

Electronic Supplementary Materials

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Rapid, material-aware inverse design of one-dimensional photonic crystals using a mixture-of-physics-expert framework

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Section S1: Introduction of the differentiable transfer matrix method

In order to train the PINN model, a forward physics model is required. The forward physics model is a part of loss function when training the PINN model. In this work, TMM is used as the forward physics model. The TMM adopts a series of complex number calculations derived from the Maxwell equations, as provided in the supporting information section, to compute the reflectance and transmittance at the specified wavelength and incidence angle of a 1D-PhC with specific refractive indices and thicknesses. Instead of using TMM to generate plenty of spectra as the input training data, it serves as a physical constraint term within the loss function to guide the gradient backpropagation. Two-dimensional real-valued matrices are used to represent the complex numbers in the TMM equations and reformulate TMM's complex-number operations into real-valued matrix representations. This representation enables direct automatic differentiation on the TMM and gradient backpropagation using the computation graph of PyTorch (Paszke et al., 2019). The details of the real-value TMM used in this study can be found in the supporting information section.

The transfer matrix method (TMM) is widely used in many studies (Zhan et al., 2022; Luce et al., 2022) involving the multilayer one-dimensional photonic crystals (1D PhC). To put it succinctly, in mathematical method, each layer of the 1D PhC can be represented by a 2×2 complex-valued matrix. When the incident angle is 0, the characteristic matrix of the j th layer ($\mathbf{M}_{j,\lambda}$) is given by

$$\mathbf{M}_{j,\lambda} = \begin{bmatrix} \cos k_{0,\lambda} n_{j,\lambda} d_j & \frac{(i \sin k_{0,\lambda} n_{j,\lambda} d_j)}{Y_j} \\ Y_j i \sin k_{0,\lambda} n_{j,\lambda} d_j & \cos k_{0,\lambda} n_{j,\lambda} d_j \end{bmatrix} \quad (\text{S1})$$

where k_0 is the magnitude of the vacuum wavevector, whose value is $2\pi/\lambda$, λ represents the wavelength of the light. The $n_{j,\lambda}$ and d_j denote the refractive index and thickness of the j th layer, respectively. And the Y_j denotes the optical admittance of each layer. It can be calculated by

$$Y_{j,\lambda} = \sqrt{\frac{\epsilon_0}{\mu_0}} n_{j,\lambda} \quad (\text{S2})$$

where ϵ_0 and μ_0 are vacuum permittivity and vacuum permeability, respectively.

The characteristic matrix of the entire multilayer 1D PhC system is

$$\mathbf{M}_\lambda = \mathbf{M}_{1,\lambda} \mathbf{M}_{2,\lambda} \cdots \mathbf{M}_{p,\lambda} = \begin{bmatrix} m_{11,\lambda} & m_{12,\lambda} \\ m_{21,\lambda} & m_{22,\lambda} \end{bmatrix} \quad (\text{S3})$$

where p is the total number of layers in the multilayer 1D PhC.

The reflectance value of the 1D PhC at the wavelength λ can be calculated by

$$r_\lambda = \frac{Y_0 m_{11,\lambda} + Y_0 Y_s m_{12,\lambda} - m_{21,\lambda} - Y_s m_{22,\lambda}}{Y_0 m_{11,\lambda} + Y_0 Y_s m_{12,\lambda} + m_{21,\lambda} + Y_s m_{22,\lambda}} \quad (\text{S4})$$

where Y_0 and Y_s are the admittance of the incident medium and the substrate of the 1D PhC, respectively. In this study, the incident medium is air, and the substrate is glass. The admittances can be calculated by the equation S. Eq. 2, where the refractive indices $n_{j,\lambda}$ are substituted by the refractive indices of air (n_0) and glass (n_s) accordingly. In this work, we used matrices to represent the complex value in the above equations. For instance, the complex values $z_1 = a_1 + b_1 i$ and $z_2 = a_2 + b_2 i$ can be represented as matrices $\mathbf{z}_1 = \begin{bmatrix} a_1 & b_1 \end{bmatrix}$ and $\mathbf{z}_2 = \begin{bmatrix} a_2 & b_2 \end{bmatrix}$. The multiplication of complex values z_1 and z_2 is thereby represented as

$$\mathbf{z}_1 \mathbf{z}_2 = \mathbf{z}_1 \otimes \mathbf{z}_2 = \begin{bmatrix} a_1 a_2 - b_1 b_2 \\ a_1 b_2 + b_1 a_2 \end{bmatrix} = \begin{bmatrix} a_1 & -b_1 \\ b_1 & a_1 \end{bmatrix} \begin{bmatrix} a_2 \\ b_2 \end{bmatrix} \quad (\text{S5})$$

Then, the whole TMM can be purely represented as a real-value matrix calculation, and can be readily differentiated by deep learning frameworks such as PyTorch.

Section S2: Regulation loss function

In order to prevent the trained neural network from predicting too thick or physical-impossible thicknesses such as negative thickness, the neural network model should be punished when it outputs such thicknesses during the training. One of the punishment method is introducing a term to add more loss in the loss function or reduce the

reward in the reward function(Wankerl et al., 2021). In this work, a regulation loss function is applied to restrain the layer thickness in a reasonable range, the range of layer thickness is 20-300 nm. The regulation loss function is defined by

$$L_{reg,i} = 0.5 * (\text{ReLU}(20 \text{ nm} - d_i) + \text{ReLU}(d_i - 300 \text{ nm})) \quad (\text{S6})$$

where i represents the i th layer of the 1D PhC, d_i denotes the thickness of i th layer.

The ReLU function is defined as:

$$\text{ReLU}(x) = \begin{cases} 0 & \text{if } x < 0 \\ x & \text{if } x \geq 0 \end{cases} \quad (\text{S7})$$

Section S3: Utilized neural network structure and training hyperparameters

Either PINN or traditional data-driven CNN is based on the same CNN structure. This CNN structure is described in the table below.

Table S1 CNN/PINN structure and other parameters.

Type of layer ^a	Input shape ^b	Output shape ^b	Activation function ^c	Parameters ^d
Conv1d	(1, 161)	(64, 161)	ReLU	kernel_size=4, padding=1
MaxPool1d	(64, 161)	(64, 80)	-	kernel_size=2
Conv1d	(64, 80)	(64, 80)	ReLU	kernel_size=4, padding=2
MaxPool1d	(64, 80)	(64, 40)	-	kernel_size=2
Conv1d	(64, 40)	(64, 40)	ReLU	kernel_size=4, padding=2
MaxPool1d	(64, 40)	(64, 20)	-	kernel_size=2
Flatten	(64, 20)	1280	-	-
Linear	1280	128	ReLU	Dropout=0.1
Linear	128	128	ReLU	Dropout=0.1
Linear	128	128	ReLU	Dropout=0.1
Linear	128	128	ReLU	Dropout=0.1
Linear	128	128	ReLU	Dropout=0.1
Output	128	11	-	-

^a**Layer types:** Conv1d (1D convolution for local feature extraction), MaxPool1d (spatial downsampling), Flatten (tensor vectorization), Linear (fully-connected dense layers).

^b**Shapes:** Input/output tensor dimensions denoted as (channels, sequence length).

^c**Activation:** Non-linear activation functions (ReLU: Rectified Linear Unit).

