Supplementary Information for

Global optimization of dielectric metasurfaces using a physics-driven neural network

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Network architecture and training process of the conditional GLOnet

The network architecture of the conditional GLOnet is shown in Figure S1. The input to the generator is a 1x256 vector of uniformly distributed variables, the operating wavelength, and the output deflection angle. All of these variables are normalized to numbers between -1 and 1. The output of the generator is a 1x256 vector. We add a Gaussian filter at the end of the generator, before the tanh layer, to eliminate extra-fine spatial features in the generated devices.

During the training process, the generator uses the Adam optimizer with a batch size of 1250, learning rate of 0.001, β_1 of 0.9, β_2 of 0.99, and σ of 0.6. We train the conditional GLOnet for 1000 iterations. β is 0 for the first 500 iterations and becomes 0.2 for the last 500 iterations. The network is implemented using pytorch-1.0.0. The forward simulations and adjoint simulations are performed using the Reticolo RCWA solver in MATLAB. The network trains on an Nvidia Titan V GPU and 8 CPUs, and the total training time is 4.5 hours.

Formulation of the loss function for the conditional GLOnet

The optimization objective of the conditional GLOnet follows that of the unconditional GLOnet, which is discussed in Ref. [32] of the main text, and it is to maximize the probability of generating the highest efficiency device for all possible (λ, θ):

$$\mathbf{w}^* := \arg\max_{\mathbf{w}} \iint d\lambda\, d\theta \int d\mathbf{n} \cdot \delta\left(\mathrm{Eff}\left(\mathbf{n};\lambda,\theta\right) - \mathrm{Eff}_{\max}\left(\lambda,\theta\right)\right) \cdot P_{\mathbf{w}}\left(\mathbf{n};\lambda,\theta\right) \tag{1}$$

By approximating the δ-function with an exponential function and using a Monte Carlo estimation, we simplify the objection function in the following way:

$$\begin{aligned}
\mathbf{w}^* &:= \arg\max_{\mathbf{w}} \iint d\lambda\, d\theta \int d\mathbf{n} \cdot \exp\left(\frac{\mathrm{Eff}\left(\mathbf{n};\lambda,\theta\right) - \mathrm{Eff}_{\max}\left(\lambda,\theta\right)}{\sigma}\right) \cdot P_{\mathbf{w}}\left(\mathbf{n};\lambda,\theta\right) \\
&= \arg\max_{\mathbf{w}} \iint d\lambda\, d\theta \exp\left(\frac{-\mathrm{Eff}_{\max}\left(\lambda,\theta\right)}{\sigma}\right) \mathop{\mathbb{E}}_{\mathbf{n}\sim P_{\mathbf{w}}\left(\lambda,\theta\right)} \exp\left(\frac{\mathrm{Eff}\left(\mathbf{n};\lambda,\theta\right)}{\sigma}\right) \\
&\approx \arg\max_{\mathbf{w}} \iint d\lambda\, d\theta \exp\left(\frac{-\mathrm{Eff}_{\max}\left(\lambda,\theta\right)}{\sigma}\right) \frac{1}{K} \sum_{k=1}^{K} \exp\left(\frac{\mathrm{Eff}\left(\mathbf{n}^{(k)};\lambda,\theta\right)}{\sigma}\right) \\
&\approx \arg\max_{\mathbf{w}} \frac{1}{M} \sum_{m=1}^{M} \exp\left(\frac{\mathrm{Eff}\left(\mathbf{n}^{(m)};\lambda^{(m)},\theta^{(m)}\right) - \mathrm{Eff}_{\max}\left(\lambda^{(m)},\theta^{(m)}\right)}{\sigma}\right)
\end{aligned} \tag{2}$$

