Supplementary Materials for：

Optimization of metamaterials and metamaterial-microcavity based on deep neural networks

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Figure S1 compares the training and validation loss for different spectral responses after 1,000 epochs. The final training and validation loss are approximately 10^{-3}, indicating that there is no obvious overfitting in each case; hence, regularization is not needed in forward prediction.

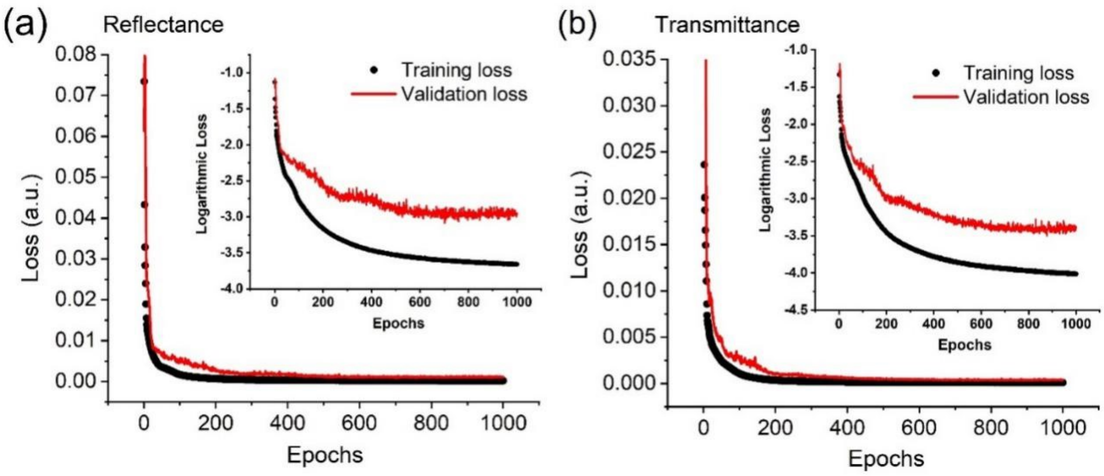

Fig. S1. Training and validation losses for the reflectance (a) and transmittance (b) of the split-ring in forward NN training. Insets are the logarithmic scales of the losses.

The networks of different inverse design methods are shown in Fig. S2. For the architecture of optimization of input data, we applied the forward prediction NN (Fig. 1 in the manuscript) but fixed all the pretrained weights from forward prediction NN and only set the input data as trainable. For the architecture of inverse training network, the input layer has 86 elements based on the spectral response of the split-ring, and the output layer has seven elements representing the predicted parameters of the split-ring. For the architecture of training the tandem NNs, composed of an inverse design NN and a forward prediction NN, and all the pretrained weights from the forward prediction NN are fixed in the new network. The spectral response is both the input and output data for training the tandem NNs. All different fully connected neural layers use the mean squared error 'mse' as the loss function, 'adam' as the optimizer, mean absolute error 'mae' as the metric, and 'sigmoid' as the activation, respectively.

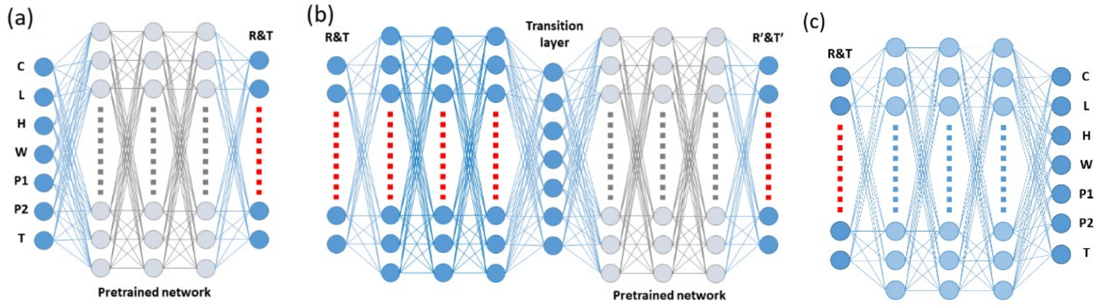

Fig. S2. (a) NN for optimization of input data (R&T are the reflectance and transmittance of the split-ring). (b) Architecture of the tandem NNs, comprising a trainable network (left, blue network) and pretrained network (right, gray network). (c) Architecture for training NN inversely.