^d**Parameters:** Layer-specific hyperparameters including kernel sizes, padding, and dropout rates for regularization.

The initial learning rate is set to 5×10^{-4} , and the learning rate decays by a factor of 0.1 every 500 training epochs. The hyperparameters of both data-driven CNN and PINN are the same in order to ensure the fairness of the comparison.

Section S4: Material parameters and configurations in case 2

In case 2, the refractive index of SiO₂ is fixed to 1.46, and the spectra of refractive indices of Al₂O₃, TiO₂(Andryieuski et al., 2015), Ta₂O₅ (Gao et al., 2012) are from the literature and the refractiveindex.info database(Polyanskiy, 2024). The 8 material configurations are shown in the Fig. S1(a) below.

(a)

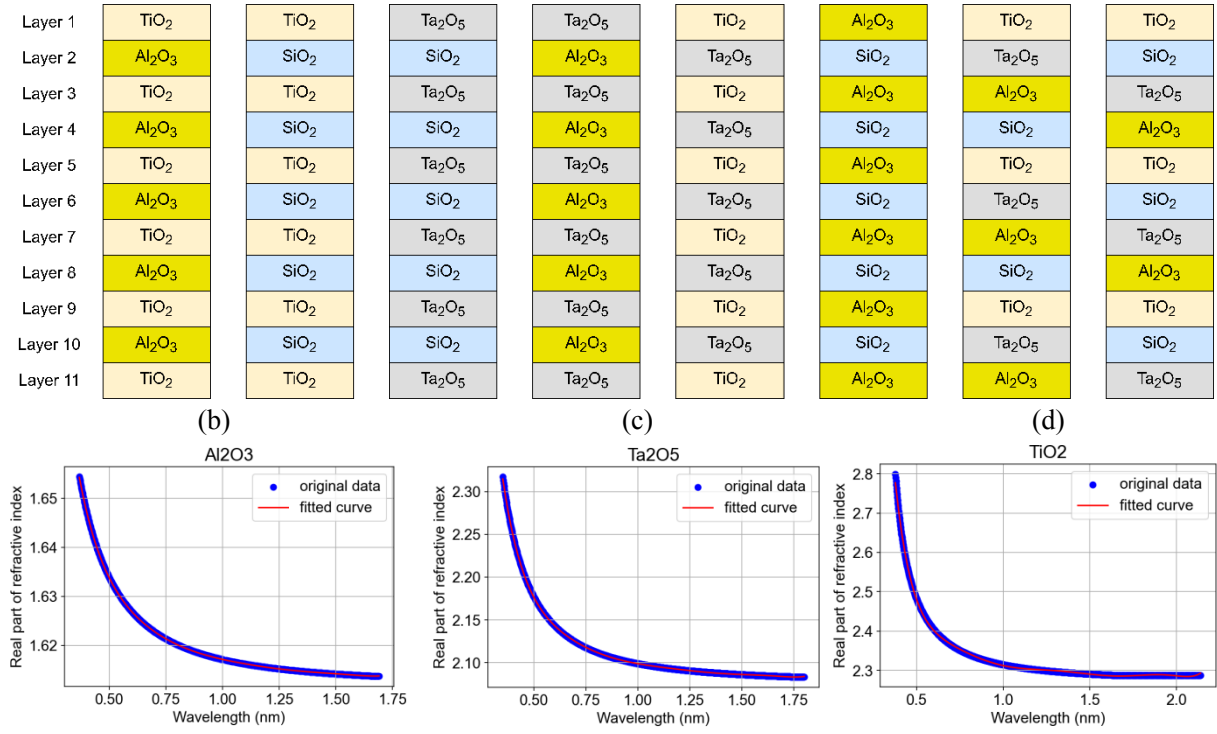


Fig. S1 (a) The 8 material configurations in case 2. (b-d) The wavelength-dependent refractive indices of Al₂O₃, Ta₂O₅ and TiO₂ in case 2.

A real-world dataset was constructed, including 12,800 randomly generated 11-layer TiO₂-SiO₂ periodic 1D-PhCs' structures and their corresponding reflectance spectra calculated by TMM. The dataset generation process follows these steps: (1) For each structure, the thickness of each layer is randomly sampled from a uniform distribution ranging from 0.02 to 0.3 μm ; (2) The material sequence is fixed as alternating TiO₂ and SiO₂ layers; (3) As shown in Fig. S2, the reflectance spectrum for each structure is computed using the TMM algorithm across the wavelength range of 400-700 nm with 161 sampling points; (4) The dataset is split into training data (80%, 10,240 pairs), validation data (12%, 1,536 pairs), and test data (8%, 1,024 pairs).

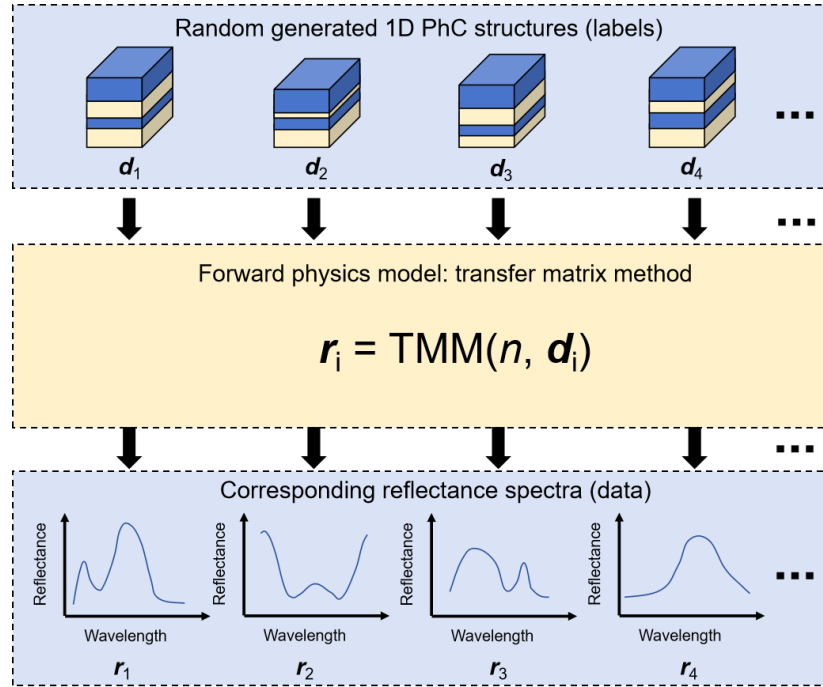


Fig. S2 The generation of real-word dataset. The dataset consists of the 1D PhC structure (labels) and their response spectra as the data.

Section S5: Material parameters and configurations in case 3

The material configurations of TAM, TA, TM, TSM and TS are shown in Fig. S3.

Layer 1	TiO ₂	TiO ₂	TiO ₂	TiO ₂	TiO ₂
Layer 2	Al ₂ O ₃	Al ₂ O ₃	MgF ₂	SiO ₂	SiO ₂
Layer 3	TiO ₂	TiO ₂	TiO ₂	TiO ₂	TiO ₂
Layer 4	MgF ₂	Al ₂ O ₃	MgF ₂	MgF ₂	SiO ₂
Layer 5	TiO ₂	TiO ₂	TiO ₂	TiO ₂	TiO ₂
Layer 6	MgF ₂	Al ₂ O ₃	MgF ₂	MgF ₂	SiO ₂
Layer 7	TiO ₂	TiO ₂	TiO ₂	TiO ₂	TiO ₂
Layer 8	Al ₂ O ₃	Al ₂ O ₃	MgF ₂	SiO ₂	SiO ₂
Layer 9	TiO ₂	TiO ₂	TiO ₂	TiO ₂	TiO ₂
	TAM	TA	TM	TSM	TS

Fig. S3 The 5 material configurations in case 3.