In the last step, the integral is approximated as a summation, which represents our use of a minibatch during training. The loss function of the conditional GLOnet at this stage is defined as:

$$L_0(\mathbf{n}) = -\frac{1}{M} \sum_{m=1}^{M} \exp\left(\frac{\mathrm{Eff}\left(\mathbf{n}^{(m)};\lambda^{(m)},\theta^{(m)}\right) - \mathrm{Eff}_{\max}\left(\lambda^{(m)},\theta^{(m)}\right)}{\sigma}\right) \tag{3}$$

The gradient of the loss function with respect to neuron weights $\mathbf{w}$, used for network updating, can be expressed in the following form using the chain rule:

$$\frac{\partial L_0}{\partial \mathbf{w}} = \sum_{m=1}^{M} \frac{\partial L_0}{\partial \mathrm{Eff}\left(\mathbf{n}^{(m)};\lambda^{(m)},\theta^{(m)}\right)} \frac{\partial \mathrm{Eff}\left(\mathbf{n}^{(m)};\lambda^{(m)},\theta^{(m)}\right)}{\partial \mathbf{n}^{(m)}} \cdot \frac{\partial \mathbf{n}^{(m)}}{\partial \mathbf{w}} \tag{4}$$

As the relation between the deflection efficiency and the device pattern is implicit, the current form of the loss function, L_0, cannot be used for backpropagation in implementation. However, the efficiency gradient with respect to the indices $\mathbf{g} = \frac{\partial \mathrm{Eff}}{\partial \mathbf{n}}$ can be calculated using adjoint variable method. We can therefore first calculate $\mathrm{Eff}^{(m)}$ and $\mathbf{g}^{(m)}$ using an EM solver and then treat $\mathrm{Eff}^{(m)}$, $\mathbf{g}^{(m)}$, and $\mathbf{n}^{(m)}$ as independent variables to define an equivalent loss function $L(\mathbf{n}, \mathbf{g}, \mathrm{Eff})$ that satisfies:

$$\frac{\partial L}{\partial \mathbf{w}} = \sum_{m=1}^{M} \frac{\partial L_0}{\partial \mathrm{Eff}^{(m)}} \mathbf{g}^{(m)} \cdot \frac{\partial \mathbf{n}^{(m)}}{\partial \mathbf{w}} = \frac{\partial L_0}{\partial \mathbf{w}} \tag{5}$$

Finally, we get the expression of $L(\mathbf{n}, \mathbf{g}, \mathrm{Eff})$ by integrating this gradient of the loss function:

$$\begin{aligned} L(\mathbf{n},\mathbf{g},\mathrm{Eff}) &= \int \frac{\partial L}{\partial \mathbf{w}} \cdot d\mathbf{w} \\ &= \int \sum_{m=1}^{M} \frac{\partial L_0}{\partial \mathrm{Eff}^{(m)}} \mathbf{g}^{(m)} \cdot \frac{\partial \mathbf{n}^{(m)}}{\partial \mathbf{w}} d\mathbf{w} \\ &= \sum_{m=1}^{M} \frac{\partial L_0}{\partial \mathrm{Eff}^{(m)}} \mathbf{g}^{(m)} \cdot \mathbf{n}^{(m)} \\ &= -\frac{1}{\sigma M} \sum_{m=1}^{M} \exp\left(\frac{\mathrm{Eff}^{(m)} - \mathrm{Eff}_{\max}\left(\lambda^{(m)},\theta^{(m)}\right)}{\sigma} \right) \mathbf{n}^{(m)} \cdot \mathbf{g}^{(m)} \end{aligned} \tag{6}$$

Computational cost of the conditional GLOnet versus adjoint-based topology optimization

The total number of simulations used to train the conditional GLOnet is 2,500,000: the network trains over 1,000 iterations, uses batch sizes of M = 1,250 device instances per iteration, and uses a forward and adjoint simulation per device to compute its efficiency gradient. When divided by the 135 unique wavelength and angle combinations displayed in Figures 3A and 3B, the number of simulations per wavelength and angle pair is 18,500, which amounts to 46 adjoint-based topology optimization runs (one run has 200 iterations and 2 simulations/iteration). As a point of comparison, 500 adjoint-based topology optimization runs were used to produce each point in Figure 3A.