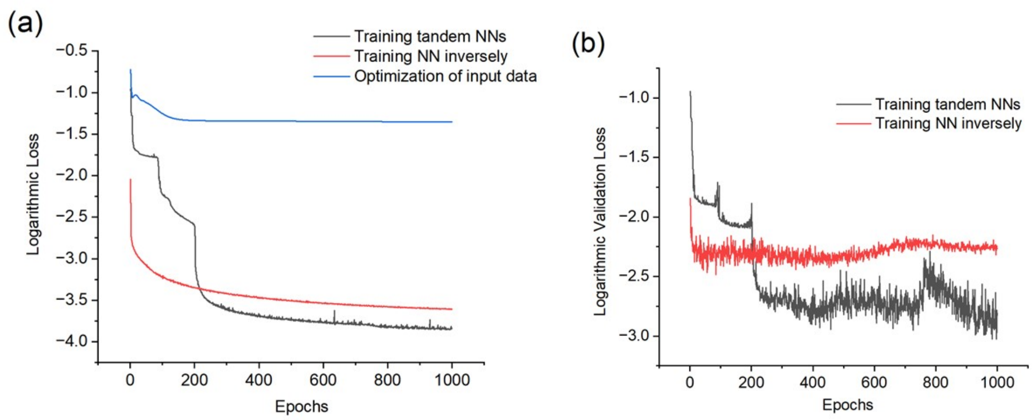

Fig. S3 Training loss and validation loss for three inverse design methods in the manuscript. There is no validation loss for optimization of input data.

From Fig. S3 we can see that there is significant training loss for optimization of input data. In this architecture, only seven parameters are trainable, which makes it difficult to find solution to converge. Inverse design of metamaterial is a typical one-to-many problem. This nonunique feature creates conflicting training instances, when such conflicting instances with the same input but different output labels exist in the training data set, the neural network would also be hard to converge, such as training NN inversely. However, the architecture of training tandem NNs has such unique feature because input data and output data are same. Both training loss and validation loss of training NN inversely are all higher than those of training tandem NNs (see Fig. S3). At the same time, training tandem NNs really performs best in practical application (see Fig. 3 in the manuscript). Therefore, we chose training tandem NNs for the inverse design of split-ring metamaterial in our experimental section.

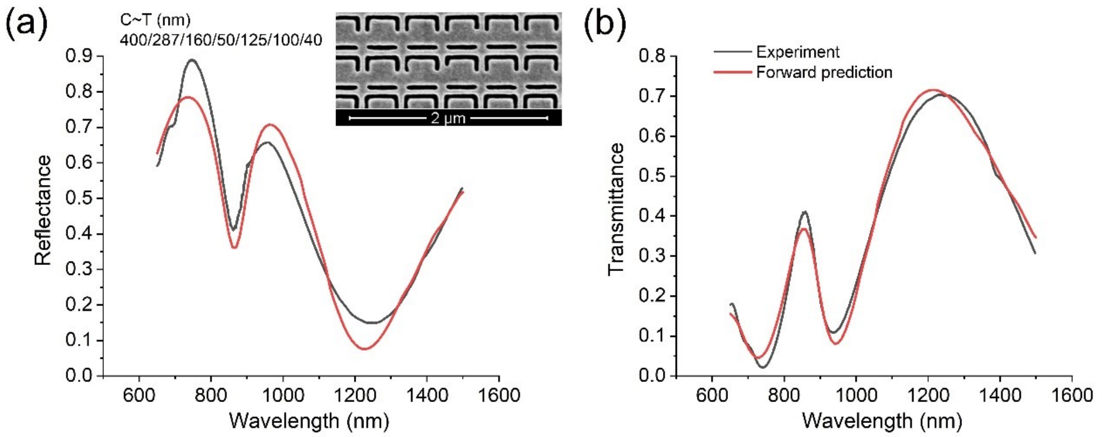

Fig. S4. Comparison of the experimental and forward predicted values by the pretrained NNs. (a) Experimental reflectance and forward predicted reflectance of the metamaterial with a cell-size of 400 nm (The measured parameters of the split-ring metamaterial are shown in the figure). (b) Experimental transmittance and forward predicted transmittance of the metamaterial. Inset is the SEM image of the metamaterial sample.

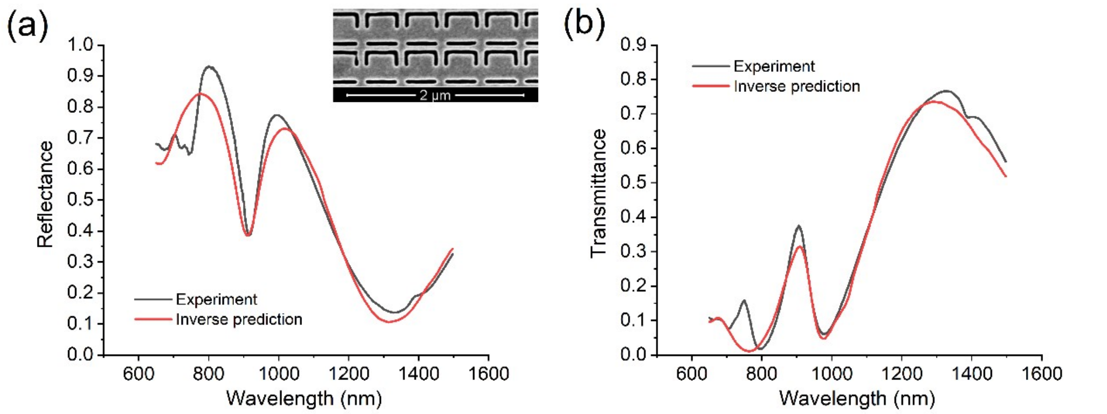

Fig. S5. Inverse prediction of the experimental spectral data by the pretrained tandem NNs. Experimental reflectance (a) and transmittance (b) of the metamaterial sample compared with corresponding inverse predicted reflectance and transmittance. Inset is the SEM image of the metamaterial sample.