Section S6: Refractive indices of the materials in case 3

The refractive indices utilized in this work are provided in this section. The real part of the refractive indices of TiO₂, SiO₂ and Al₂O₃ are from the literature (Franta et al., 2015; Franta et al., 2016; Boidin et al., 2016), respectively. In the calculation, the refractive indices are approximated by the curves (yellow curves in the following figures) fitted from the data points. According to literature (Rodríguez-de Marcos et al., 2017), the index of MgF₂ in the visible-to-near-infrared (VIS-NIR) band is very close to 1.38, so the index of MgF₂ in this work is a constant of 1.38. The imaginary part of the refractive indices of the materials is fixed to 0 since these materials are lossless dielectric materials in the VIS-NIR band.

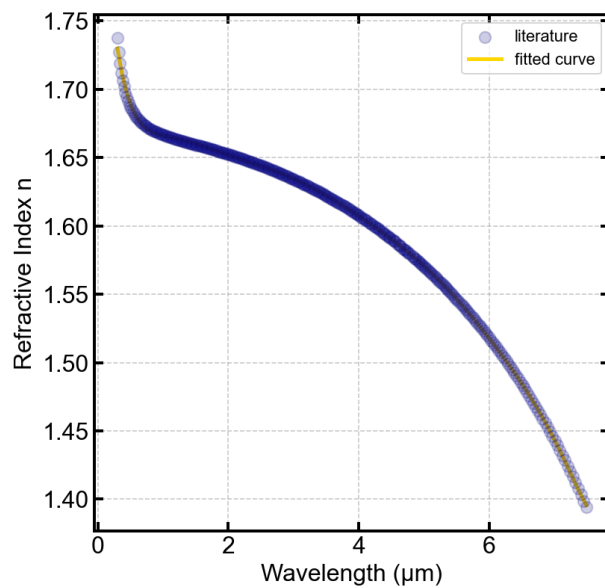


Fig. S4 The real part of the refractive index of Al_2O_3 .

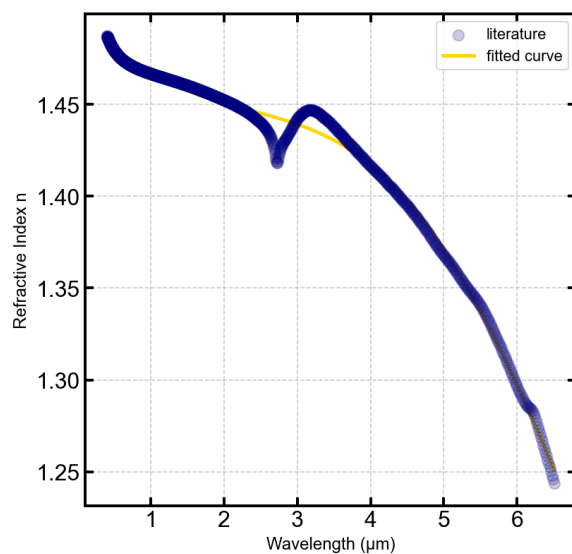


Fig. S5 The real part of the refractive index of SiO_2 .

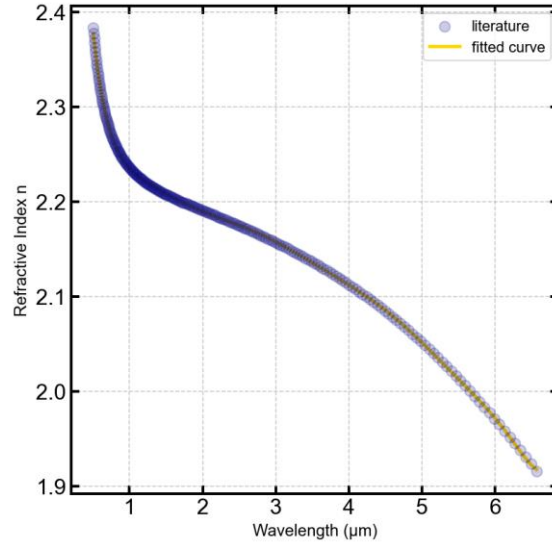


Fig. S6 The real part of the refractive index of TiO₂.

Section S7: Predicted 1D PhC structures in case 2

Photonic Crystal Al₂O₃_SiO₂:

Task1: [Incident-->/Layer 1 Al₂O₃: 80.48nm/Layer 2 SiO₂: 95.57nm/Layer 3 Al₂O₃: 137.79nm/Layer 4 SiO₂: 95.94nm/Layer 5 Al₂O₃: 84.02nm/Layer 6 SiO₂: 102.81nm/Layer 7 Al₂O₃: 120.73nm/Layer 8 SiO₂: 99.83nm/Layer 9 Al₂O₃: 84.60nm/Layer 10 SiO₂: 121.29nm/Layer 11 Al₂O₃: 98.63nm]

Task2: [Incident-->/Layer 1 Al₂O₃: 71.86nm/Layer 2 SiO₂: 80.51nm/Layer 3 Al₂O₃: 70.46nm/Layer 4 SiO₂: 81.92nm/Layer 5 Al₂O₃: 73.08nm/Layer 6 SiO₂: 85.24nm/Layer 7 Al₂O₃: 93.70nm/Layer 8 SiO₂: 101.51nm/Layer 9 Al₂O₃: 81.81nm/Layer 10 SiO₂: 85.41nm/Layer 11 Al₂O₃: 75.02nm]

Task3: [Incident-->/Layer 1 Al₂O₃: 69.70nm/Layer 2 SiO₂: 78.34nm/Layer 3 Al₂O₃: 65.92nm/Layer 4 SiO₂: 68.88nm/Layer 5 Al₂O₃: 69.86nm/Layer 6 SiO₂: 79.16nm/Layer 7 Al₂O₃: 66.45nm/Layer 8 SiO₂: 83.70nm/Layer 9 Al₂O₃: 182.01nm/Layer 10 SiO₂: 81.05nm/Layer 11 Al₂O₃: 162.86nm]

Task4: [Incident-->/Layer 1 Al₂O₃: 72.11nm/Layer 2 SiO₂: 80.85nm/Layer 3 Al₂O₃: 70.95nm/Layer 4 SiO₂: 82.67nm/Layer 5 Al₂O₃: 73.33nm/Layer 6 SiO₂: 85.14nm/Layer 7 Al₂O₃: 91.80nm/Layer 8 SiO₂: 100.10nm/Layer 9 Al₂O₃: 81.47nm/Layer 10 SiO₂: 85.66nm/Layer 11 Al₂O₃: 75.64nm]

