter spaces $(\lambda, \theta_x, \theta_y, \boldsymbol{p})$
- The response matrix $\mathbf{M}$ and derived quantities
- Forward and inverse queries
- Analysis tools for understanding meta-atom physics
- Validation methods

For the theoretical foundation of phase extraction — including the definition of the local common phase Ψ, the quality criterion $\sigma^2(\boldsymbol{J}^{\text{in}}, \boldsymbol{p})$ and $\Sigma^2(\boldsymbol{J}^{\text{in}})$, optimal basis selection $(\boldsymbol{J}_1, \boldsymbol{J}_2)$, and design/simulation strategies — see the Phase Response Paper [1].

2 Local Electromagnetic Interaction

Consider a local meta-atom within a metasurface. Locally, the incident field interacts with this meta-atom and is transformed into an output field. In the local coordinate system of the metasurface (with $\hat{\boldsymbol{z}}$ normal to the surface), this transformation is described by a 2×2 Jones matrix acting on Jones vectors:

$$\boldsymbol{J}^{\text{out}} = \mathbf{M} \cdot \boldsymbol{J}^{\text{in}} \tag{1}$$

where:

- $\boldsymbol{J}^{\text{in}} = (J_x^{\text{in}}, J_y^{\text{in}})^T$ is the incident Jones vector (non-normalized, representing the local transverse electric field)
- $\boldsymbol{J}^{\text{out}} = (J_x^{\text{out}}, J_y^{\text{out}})^T$ is the output Jones vector
- $\mathbf{M} = \begin{pmatrix} M_{xx} & M_{xy} \\ M_{yx} & M_{yy} \end{pmatrix}$ with complex coefficients $M_{ij} = |M_{ij}|e^{\mathrm{i}\phi_{ij}}$

The Jones vector formalism is sufficient for the surrogate model, as it describes the local polarization state. The extension to full electromagnetic fields (including

wavefront phase and lateral variation) is discussed in the Phase Response Paper [1].

2.1 Determination of the Jones Matrix via PCA

The Jones matrix **M** is determined using the Periodic Cell Array (PCA) approximation [2]. The PCA approximation replaces the actual varying neighborhood of a meta-atom with an idealized periodic array of identical structures. Within this substituted periodic structure, Maxwell's equations are solved rigorously using RCWA. The response for a given geometry thus includes electromagnetic coupling with assumed-identical neighbors.

2.2 Dependence on Local Direction

The matrix **M** depends on the local direction of the incident field. Within the PCA framework, the incident field at each meta-atom is treated as a local plane wave. The local direction is encoded in the spatial frequency vector:

$$\boldsymbol{\kappa} = \nabla_\perp \psi^{\text{in}} = k_0 n\, \hat{\boldsymbol{s}} \tag{2}$$

where $\nabla_\perp = (\partial_x, \partial_y)$ is the lateral gradient operator, ψ^{in} is the wavefront phase of the incident field, $k_0 = 2\pi/\lambda$, and n is the refractive index of the incident medium. In the surrogate model the direction $\hat{\boldsymbol{s}}$ is directly selected. Its dependency from $\boldsymbol{\kappa} = \nabla_\perp \psi^{\text{in}}$ is used in the design and simulation of metasurfaces via the surrogate model for specified input fields and input wavefront phases ψ^{in} [1].

2.3 Parameterization of Local Direction

The local direction can be parameterized in two ways:

Cartesian angles (θ_x, θ_y)**:**

$$k_x = k_0 n \sin\theta_x, \qquad k_y = k_0 n \sin\theta_y \tag{3}$$

Spherical coordinates (θ, φ)**:**

$$k_x = k_0 n \sin\theta\cos\varphi, \qquad k_y = k_0 n \sin\theta\sin\varphi \tag{4}$$

Both representations are supported. The choice depends on the symmetry of the problem and the preference of the user. The surrogate model samples the direction space equidistantly in k_x and k_y.

2.4 Full Parameter Dependence

In addition to the incident direction and wavelength, the matrix depends on the meta-atom geometry $\boldsymbol{p}$, i.e., the components of the vector $\boldsymbol{p}$ define the parameters which define the shape and orientation of the meta-atom:

$$\mathbf{M} = \mathbf{M}(\lambda, \theta_x, \theta_y, \boldsymbol{p}) \tag{5}$$

This is the function that the surrogate model provides at inference time and can be applied to any given input polarization $\boldsymbol{J}^{\text{in}}$.