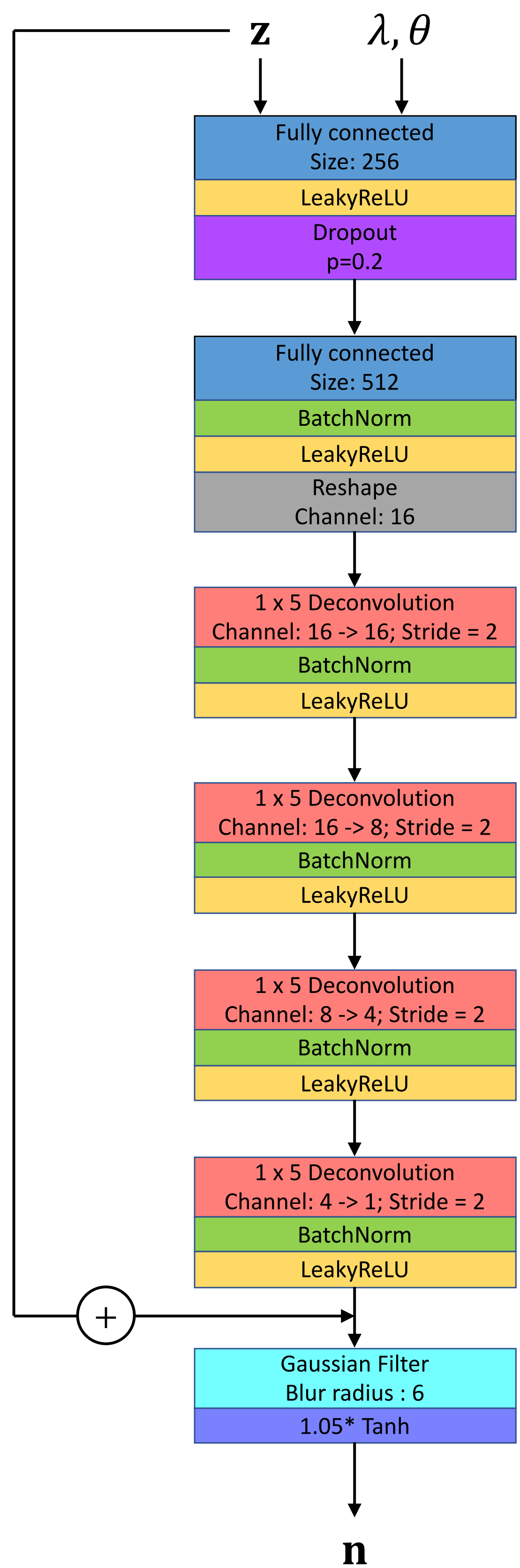


Figure S1. Network structures and parameters of GLOnet.