Task5: [Incident-->/Layer 1 Al₂O₃: 77.14nm/Layer 2 SiO₂: 86.60nm/Layer 3 Al₂O₃: 77.56nm/Layer 4 SiO₂: 89.75nm/Layer 5 Al₂O₃: 77.26nm/Layer 6 SiO₂: 87.46nm/Layer 7 Al₂O₃: 77.14nm/Layer 8 SiO₂: 84.36nm/Layer 9 Al₂O₃: 77.48nm/Layer 10 SiO₂: 88.11nm/Layer 11 Al₂O₃: 79.88nm]

Task6: [Incident-->/Layer 1 Al₂O₃: 93.82nm/Layer 2 SiO₂: 107.20nm/Layer 3 Al₂O₃: 91.65nm/Layer 4 SiO₂: 103.86nm/Layer 5 Al₂O₃: 93.39nm/Layer 6 SiO₂: 108.12nm/Layer 7 Al₂O₃: 92.28nm/Layer 8 SiO₂: 103.67nm/Layer 9 Al₂O₃: 94.28nm/Layer 10 SiO₂: 108.29nm/Layer 11 Al₂O₃: 98.96nm]

Task7: [Incident-->/Layer 1 Al₂O₃: 83.16nm/Layer 2 SiO₂: 94.41nm/Layer 3 Al₂O₃: 86.82nm/Layer 4 SiO₂: 101.93nm/Layer 5 Al₂O₃: 94.55nm/Layer 6 SiO₂: 155.80nm/Layer 7 Al₂O₃: 93.23nm/Layer 8 SiO₂: 98.50nm/Layer 9 Al₂O₃: 86.39nm/Layer 10 SiO₂: 98.98nm/Layer 11 Al₂O₃: 89.06nm]

Task8: [Incident-->/Layer 1 Al₂O₃: 92.04nm/Layer 2 SiO₂: 106.52nm/Layer 3 Al₂O₃: 92.65nm/Layer 4 SiO₂: 103.20nm/Layer 5 Al₂O₃: 94.56nm/Layer 6 SiO₂: 109.16nm/Layer 7 Al₂O₃: 93.79nm/Layer 8 SiO₂: 104.21nm/Layer 9 Al₂O₃: 95.21nm/Layer 10 SiO₂: 108.64nm/Layer 11 Al₂O₃: 97.74nm]

Photonic Crystal Ta₂O₅_Al₂O₃:

Task1: [Incident-->/Layer 1 Ta₂O₅: 56.79nm/Layer 2 Al₂O₃: 75.61nm/Layer 3 Ta₂O₅: 28.28nm/Layer 4 Al₂O₃: 31.61nm/Layer 5 Ta₂O₅: 59.44nm/Layer 6 Al₂O₃: 79.87nm/Layer 7 Ta₂O₅: 59.59nm/Layer 8 Al₂O₃: 91.40nm/Layer 9 Ta₂O₅: 94.00nm/Layer 10 Al₂O₃: 88.42nm/Layer 11 Ta₂O₅: 75.86nm]

Task2: [Incident-->/Layer 1 Ta2O5: 51.34nm/Layer 2 Al2O3: 73.84nm/Layer 3 Ta2O5: 49.23nm/Layer 4 Al2O3: 70.98nm/Layer 5 Ta2O5: 51.05nm/Layer 6 Al2O3: 74.78nm/Layer 7 Ta2O5: 59.17nm/Layer 8 Al2O3: 104.00nm/Layer 9 Ta2O5: 93.10nm/Layer 10 Al2O3: 149.34nm/Layer 11 Ta2O5: 82.30nm]

Task3: [Incident-->/Layer 1 Ta2O5: 24.99nm/Layer 2 Al2O3: 49.63nm/Layer 3 Ta2O5: 69.59nm/Layer 4 Al2O3: 70.66nm/Layer 5 Ta2O5: 34.66nm/Layer 6 Al2O3: 59.30nm/Layer 7 Ta2O5: 45.16nm/Layer 8 Al2O3: 66.28nm/Layer 9 Ta2O5: 144.04nm/Layer 10 Al2O3: 52.95nm/Layer 11 Ta2O5: 134.47nm]

Task4: [Incident-->/Layer 1 Ta2O5: 51.07nm/Layer 2 Al2O3: 73.09nm/Layer 3 Ta2O5: 50.56nm/Layer 4 Al2O3: 71.34nm/Layer 5 Ta2O5: 51.92nm/Layer 6 Al2O3: 73.95nm/Layer 7 Ta2O5: 59.38nm/Layer 8 Al2O3: 99.11nm/Layer 9 Ta2O5: 98.29nm/Layer 10 Al2O3: 144.76nm/Layer 11 Ta2O5: 91.24nm]

Task5: [Incident-->/Layer 1 Ta2O5: 77.85nm/Layer 2 Al2O3: 53.64nm/Layer 3 Ta2O5: 46.66nm/Layer 4 Al2O3: 92.18nm/Layer 5 Ta2O5: 52.16nm/Layer 6 Al2O3: 85.59nm/Layer 7 Ta2O5: 53.19nm/Layer 8 Al2O3: 74.56nm/Layer 9 Ta2O5: 168.08nm/Layer 10 Al2O3: 113.14nm/Layer 11 Ta2O5: 30.23nm]

Task6: [Incident-->/Layer 1 Ta2O5: 73.68nm/Layer 2 Al2O3: 30.74nm/Layer 3 Ta2O5: 23.24nm/Layer 4 Al2O3: 37.84nm/Layer 5 Ta2O5: 57.84nm/Layer 6 Al2O3: 108.82nm/Layer 7 Ta2O5: 69.99nm/Layer 8 Al2O3: 71.53nm/Layer 9 Ta2O5: 81.90nm/Layer 10 Al2O3: 85.33nm/Layer 11 Ta2O5: 87.03nm]

Task7: [Incident-->/Layer 1 Ta2O5: 66.33nm/Layer 2 Al2O3: 100.94nm/Layer 3 Ta2O5: 72.34nm/Layer 4 Al2O3: 85.15nm/Layer 5 Ta2O5: 61.95nm/Layer 6 Al2O3: 84.33nm/Layer 7 Ta2O5: 71.63nm/Layer 8 Al2O3: 82.49nm/Layer 9 Ta2O5: 142.44nm/Layer 10 Al2O3: 81.49nm/Layer 11 Ta2O5: 58.63nm]

Task8: [Incident-->/Layer 1 Ta2O5: 72.04nm/Layer 2 Al2O3: 32.04nm/Layer 3 Ta2O5: 24.10nm/Layer 4 Al2O3: 43.00nm/Layer 5 Ta2O5: 63.37nm/Layer 6 Al2O3: 96.57nm/Layer 7 Ta2O5: 78.20nm/Layer 8 Al2O3: 93.73nm/Layer 9 Ta2O5: 66.45nm/Layer 10 Al2O3: 97.88nm/Layer 11 Ta2O5: 85.98nm]

Photonic Crystal Ta2O5_SiO2:

Task1: [Incident-->/Layer 1 Ta2O5: 60.68nm/Layer 2 SiO2: 25.38nm/Layer 3 Ta2O5: 34.85nm/Layer 4 SiO2: 89.28nm/Layer 5 Ta2O5: 55.99nm/Layer 6 SiO2: 82.65nm/Layer 7 Ta2O5: 103.79nm/Layer 8 SiO2: 115.64nm/Layer 9 Ta2O5: 58.55nm/Layer 10 SiO2: 101.41nm/Layer 11 Ta2O5: 103.86nm]