3 Parameter Spaces

3.1 Incident Parameter Space

The incident parameters define the illumination conditions:

Parameter	Symbol	Unit	Typical Range
Wavelength	λ	nm	450–700 (visible) or 1000–1600 (telecom)
Cartesian angle x	θ_x	deg	$-30°$ to $30°$
Cartesian angle y	θ_y	deg	$-30°$ to $30°$
Polar angle (spherical)	θ	deg	$0°$ to $30°$
Azimuthal angle (spherical)	φ	deg	$0°$ to $360°$

Table 1: Incident parameter space. The ranges shown are typical examples; the surrogate model can be trained over any user-defined ranges.

3.2 Structure Parameter Space

The structure parameters $\boldsymbol{p}$ define the meta-atom geometry. Critically, the parameter space reflects **fabrication constraints**: each parameter has a defined range and a minimum increment (the fabrication grid step). This is not merely a numerical sampling choice — it represents what can physically be manufactured.

The surrogate model can be trained for any meta-atom geometry with one or more parameters represented by the vector $\boldsymbol{p}$. Additional meta-atom types will be added on demand. Currently supported meta-atom geometries are:

3.2.1 Pillar Meta-Atoms

- **Single parameter:** Diameter d
- **Fixed parameters:** Height h, pitch p, material
- **Phase mechanism:** Varying diameter controls the effective index and thus the phase delay
- **Fabrication constraints:** $d_{\min} \leq d \leq d_{\max}$ with increment Δd

3.2.2 Nanofin Meta-Atoms

- **Single parameter:** Rotation angle θ_r
- **Fixed parameters:** Dimensions (length, width, height), pitch p, material

- **Phase mechanism:** Geometric phase (Pancharatnam–Berry phase)
- **Fabrication constraints:** $0° \leq \theta_r \leq 180°$ with increment $\Delta\theta_r$

Parameter	Symbol	Unit	Typical Range
Pillar diameter	d	nm	50–300, $\Delta d = 10$ nm
Nanofin rotation	θ_r	deg	0°–180°, $\Delta\theta_r = 1°$

Table 2: Structure parameter space with fabrication increments. The ranges and increments shown are typical examples; the surrogate model can be trained over any user-defined ranges and increments.

3.3 Pitch and Subwavelength Condition

The meta-atoms are arranged on a periodic grid with pitch p (unit cell size). The pitch is a fixed parameter for a given surrogate model training. The pitch must satisfy the subwavelength condition:

$$p < \frac{\lambda}{n} \tag{6}$$

where n is the refractive index of the medium into which the metasurface focuses. This condition ensures that higher diffraction orders become evanescent for orthogonal incident light.

3.4 Complete Parameter Space

$$(\lambda, \theta_x, \theta_y, \boldsymbol{p}) \in \mathcal{P}_{\text{inc}} \times \mathcal{P}_{\text{struct}} \tag{7}$$

where $\mathcal{P}_{\text{inc}}$ is continuous and $\mathcal{P}_{\text{struct}}$ is discrete. The pitch p and meta-atom type are fixed for a given surrogate model instance.

3.5 Interpolation Methods

The surrogate model uses different interpolation strategies for different parameter spaces:

- **Continuous parameters** $(\lambda, \theta_x, \theta_y)$**:** Linear interpolation between sampled points.
- **Discrete parameters** $\boldsymbol{p} \in \mathcal{P}_{\text{struct}}$**:** Nearest-neighbor interpolation to maintain the discrete nature of the fabrication grid.

4 Surrogate Model Response

4.1 Forward Query

A forward query asks: Given a complete input specification — incident parameters $(\lambda, \theta_x, \theta_y)$, structure parameter $\boldsymbol{p}$, and input Jones vector $\boldsymbol{J}^{\text{in}}$ — what is the output?

The trained surrogate model provides the Jones matrix $\mathbf{M}(\lambda, \theta_x, \theta_y, \boldsymbol{p})$ at inference time. The output Jones vector is:

$$\boldsymbol{J}^{\text{out}} = \mathbf{M}(\lambda, \theta_x, \theta_y, \boldsymbol{p}) \cdot \boldsymbol{J}^{\text{in}} \tag{8}$$

4.2 Derived Quantities

From the output Jones vector, the surrogate model computes the following derived quantities:

1. **Amplitude components:**[1]

$$|J_x^{\text{out}}|, \quad |J_y^{\text{out}}|$$

2. **Transverse squared sum (relative power):**[2] [3]

$$P^{\text{out}} = |J_x^{\text{out}}|^2 + |J_y^{\text{out}}|^2$$

3. **Phase components:**[1]

$$\phi_x = \arg(J_x^{\text{out}}), \quad \phi_y = \arg(J_y^{\text{out}})$$

4. **Local common phase:**[2]

$$\Psi = \arg\left(J_x^{\text{out}} + J_y^{\text{out}}\right)$$

   This is the phase common to both field components. It is the reference for design. For a detailed theoretical foundation, see the Phase Response Paper [1].