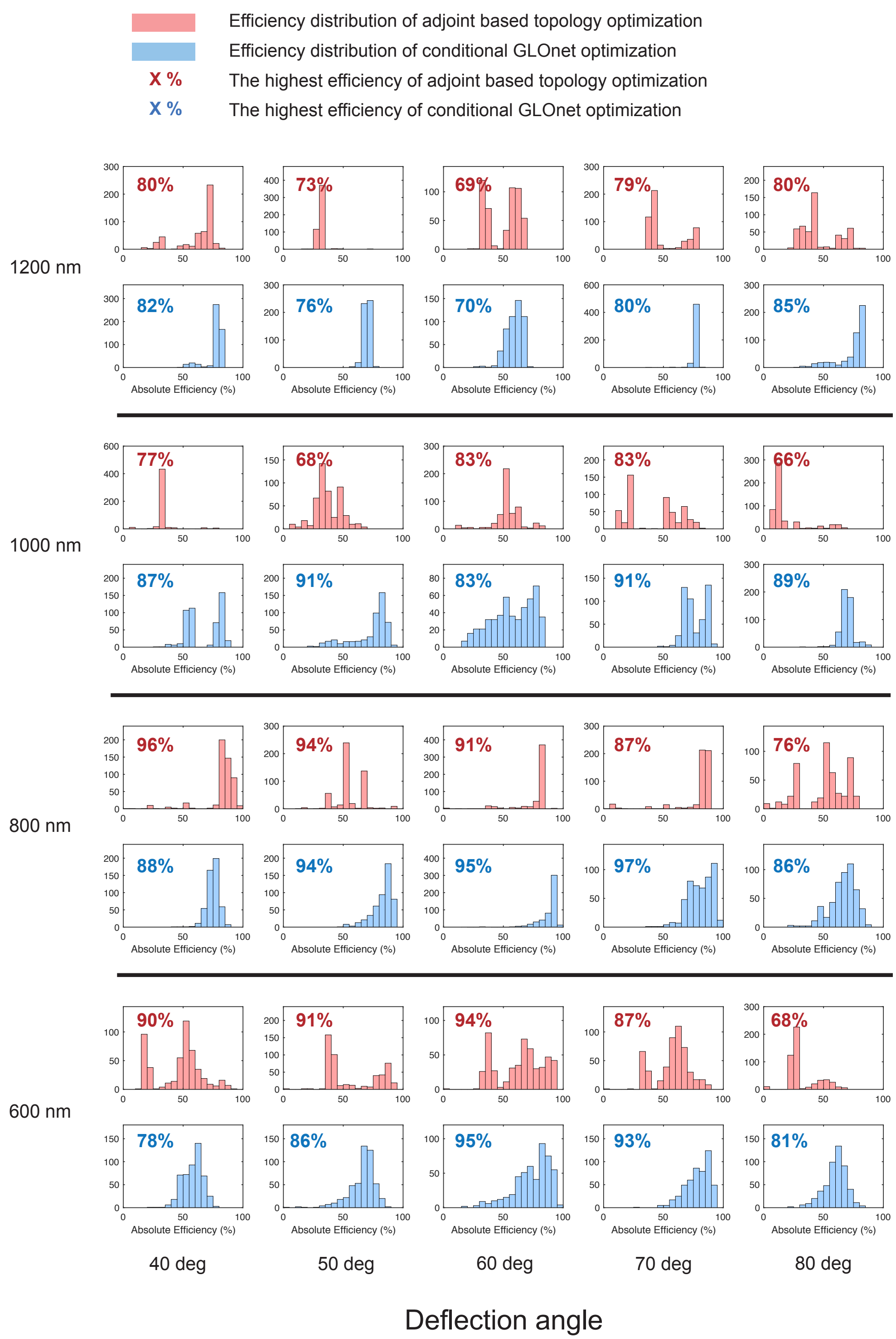


Figure S2. Representative efficiency distributions of devices designed using adjoint-based topology optimization (red histograms, 500 devices/histogram) and GLOnet (blue histograms, 500 devices/histogram). The highest efficiencies of adjoint-based topology optimization in each distribution are denoted by the red numbers, and the highest efficiencies of GLOnet-generated devices in each distribution are denoted by the blue numbers.