Task2: [Incident-->/Layer 1 Ta2O5: 57.60nm/Layer 2 SiO2: 73.18nm/Layer 3 Ta2O5: 47.54nm/Layer 4 SiO2: 73.80nm/Layer 5 Ta2O5: 53.24nm/Layer 6 SiO2: 83.53nm/Layer 7 Ta2O5: 61.43nm/Layer 8 SiO2: 91.91nm/Layer 9 Ta2O5: 121.65nm/Layer 10 SiO2: 162.96nm/Layer 11 Ta2O5: 69.02nm]

Task3: [Incident-->/Layer 1 Ta2O5: 34.52nm/Layer 2 SiO2: 53.49nm/Layer 3 Ta2O5: 54.48nm/Layer 4 SiO2: 77.98nm/Layer 5 Ta2O5: 42.16nm/Layer 6 SiO2: 43.80nm/Layer 7 Ta2O5: 158.03nm/Layer 8 SiO2: 109.35nm/Layer 9 Ta2O5: 122.77nm/Layer 10 SiO2: 134.88nm/Layer 11 Ta2O5: 117.54nm]

Task4: [Incident-->/Layer 1 Ta2O5: 52.60nm/Layer 2 SiO2: 69.48nm/Layer 3 Ta2O5: 58.60nm/Layer 4 SiO2: 80.35nm/Layer 5 Ta2O5: 52.80nm/Layer 6 SiO2: 79.06nm/Layer 7 Ta2O5: 56.96nm/Layer 8 SiO2: 86.90nm/Layer 9 Ta2O5: 128.09nm/Layer 10 SiO2: 162.30nm/Layer 11 Ta2O5: 79.94nm]

Task5: [Incident-->/Layer 1 Ta2O5: 57.32nm/Layer 2 SiO2: 25.90nm/Layer 3 Ta2O5: 99.56nm/Layer 4 SiO2: 77.04nm/Layer 5 Ta2O5: 58.07nm/Layer 6 SiO2: 59.51nm/Layer 7 Ta2O5: 79.19nm/Layer 8 SiO2: 83.13nm/Layer 9 Ta2O5: 157.89nm/Layer 10 SiO2: 106.76nm/Layer 11 Ta2O5: 115.38nm]

Task6: [Incident-->/Layer 1 Ta2O5: 27.18nm/Layer 2 SiO2: 22.98nm/Layer 3 Ta2O5: 39.01nm/Layer 4 SiO2: 150.48nm/Layer 5 Ta2O5: 37.08nm/Layer 6 SiO2: 30.45nm/Layer 7 Ta2O5: 112.53nm/Layer 8 SiO2: 108.47nm/Layer 9 Ta2O5: 78.54nm/Layer 10 SiO2: 111.32nm/Layer 11 Ta2O5: 86.24nm]

Task7: [Incident-->/Layer 1 Ta2O5: 30.37nm/Layer 2 SiO2: 29.09nm/Layer 3 Ta2O5: 73.74nm/Layer 4 SiO2: 115.58nm/Layer 5 Ta2O5: 62.24nm/Layer 6 SiO2: 88.78nm/Layer 7 Ta2O5: 66.53nm/Layer 8 SiO2: 97.33nm/Layer 9 Ta2O5: 65.23nm/Layer 10 SiO2: 107.10nm/Layer 11 Ta2O5: 84.65nm]

Task8: [Incident-->/Layer 1 Ta2O5: 23.59nm/Layer 2 SiO2: 23.07nm/Layer 3 Ta2O5: 45.19nm/Layer 4 SiO2: 131.03nm/Layer 5 Ta2O5: 63.37nm/Layer 6 SiO2: 48.37nm/Layer 7 Ta2O5: 100.96nm/Layer 8 SiO2: 97.51nm/Layer 9 Ta2O5: 87.34nm/Layer 10 SiO2: 105.41nm/Layer 11 Ta2O5: 87.72nm]

Photonic Crystal TiO₂_Al₂O₃:

Task1: [Incident-->/Layer 1 TiO₂: 103.11nm/Layer 2 Al₂O₃: 70.49nm/Layer 3 TiO₂: 43.65nm/Layer 4 Al₂O₃: 79.74nm/Layer 5 TiO₂: 92.99nm/Layer 6 Al₂O₃: 85.95nm/Layer 7 TiO₂: 49.49nm/Layer 8 Al₂O₃: 113.62nm/Layer 9 TiO₂: 80.28nm/Layer 10 Al₂O₃: 89.88nm/Layer 11 TiO₂: 102.98nm]

Task2: [Incident-->/Layer 1 TiO₂: 48.80nm/Layer 2 Al₂O₃: 69.82nm/Layer 3 TiO₂: 40.05nm/Layer 4 Al₂O₃: 72.29nm/Layer 5 TiO₂: 46.47nm/Layer 6 Al₂O₃: 76.21nm/Layer 7 TiO₂: 61.81nm/Layer 8 Al₂O₃: 122.54nm/Layer 9 TiO₂: 89.80nm/Layer 10 Al₂O₃: 135.02nm/Layer 11 TiO₂: 82.95nm]

Task3: [Incident-->/Layer 1 TiO₂: 118.95nm/Layer 2 Al₂O₃: 69.42nm/Layer 3 TiO₂: 25.78nm/Layer 4 Al₂O₃: 189.23nm/Layer 5 TiO₂: 54.62nm/Layer 6 Al₂O₃: 162.45nm/Layer 7 TiO₂: 58.14nm/Layer 8 Al₂O₃: 159.21nm/Layer 9 TiO₂: 112.36nm/Layer 10 Al₂O₃: 169.19nm/Layer 11 TiO₂: 111.90nm]

Task4: [Incident-->/Layer 1 TiO₂: 38.56nm/Layer 2 Al₂O₃: 75.86nm/Layer 3 TiO₂: 51.04nm/Layer 4 Al₂O₃: 71.20nm/Layer 5 TiO₂: 41.91nm/Layer 6 Al₂O₃: 73.72nm/Layer 7 TiO₂: 75.71nm/Layer 8 Al₂O₃: 133.75nm/Layer 9 TiO₂: 82.33nm/Layer 10 Al₂O₃: 149.76nm/Layer 11 TiO₂: 96.26nm]

Task5: [Incident-->/Layer 1 TiO₂: 84.28nm/Layer 2 Al₂O₃: 25.21nm/Layer 3 TiO₂: 36.67nm/Layer 4 Al₂O₃: 99.91nm/Layer 5 TiO₂: 53.45nm/Layer 6 Al₂O₃: 75.50nm/Layer 7 TiO₂: 146.05nm/Layer 8 Al₂O₃: 84.91nm/Layer 9 TiO₂: 92.37nm/Layer 10 Al₂O₃: 157.12nm/Layer 11 TiO₂: 97.12nm]

Task6: [Incident-->/Layer 1 TiO₂: 101.01nm/Layer 2 Al₂O₃: 36.95nm/Layer 3 TiO₂: 21.83nm/Layer 4 Al₂O₃: 135.51nm/Layer 5 TiO₂: 73.70nm/Layer 6 Al₂O₃: 87.32nm/Layer 7 TiO₂: 77.66nm/Layer 8 Al₂O₃: 84.26nm/Layer 9 TiO₂: 79.36nm/Layer 10 Al₂O₃: 225.36nm/Layer 11 TiO₂: 88.60nm]