5. **Non-common phases:**[2]

$$\Delta\phi_x = \phi_x - \Psi, \qquad \Delta\phi_y = \phi_y - \Psi$$

   These indicate polarization-dependent phase effects that are not captured by the common phase.

6. **Non-common phase variance:**[2]

$$\sigma^2(\boldsymbol{J}^{\text{in}}, \boldsymbol{p}) = \frac{|J_x^{\text{out}}|^2(\Delta\phi_x)^2 + |J_y^{\text{out}}|^2(\Delta\phi_y)^2}{|J_x^{\text{out}}|^2 + |J_y^{\text{out}}|^2}$$

   This quantifies how well the output field approximates a common-phase behavior. A small σ^2 indicates that the common phase is a good representation

[1] Available in VirtualLab Fusion from version 2026.1.

[2] Available in VirtualLab Fusion from version 2026.2.

[3] This quantity is proportional to the local power carried by the plane wave. For a plane wave in a homogeneous medium, the time-averaged Poynting vector magnitude is $I = \frac{1}{2}\sqrt{\varepsilon/\mu}\, P^{\text{out}}$. The constant factors are the same for all meta-atoms, so P^{out} serves as a relative measure.

of the meta-atom's phase response.

4.3 Scan Modes

4.3.1 Customized Scans

The user can perform 1D or 2D scans over arbitrary combinations of the parameters $(\lambda, \theta_x, \theta_y, \boldsymbol{p})$. For each scan, the user selects which output quantities to display (amplitudes, square sum, phases, common phase, non-common phases, σ^2).

4.3.2 Design-Related Scans

For design purposes, the surrogate model offers a specialized mode: the generation of meta-atoms for the realization of a linear phase ramp from 0 to 2π with respect to the common phase Ψ for a selected input polarization $\boldsymbol{J}^{\text{in}}$.[2]

1. A set of equidistant target phase values $\Psi_k^{\text{target}} = k \cdot \frac{2\pi}{N}$ for $k = 0, \ldots, N-1$ is defined.
2. For each target phase, the inverse query finds the best matching $\boldsymbol{p}_k \in \mathcal{P}_{\text{struct}}$.
3. The resulting pairs $(\Psi_k^{\text{target}}, \boldsymbol{p}_k)$ form the design lookup table.

The x-axis corresponds to the design index $k = 0, \ldots, N-1$ (equidistant steps). The tick labels can be toggled between:

- The target phase values Ψ_k^{target}
- The associated geometry parameters $\boldsymbol{p}_k$

The y-axis displays the selected derived quantity (e.g., actual common phase $\Psi(\boldsymbol{p}_k)$,$\boldsymbol{p}_k$, amplitudes, squared sum, non-common phases, or σ^2).

4.4 Step Size and Quantization Analysis

For design evaluation, the following metrics are available:[2]

1. **Step-to-step changes:** For any quantity $Q(\boldsymbol{p})$ (e.g., Ψ, amplitudes, phases), the difference to the neighboring $\boldsymbol{p}$ is computed:

$$\Delta Q^{\text{step}}(\boldsymbol{p}_k) = |Q(\boldsymbol{p}_{k+1}) - Q(\boldsymbol{p}_k)|$$

   Statistical values (peak, variance) are provided.

2. **Quantization error:** The difference between target phase and achieved common phase:

$$\delta\Psi_k^{\text{quanta}} = \Psi(\boldsymbol{p}_k) - \Psi_k^{\text{target}}$$

   Statistical values (peak, variance) are provided. The peak error can be expressed in radians, wavelengths ($\lambda/2\pi$), or fractions of 2π.