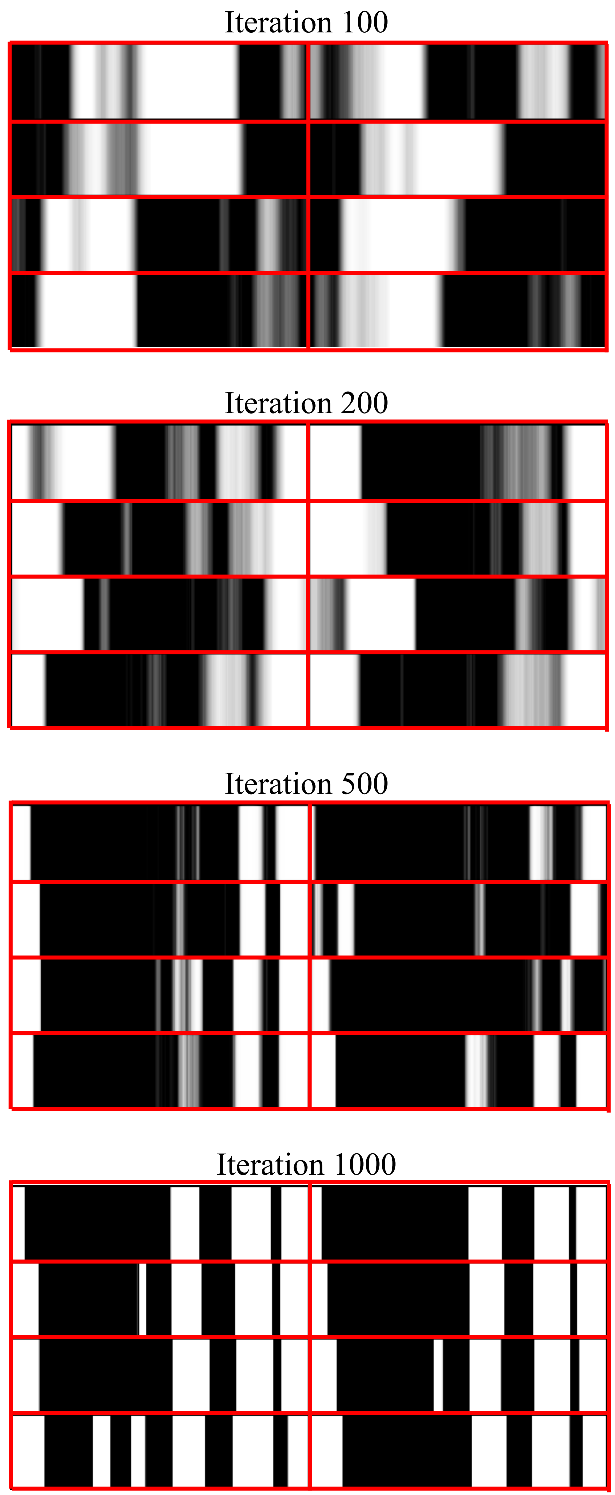
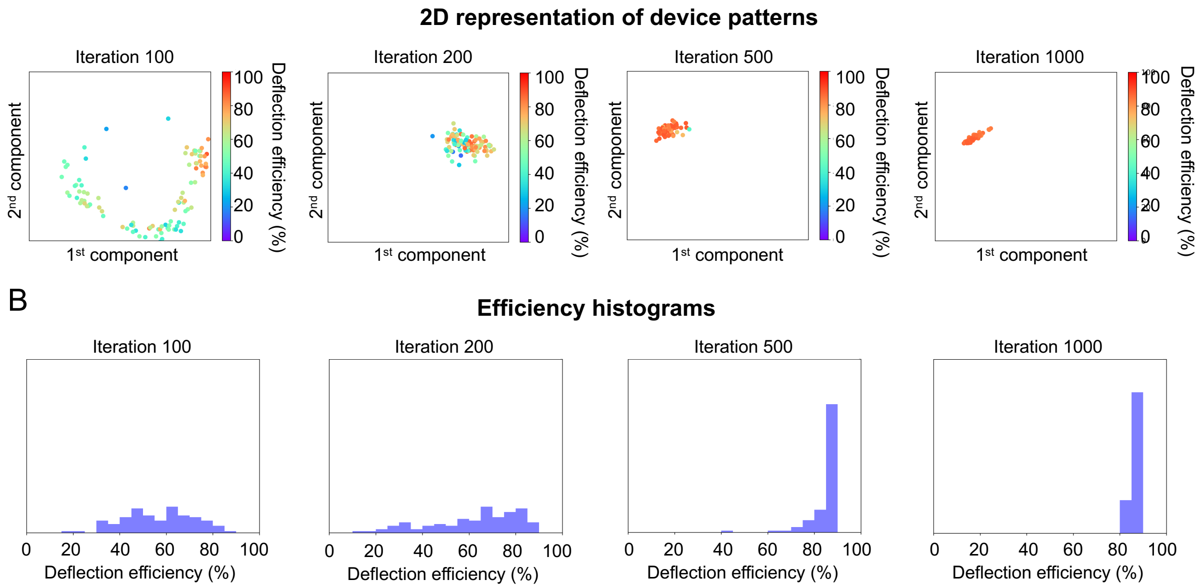