Task7: [Incident-->/Layer 1 TiO₂: 61.92nm/Layer 2 Al₂O₃: 82.50nm/Layer 3 TiO₂: 50.88nm/Layer 4 Al₂O₃: 82.63nm/Layer 5 TiO₂: 55.50nm/Layer 6 Al₂O₃: 87.06nm/Layer 7 TiO₂: 61.10nm/Layer 8 Al₂O₃: 111.39nm/Layer 9 TiO₂: 80.62nm/Layer 10 Al₂O₃: 95.77nm/Layer 11 TiO₂: 76.29nm]

Task8: [Incident-->/Layer 1 TiO₂: 98.12nm/Layer 2 Al₂O₃: 53.09nm/Layer 3 TiO₂: 24.20nm/Layer 4 Al₂O₃: 151.38nm/Layer 5 TiO₂: 57.09nm/Layer 6 Al₂O₃: 110.99nm/Layer 7 TiO₂: 64.59nm/Layer 8 Al₂O₃: 105.28nm/Layer 9 TiO₂: 73.65nm/Layer 10 Al₂O₃: 249.90nm/Layer 11 TiO₂: 87.48nm]

Photonic Crystal TiO₂_SiO₂_Ta₂O₅_Al₂O₃:

Task1: [Incident-->/Layer 1 TiO₂: 95.05nm/Layer 2 SiO₂: 100.10nm/Layer 3 Ta₂O₅: 57.78nm/Layer 4 Al₂O₃: 75.53nm/Layer 5 TiO₂: 100.36nm/Layer 6 SiO₂: 88.87nm/Layer 7 Ta₂O₅: 58.63nm/Layer 8 Al₂O₃: 68.30nm/Layer 9 TiO₂: 24.37nm/Layer 10 SiO₂: 33.30nm/Layer 11 Ta₂O₅: 53.87nm]

Task2: [Incident-->/Layer 1 TiO₂: 102.95nm/Layer 2 SiO₂: 181.27nm/Layer 3 Ta₂O₅: 64.84nm/Layer 4 Al₂O₃: 95.76nm/Layer 5 TiO₂: 171.86nm/Layer 6 SiO₂: 80.05nm/Layer 7 Ta₂O₅: 48.86nm/Layer 8 Al₂O₃: 70.48nm/Layer 9 TiO₂: 46.86nm/Layer 10 SiO₂: 80.70nm/Layer 11 Ta₂O₅: 55.46nm]

Task3: [Incident-->/Layer 1 TiO₂: 115.21nm/Layer 2 SiO₂: 103.26nm/Layer 3 Ta₂O₅: 132.07nm/Layer 4 Al₂O₃: 72.08nm/Layer 5 TiO₂: 110.87nm/Layer 6 SiO₂: 138.05nm/Layer 7 Ta₂O₅: 21.54nm/Layer 8 Al₂O₃: 51.21nm/Layer 9 TiO₂: 41.11nm/Layer 10 SiO₂: 38.00nm/Layer 11 Ta₂O₅: 35.05nm]

Task4: [Incident-->/Layer 1 TiO₂: 110.99nm/Layer 2 SiO₂: 192.15nm/Layer 3 Ta₂O₅: 60.25nm/Layer 4 Al₂O₃: 100.44nm/Layer 5 TiO₂: 164.57nm/Layer 6 SiO₂: 76.64nm/Layer 7 Ta₂O₅: 53.04nm/Layer 8 Al₂O₃: 70.21nm/Layer 9 TiO₂: 50.41nm/Layer 10 SiO₂: 76.31nm/Layer 11 Ta₂O₅: 48.69nm]

Task5: [Incident-->/Layer 1 TiO₂: 98.97nm/Layer 2 SiO₂: 194.81nm/Layer 3 Ta₂O₅: 103.05nm/Layer 4 Al₂O₃: 76.79nm/Layer 5 TiO₂: 151.20nm/Layer 6 SiO₂: 90.22nm/Layer 7 Ta₂O₅: 79.14nm/Layer 8 Al₂O₃: 34.36nm/Layer 9 TiO₂: 71.26nm/Layer 10 SiO₂: 28.83nm/Layer 11 Ta₂O₅: 84.15nm]

Task6: [Incident-->/Layer 1 TiO₂: 93.55nm/Layer 2 SiO₂: 61.89nm/Layer 3 Ta₂O₅: 93.70nm/Layer 4 Al₂O₃: 98.71nm/Layer 5 TiO₂: 161.21nm/Layer 6 SiO₂: 134.25nm/Layer 7 Ta₂O₅: 63.69nm/Layer 8 Al₂O₃: 136.58nm/Layer 9 TiO₂: 28.04nm/Layer 10 SiO₂: 26.86nm/Layer 11 Ta₂O₅: 127.36nm]

Task7: [Incident-->/Layer 1 TiO₂: 97.42nm/Layer 2 SiO₂: 141.27nm/Layer 3 Ta₂O₅: 57.88nm/Layer 4 Al₂O₃: 97.65nm/Layer 5 TiO₂: 202.49nm/Layer 6 SiO₂: 94.38nm/Layer 7 Ta₂O₅: 60.71nm/Layer 8 Al₂O₃: 83.37nm/Layer 9 TiO₂: 51.84nm/Layer 10 SiO₂: 88.85nm/Layer 11 Ta₂O₅: 67.93nm]

Task8: [Incident-->/Layer 1 TiO₂: 90.18nm/Layer 2 SiO₂: 92.02nm/Layer 3 Ta₂O₅: 83.82nm/Layer 4 Al₂O₃: 97.46nm/Layer 5 TiO₂: 171.89nm/Layer 6 SiO₂: 123.47nm/Layer 7 Ta₂O₅: 74.12nm/Layer 8 Al₂O₃: 122.55nm/Layer 9 TiO₂: 27.71nm/Layer 10 SiO₂: 24.15nm/Layer 11 Ta₂O₅: 131.13nm]

Photonic Crystal TiO₂_Ta₂O₅:

Task1: [Incident-->/Layer 1 TiO₂: 196.58nm/Layer 2 Ta₂O₅: 62.80nm/Layer 3 TiO₂: 91.15nm/Layer 4 Ta₂O₅: 62.42nm/Layer 5 TiO₂: 74.69nm/Layer 6 Ta₂O₅: 74.93nm/Layer 7 TiO₂: 64.30nm/Layer 8 Ta₂O₅: 89.25nm/Layer 9 TiO₂: 57.79nm/Layer 10 Ta₂O₅: 61.06nm/Layer 11 TiO₂: 89.43nm]

Task2: [Incident-->/Layer 1 TiO₂: 169.17nm/Layer 2 Ta₂O₅: 58.82nm/Layer 3 TiO₂: 44.46nm/Layer 4 Ta₂O₅: 53.84nm/Layer 5 TiO₂: 43.49nm/Layer 6 Ta₂O₅: 52.32nm/Layer 7 TiO₂: 39.00nm/Layer 8 Ta₂O₅: 45.33nm/Layer 9 TiO₂: 41.73nm/Layer 10 Ta₂O₅: 54.39nm/Layer 11 TiO₂: 48.47nm]