3. **Average σ^2:** When σ^2 is selected, the average over the design set is calculated

as a figure of merit for the input polarization $\boldsymbol{J}^{\text{in}}$:

$$\overline{\sigma^2}(\boldsymbol{J}^{\text{in}}) = \frac{1}{N} \sum_k \sigma^2(\boldsymbol{J}^{\text{in}}, \boldsymbol{p}_k)$$

4.5 Optimal Basis Analysis

For a fixed meta-atom $(\lambda, \theta_x, \theta_y, \boldsymbol{p})$, the surrogate model can compute $\sigma^2(\boldsymbol{J}^{\text{in}}, \boldsymbol{p})$ over the Poincaré sphere.[2] The user can choose:

- **Single $\boldsymbol{p}$:** Heatmap of $\sigma^2(\psi, \chi)$ for one geometry parameter.
- **Averaged over all $\boldsymbol{p}$:** Heatmap of $\Sigma^2(\boldsymbol{J}^{\text{in}}) = \sum_{\boldsymbol{p} \in \mathcal{P}_{\text{struct}}} \sigma^2(\boldsymbol{J}^{\text{in}}, \boldsymbol{p})$ to identify polarizations that work well across the entire fabrication range.

The minimum of $\Sigma^2(\boldsymbol{J}^{\text{in}})$ identifies the optimal input polarization $\boldsymbol{J}_1$. The orthogonal polarization $\boldsymbol{J}_2$ is the antipodal point on the sphere.

For pillars, the optimal basis is linear polarization. For nanofins, the optimal basis is circular polarization. For a detailed discussion of optimal basis selection and its consequences for design, see the Phase Response Paper [1].

5 Inverse Queries (Design Support)

An inverse query asks:[2] Given incident parameters $(\lambda, \theta_x, \theta_y)$ and a desired local common phase value Ψ^{target}, which geometry parameter $\boldsymbol{p} \in \mathcal{P}_{\text{struct}}$ best matches?

$$\boldsymbol{p} = \underset{\boldsymbol{p} \in \mathcal{P}_{\text{struct}}}{\arg\min} \left| \Psi(\lambda, \theta_x, \theta_y, \boldsymbol{p}) - \Psi^{\text{target}} \right| \tag{9}$$

Because $\mathcal{P}_{\text{struct}}$ is discrete due to fabrication constraints, this is a nearest-neighbor search. This discrete selection introduces a **phase quantization error**:

$$\delta\Psi^{\text{quanta}} = \Psi(\lambda, \theta_x, \theta_y, \boldsymbol{p}) - \Psi^{\text{target}}. \tag{10}$$

This inverse query is the fundamental operation for metasurface design. When bound to a metasurface twin (e.g., Metalens [PCA] [3]), the twin calls this query for each position $\boldsymbol{\rho}$ using $\Psi^{\text{target}} = \Delta\psi^{\text{profile}}(\boldsymbol{\rho})$ to generate the full design, as described in the Phase Response Paper [1].

5.1 Additional Filters for Design

Beyond the basic range and increment, additional **filters** may be applied to exclude certain meta-atom parameters $\boldsymbol{p}$ from the design process, for example:[2]

- Minimum transmission amplitude (e.g., exclude pillars with $|t| < 0.8$)
- Enforcing stricter fabrication constraints by increasing the effective increment — excluding intermediate $\boldsymbol{p}$ values without retraining

- Excluding pillars with critical aspect ratio (height-to-diameter)
- Customized user-defined rules

When a filter excludes a geometry parameter (and thus the corresponding meta-atom), it is removed from the set of available choices during the inverse query. The design then selects the next-best available $\boldsymbol{p}$.

6 Validation Using Queries

The queries provided by the surrogate model can be used to validate its suitability for a given application. In particular:

- The **step size analysis** (difference between neighboring $\boldsymbol{p}$ values) reveals whether the fabrication grid is sufficiently fine for the desired phase accuracy.
- The **quantization error** $\delta\Psi^{\text{quanta}}$ quantifies the deviation between target and achievable common phase.
- The **non-common phase variance** σ^2 indicates how well the common phase represents the meta-atom's response for the chosen input polarization.

The user should verify that these metrics meet the requirements of the intended application before proceeding to full metasurface design.

7 Limitations

7.1 Trained Parameter Range

The surrogate model is valid only within the trained ranges of $(\lambda, \theta_x, \theta_y, \boldsymbol{p})$.

Queries outside these ranges:

- Return the closest available response (nearest neighbor in parameter space)
- Issue a warning to the user
- Prompt the user to extend training to cover the requested range

Extrapolation is not supported and results should not be trusted.