The method to design single-layer split-ring metamaterial with the minimum reflectance at the wavelength of 1310 nm.

We use the combination of several Gaussian functions (as described in Equation (1)) to generate a reflectance curve which has the minimum reflectance at the wavelength of 1310nm. Reflectance curve generated from Gaussian equations is given by:

$$R = D - \left(a_1 e^{-\frac{(x-b_1)^2}{2c_1^2}} + a_2 e^{-\frac{(x-b_2)^2}{2c_2^2}} + a_3 e^{-\frac{(x-b_3)^2}{2c_3^2}}\right) \qquad (1)$$

where *x* represents wavelength and *R* is reflectance; *D* is a constant to reverse the whole curve; *a*, *b* and *c* in each Gaussian function are any real numbers. We can set different coefficient values ($D, a_i, b_i, c_i; i = 1,2,3$) to obtain different reflectance curves. Here, $b_1 = 1310\ nm$ is fixed to maintain all the generated reflectance curves have the minimum reflectance at the wavelength of 1310 nm. All the generated reflectance data will be used as the input data of the pretrained tandem NNs, and the corresponding output data can be obtained. We calculate the 'root mean square' value of each group of input and output data, and then find the minimum value of all data, which indicates the optimal input and output data we want. The expected inverse design parameters of split-ring metamaterial can be extracted from the transition layer of the tandem NNs with optimal input and output data. It is particularly pointed out that the minimum root mean square value represents that the input data are closer to the real reflectance of the metamaterial, so that the pretrained tandem NNs can easily find the convergence solution. All above calculations can be done easily and quickly by MATLAB (all pretrained weights of tandem NNs are included in this step). Figure S6 (a) shows two arbitrary reflectance curves with exact parameters. Figure S6 (b) shows input data and output data of pretrained tandem NNs with the minimum 'rms', then the inverse design parameters of the split-ring metamaterial (as shown in Fig. 7(b) in the manuscript) are obtained from this input data accordingly. The optimal parameters of Gaussian functions are given inset.

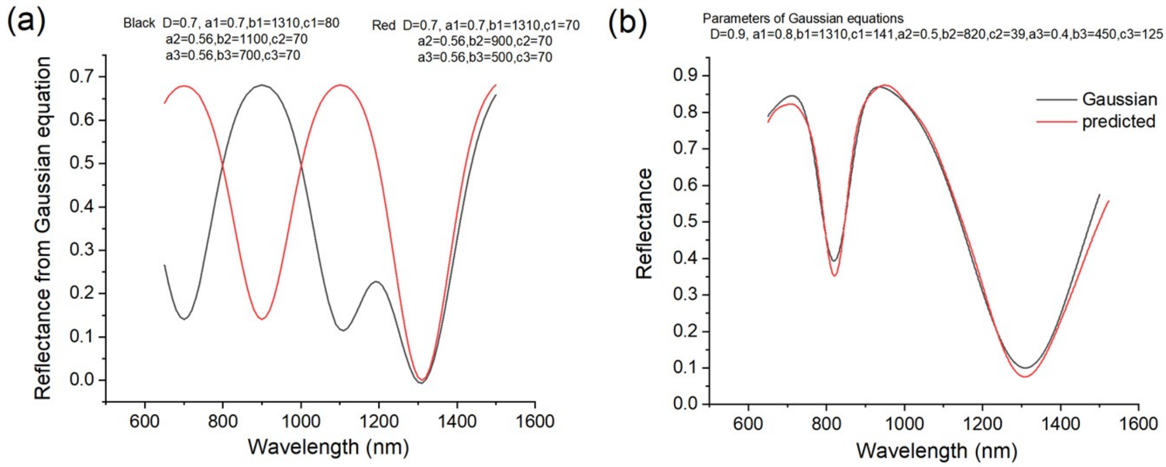

Fig. S6. Reflectance curves from Gaussian equations. (a) Two arbitrary curves from Equation (1) with exact parameters. (b) Optimal reflectance curve for input data of pretrained tandem NNs and its output data. The parameters of Gaussian equations are given inset.

Table S1. Parameters of split-ring used in forward prediction.

Units/(nm)	*C*	*L*	*H*	*W*	*P1*	*P2*	*T*
Purple	333	272	151	52	130	132	55
Green	349	237	167	60	128	135	52
Red	403	235	161	52	151	104	53

Table S2. Parameters of split-ring for true structure and inverse predicted parameters of three inverse design methods in Fig. 3.

Units/(nm)	*C*	*L*	*H*	*W*	*P1*	*P2*	*T*
original	333	272	151	52	130	132	55
Training tandem NNs	337	269	150	54	133	130	53
Optimization of input data	359	277	170	57	146	125	54
Training NN inversely	338	276	156	56	133	133	59