Task3: [Incident-->/Layer 1 TiO₂: 233.61nm/Layer 2 Ta₂O₅: 54.73nm/Layer 3 TiO₂: 111.45nm/Layer 4 Ta₂O₅: 50.60nm/Layer 5 TiO₂: 109.74nm/Layer 6 Ta₂O₅: 48.51nm/Layer 7 TiO₂: 41.69nm/Layer 8 Ta₂O₅: 50.14nm/Layer 9 TiO₂: 40.40nm/Layer 10 Ta₂O₅: 48.65nm/Layer 11 TiO₂: 39.12nm]

Task4: [Incident-->/Layer 1 TiO₂: 168.75nm/Layer 2 Ta₂O₅: 58.81nm/Layer 3 TiO₂: 44.37nm/Layer 4 Ta₂O₅: 53.73nm/Layer 5 TiO₂: 43.38nm/Layer 6 Ta₂O₅: 52.18nm/Layer 7 TiO₂: 38.89nm/Layer 8 Ta₂O₅: 45.35nm/Layer 9 TiO₂: 41.82nm/Layer 10 Ta₂O₅: 54.39nm/Layer 11 TiO₂: 48.44nm]

Task5: [Incident-->/Layer 1 TiO₂: 154.44nm/Layer 2 Ta₂O₅: 60.23nm/Layer 3 TiO₂: 82.39nm/Layer 4 Ta₂O₅: 61.70nm/Layer 5 TiO₂: 50.46nm/Layer 6 Ta₂O₅: 58.88nm/Layer 7 TiO₂: 48.53nm/Layer 8 Ta₂O₅: 56.54nm/Layer 9 TiO₂: 48.67nm/Layer 10 Ta₂O₅: 58.53nm/Layer 11 TiO₂: 50.86nm]

Task6: [Incident-->/Layer 1 TiO₂: 180.66nm/Layer 2 Ta₂O₅: 80.65nm/Layer 3 TiO₂: 62.87nm/Layer 4 Ta₂O₅: 72.29nm/Layer 5 TiO₂: 64.80nm/Layer 6 Ta₂O₅: 72.78nm/Layer 7 TiO₂: 60.83nm/Layer 8 Ta₂O₅: 75.38nm/Layer 9 TiO₂: 65.06nm/Layer 10 Ta₂O₅: 61.18nm/Layer 11 TiO₂: 79.46nm]

Task7: [Incident-->/Layer 1 TiO₂: 193.91nm/Layer 2 Ta₂O₅: 69.46nm/Layer 3 TiO₂: 63.75nm/Layer 4 Ta₂O₅: 63.51nm/Layer 5 TiO₂: 48.85nm/Layer 6 Ta₂O₅: 54.65nm/Layer 7 TiO₂: 43.94nm/Layer 8 Ta₂O₅: 56.06nm/Layer 9 TiO₂: 52.51nm/Layer 10 Ta₂O₅: 61.96nm/Layer 11 TiO₂: 54.98nm]

Task8: [Incident-->/Layer 1 TiO₂: 191.91nm/Layer 2 Ta₂O₅: 73.41nm/Layer 3 TiO₂: 77.31nm/Layer 4 Ta₂O₅: 71.57nm/Layer 5 TiO₂: 66.35nm/Layer 6 Ta₂O₅: 75.84nm/Layer 7 TiO₂: 64.14nm/Layer 8 Ta₂O₅: 76.39nm/Layer 9 TiO₂: 65.74nm/Layer 10 Ta₂O₅: 66.74nm/Layer 11 TiO₂: 79.73nm]

Photonic Crystal TiO₂_Ta₂O₅_Al₂O₃_SiO₂:

Task1: [Incident-->/Layer 1 TiO₂: 108.72nm/Layer 2 Ta₂O₅: 107.28nm/Layer 3 Al₂O₃: 245.20nm/Layer 4 SiO₂: 83.99nm/Layer 5 TiO₂: 208.15nm/Layer 6 Ta₂O₅: 135.69nm/Layer 7 Al₂O₃: 188.37nm/Layer 8 SiO₂: 106.80nm/Layer 9 TiO₂: 52.77nm/Layer 10 Ta₂O₅: 20.61nm/Layer 11 Al₂O₃: 179.32nm]

Task2: [Incident-->/Layer 1 TiO₂: 172.86nm/Layer 2 Ta₂O₅: 108.64nm/Layer 3 Al₂O₃: 152.96nm/Layer 4 SiO₂: 87.86nm/Layer 5 TiO₂: 234.07nm/Layer 6 Ta₂O₅: 104.13nm/Layer 7 Al₂O₃: 131.17nm/Layer 8 SiO₂: 82.37nm/Layer 9 TiO₂: 36.01nm/Layer 10 Ta₂O₅: 20.12nm/Layer 11 Al₂O₃: 130.71nm]

Task3: [Incident-->/Layer 1 TiO₂: 121.50nm/Layer 2 Ta₂O₅: 100.73nm/Layer 3 Al₂O₃: 143.08nm/Layer 4 SiO₂: 211.20nm/Layer 5 TiO₂: 214.93nm/Layer 6 Ta₂O₅: 186.24nm/Layer 7 Al₂O₃: 150.39nm/Layer 8 SiO₂: 192.51nm/Layer 9 TiO₂: 90.48nm/Layer 10 Ta₂O₅: 24.47nm/Layer 11 Al₂O₃: 236.80nm]

Task4: [Incident-->/Layer 1 TiO₂: 53.07nm/Layer 2 Ta₂O₅: 114.96nm/Layer 3 Al₂O₃: 158.98nm/Layer 4 SiO₂: 81.84nm/Layer 5 TiO₂: 118.18nm/Layer 6 Ta₂O₅: 99.09nm/Layer 7 Al₂O₃: 144.62nm/Layer 8 SiO₂: 83.59nm/Layer 9 TiO₂: 37.46nm/Layer 10 Ta₂O₅: 22.81nm/Layer 11 Al₂O₃: 127.85nm]

Task5: [Incident-->/Layer 1 TiO₂: 56.90nm/Layer 2 Ta₂O₅: 112.55nm/Layer 3 Al₂O₃: 161.08nm/Layer 4 SiO₂: 90.00nm/Layer 5 TiO₂: 155.32nm/Layer 6 Ta₂O₅: 157.12nm/Layer 7 Al₂O₃: 135.89nm/Layer 8 SiO₂: 120.82nm/Layer 9 TiO₂: 71.88nm/Layer 10 Ta₂O₅: 74.80nm/Layer 11 Al₂O₃: 160.10nm]

Task6: [Incident-->/Layer 1 TiO₂: 74.08nm/Layer 2 Ta₂O₅: 128.75nm/Layer 3 Al₂O₃: 184.83nm/Layer 4 SiO₂: 112.66nm/Layer 5 TiO₂: 184.21nm/Layer 6 Ta₂O₅: 150.78nm/Layer 7 Al₂O₃: 168.60nm/Layer 8 SiO₂:

134.19nm/Layer 9 TiO₂: 72.18nm/Layer 10 Ta₂O₅: 25.06nm/Layer 11 Al₂O₃: 191.45nm]