8 Conclusion

The surrogate model provides a fast, accurate approximation of meta-atom electromagnetic response:

1. **Parameter spaces** are defined for incident light $(\lambda, \theta_x, \theta_y)$ and structure $(\boldsymbol{p})$, with $\boldsymbol{p}$-space reflecting fabrication constraints (range and increment) as $\mathcal{P}_{\text{struct}}$.
2. **Interpolation:** Linear in continuous parameters, nearest-neighbor in discrete $\mathcal{P}_{\text{struct}}$.
3. **Response** provides $\mathbf{M}(\lambda, \theta_x, \theta_y, \boldsymbol{p})$ at inference; derived quantities include am-

plitudes, intensity, phases, local common phase Ψ, non-common phases, and variance $\sigma^2(\boldsymbol{J}^{\text{in}}, \boldsymbol{p})$.

4. **Forward queries** enable customized 1D and 2D scans for analysis of dispersion, angular response, and design curves.
5. **Design-related scans** generate lookup tables for linear phase ramps, with step size and quantization error analysis.
6. **Optimal basis analysis** provides heatmaps of σ^2 over the Poincaré sphere to identify optimal input polarizations (linear for pillars, circular for nanofins), using $\Sigma^2(\boldsymbol{J}^{\text{in}}) = \sum_{\boldsymbol{p}} \sigma^2(\boldsymbol{J}^{\text{in}}, \boldsymbol{p})$ for averaging over the fabrication range.
7. **Inverse queries** find $\boldsymbol{p} \in \mathcal{P}_{\text{struct}}$ that best matches a desired phase value Ψ^{target} — the foundation for metasurface design.
8. **Validation** using step size analysis, quantization error, and σ^2 ensures the surrogate model is suitable for the intended application.

For the theoretical foundation of phase extraction, optimal basis selection, and design strategies, see the Phase Response Paper [1].

Key Takeaway: The surrogate model provides fast forward and inverse queries for meta-atom response. Derived quantities include amplitudes, intensity, phases, local common phase Ψ, and the quality criterion $\sigma^2(\boldsymbol{J}^{\text{in}}, \boldsymbol{p})$. Design-related scans enable linear phase ramp generation with step size and quantization analysis. Optimal basis analysis identifies the best input polarizations for design. For the underlying phase extraction theory, see the Phase Response Paper [1].

A Complete Notation Reference

Symbol	Meaning
λ	Wavelength
θ_x, θ_y	Cartesian angles of incidence
θ, φ	Spherical coordinates of incidence
$\boldsymbol{p}$	Structure parameter(s) (e.g., d or θ_r)
$\mathcal{P}_{\text{inc}}$	Incident parameter space (continuous)
$\mathcal{P}_{\text{struct}}$	Structure parameter space (discrete, fabrication grid)
$\mathbf{M}(\lambda, \theta_x, \theta_y, \boldsymbol{p})$	Jones matrix response (2×2, complex)
$\boldsymbol{J}^{\text{in}}, \boldsymbol{J}^{\text{out}}$	Input/output Jones vectors $(J_x, J_y)^T$
Ψ	Local common phase: $\arg(J_x^{\text{out}} + J_y^{\text{out}})$
$\sigma^2(\boldsymbol{J}^{\text{in}}, \boldsymbol{p})$	Non-common phase variance (quality criterion)
$\Sigma^2(\boldsymbol{J}^{\text{in}})$	Summed variance over $\boldsymbol{p}$-space
$\overline{\sigma^2}(\boldsymbol{J}^{\text{in}})$	Average σ^2 over design set
$\boldsymbol{J}_1, \boldsymbol{J}_2$	Optimal input polarization basis
Ψ^{target}	Desired local common phase value (for inverse query)
$\Delta\Psi^{\text{step}}$	Step-to-step phase change (for validation)
$\delta\Psi^{\text{quanta}}$	Phase quantization error
$\nabla_\perp = (\partial_x, \partial_y)$	Lateral gradient operator

Table 3: Summary of notation. For theoretical foundations of phase extraction, see the Phase Response Paper [1].

B Document Version History

Version	Date	Changes
1.0	April 2026	Initial release
2.0	April 2026	Revised to reference Phase Response Paper; added $\Sigma^2(\boldsymbol{J}^{\text{in}})$; added design-related scans; added step size and quantization analysis; updated notation to use Jones vectors

References

[1] Frank Wyrowski. *Designing and Analyzing the Phase Response of Metasurfaces.* White Paper WP-META-PHASE. LightTrans International GmbH, 2026. link.

[2] Frank Wyrowski. *PCA: The Foundation for Metalens Design.* White Paper WP-META-PCA. LightTrans International GmbH, 2026. link.

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