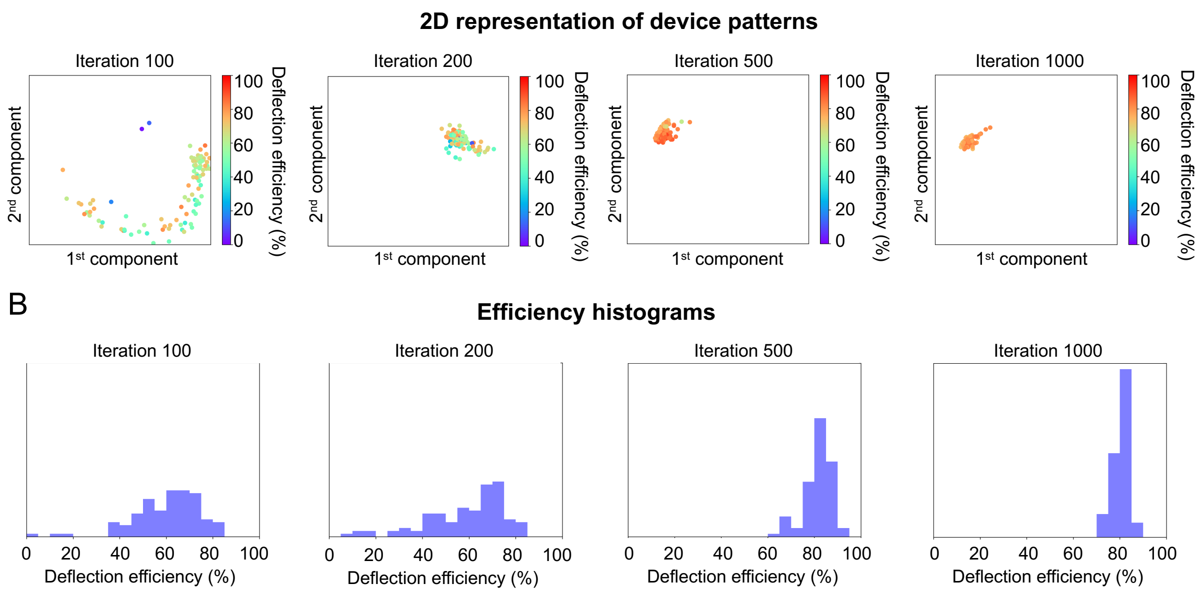


Figure S3. Evolution of device patterns as a function of iteration number. Eight patterns per iteration are randomly selected from those generated in Figure 4. The devices operate with a wavelength of 900 nm and an outgoing angle of 60 degrees.

Wavelength = 1100 nm, Deflection angle = 70 deg



Wavelength = 1100 nm, Deflection angle = 50 deg



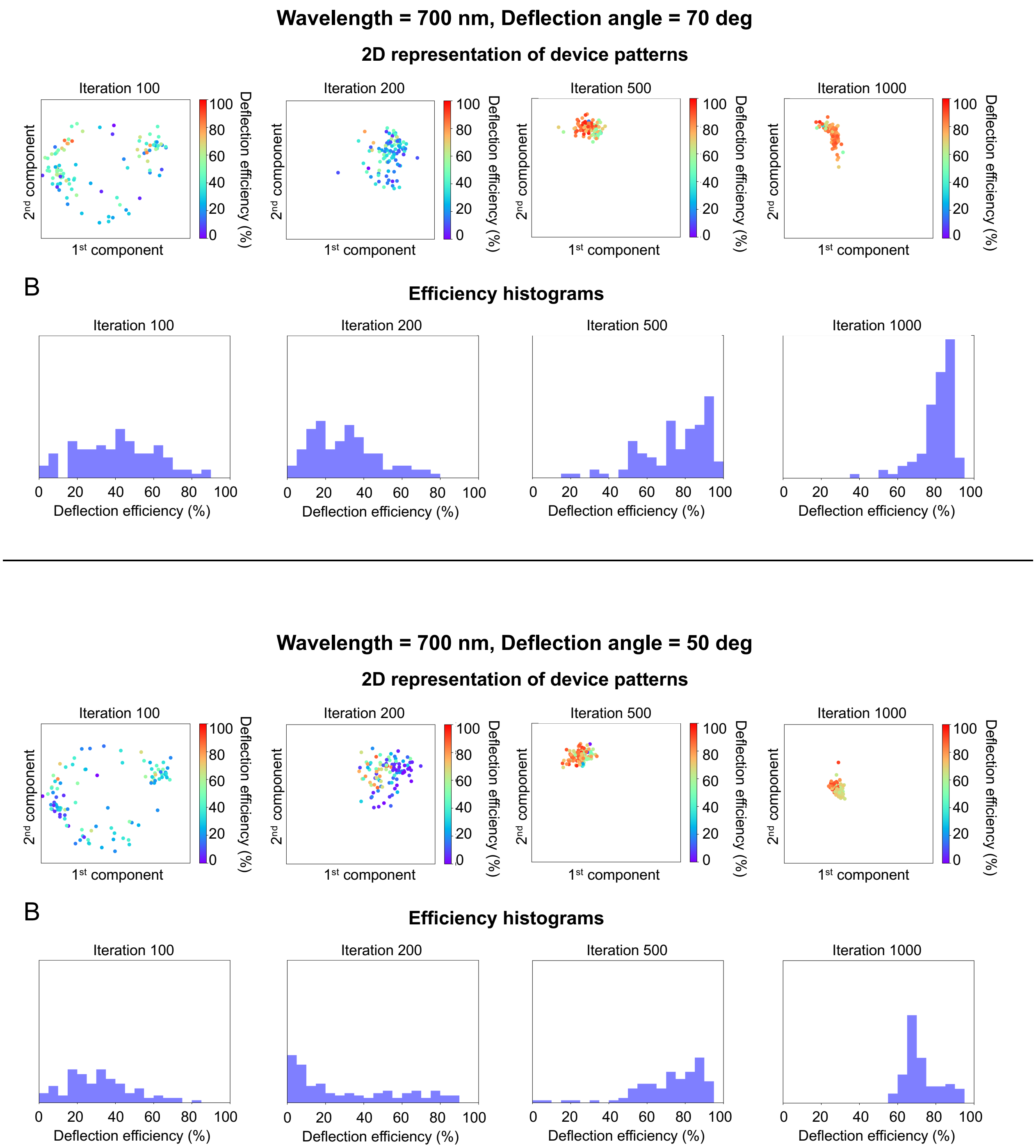


Figure S4. Evolution of device patterns and efficiency histograms as a function of GLOnet training, for four different wavelength and angle combinations. The analysis is consistent with that presented in Figure 4 of the main text.

Movie S1. Evolution of device patterns and efficiency histograms as a function of GLOnet training, for wavelength 900 nm and deflection angle 60 degrees.