Task7: [Incident-->/Layer 1 TiO₂: 66.16nm/Layer 2 Ta₂O₅: 137.25nm/Layer 3 Al₂O₃: 192.34nm/Layer 4 SiO₂: 98.58nm/Layer 5 TiO₂: 155.76nm/Layer 6 Ta₂O₅: 106.62nm/Layer 7 Al₂O₃: 160.44nm/Layer 8 SiO₂: 96.13nm/Layer 9 TiO₂: 47.30nm/Layer 10 Ta₂O₅: 22.34nm/Layer 11 Al₂O₃: 155.45nm]

Task8: [Incident-->/Layer 1 TiO₂: 72.36nm/Layer 2 Ta₂O₅: 131.20nm/Layer 3 Al₂O₃: 181.83nm/Layer 4 SiO₂: 116.60nm/Layer 5 TiO₂: 189.13nm/Layer 6 Ta₂O₅: 154.34nm/Layer 7 Al₂O₃: 178.07nm/Layer 8 SiO₂: 136.81nm/Layer 9 TiO₂: 76.10nm/Layer 10 Ta₂O₅: 23.82nm/Layer 11 Al₂O₃: 197.90nm]

Photonic Crystal TiO₂_SiO₂:

Task1: [Incident-->/Layer 1 TiO₂: 101.76nm/Layer 2 SiO₂: 88.79nm/Layer 3 TiO₂: 53.71nm/Layer 4 SiO₂: 49.65nm/Layer 5 TiO₂: 111.26nm/Layer 6 SiO₂: 85.46nm/Layer 7 TiO₂: 57.76nm/Layer 8 SiO₂: 149.32nm/Layer 9 TiO₂: 67.37nm/Layer 10 SiO₂: 101.91nm/Layer 11 TiO₂: 92.16nm]

Task2: [Incident-->/Layer 1 TiO₂: 56.30nm/Layer 2 SiO₂: 64.06nm/Layer 3 TiO₂: 41.28nm/Layer 4 SiO₂: 79.68nm/Layer 5 TiO₂: 53.31nm/Layer 6 SiO₂: 89.94nm/Layer 7 TiO₂: 59.44nm/Layer 8 SiO₂: 162.18nm/Layer 9 TiO₂: 108.97nm/Layer 10 SiO₂: 106.96nm/Layer 11 TiO₂: 83.97nm]

Task3: [Incident-->/Layer 1 TiO₂: 123.67nm/Layer 2 SiO₂: 79.42nm/Layer 3 TiO₂: 23.26nm/Layer 4 SiO₂: 60.81nm/Layer 5 TiO₂: 139.69nm/Layer 6 SiO₂: 170.57nm/Layer 7 TiO₂: 85.48nm/Layer 8 SiO₂: 157.56nm/Layer 9 TiO₂: 92.08nm/Layer 10 SiO₂: 149.91nm/Layer 11 TiO₂: 101.45nm]

Task4: [Incident-->/Layer 1 TiO₂: 53.62nm/Layer 2 SiO₂: 49.53nm/Layer 3 TiO₂: 45.36nm/Layer 4 SiO₂: 98.99nm/Layer 5 TiO₂: 49.20nm/Layer 6 SiO₂: 86.30nm/Layer 7 TiO₂: 137.11nm/Layer 8 SiO₂: 145.37nm/Layer 9 TiO₂: 61.42nm/Layer 10 SiO₂: 188.34nm/Layer 11 TiO₂: 94.60nm]

Task5: [Incident-->/Layer 1 TiO₂: 93.32nm/Layer 2 SiO₂: 29.44nm/Layer 3 TiO₂: 37.77nm/Layer 4 SiO₂: 77.20nm/Layer 5 TiO₂: 75.74nm/Layer 6 SiO₂: 82.68nm/Layer 7 TiO₂: 144.68nm/Layer 8 SiO₂: 94.09nm/Layer 9 TiO₂: 75.18nm/Layer 10 SiO₂: 192.24nm/Layer 11 TiO₂: 89.71nm]

Task6: [Incident-->/Layer 1 TiO₂: 87.74nm/Layer 2 SiO₂: 93.68nm/Layer 3 TiO₂: 21.03nm/Layer 4 SiO₂: 26.48nm/Layer 5 TiO₂: 119.76nm/Layer 6 SiO₂: 136.70nm/Layer 7 TiO₂: 66.06nm/Layer 8 SiO₂: 120.64nm/Layer 9 TiO₂: 79.31nm/Layer 10 SiO₂: 247.38nm/Layer 11 TiO₂: 89.16nm]

Task7: [Incident-->/Layer 1 TiO₂: 64.57nm/Layer 2 SiO₂: 93.12nm/Layer 3 TiO₂: 51.57nm/Layer 4 SiO₂: 80.12nm/Layer 5 TiO₂: 64.18nm/Layer 6 SiO₂: 87.24nm/Layer 7 TiO₂: 63.20nm/Layer 8 SiO₂: 125.27nm/Layer 9 TiO₂: 80.72nm/Layer 10 SiO₂: 124.75nm/Layer 11 TiO₂: 77.49nm]

Task8: [Incident-->/Layer 1 TiO₂: 83.86nm/Layer 2 SiO₂: 121.21nm/Layer 3 TiO₂: 23.23nm/Layer 4 SiO₂: 26.38nm/Layer 5 TiO₂: 113.08nm/Layer 6 SiO₂: 120.60nm/Layer 7 TiO₂: 77.86nm/Layer 8 SiO₂: 98.83nm/Layer 9 TiO₂: 78.92nm/Layer 10 SiO₂: 116.00nm/Layer 11 TiO₂: 86.13nm]

Section S8: Predicted 1D PhC structures in case 3

For the GaAs/Si system, the vectors of predicted 1D PhCs' structure are:

TAM1: [Incident--> TiO₂: 11.51nm/Al₂O₃: 31.74nm/TiO₂: 94.87nm/MgF₂: 186.66nm/TiO₂: 111.77nm/MgF₂: 169.79nm/TiO₂: 112.50nm/Al₂O₃: 24.45nm/TiO₂: 13.67nm --> Substrate]

TA1: [Incident--> TiO₂: 12.59nm/Al₂O₃: 37.09nm/TiO₂: 87.85nm/Al₂O₃: 143.52nm/TiO₂: 103.25nm/Al₂O₃: 144.07nm/TiO₂: 116.85nm/Al₂O₃: 144.32nm/TiO₂: 111.77nm --> Substrate]

TM1: [Incident--> TiO₂: 18.06nm/MgF₂: 27.31nm/TiO₂: 71.72nm/MgF₂: 194.88nm/TiO₂: 116.70nm/MgF₂: 171.50nm/TiO₂: 118.11nm/MgF₂: 31.26nm/TiO₂: 11.05nm --> Substrate]

TSM1: [Incident--> TiO₂: 12.64nm/SiO₂: 29.72nm/TiO₂: 83.12nm/MgF₂: 194.42nm/TiO₂: 116.42nm/MgF₂: 176.64nm/TiO₂: 121.32nm/SiO₂: 38.42nm/TiO₂: 11.08nm --> Substrate]

TS1: [Incident--> TiO₂: 15.15nm/SiO₂: 34.66nm/TiO₂: 81.98nm/SiO₂: 186.76nm/TiO₂: 111.83nm/SiO₂: 178.95nm/TiO₂: 120.38nm/SiO₂: 141.38nm/TiO₂: 116.38nm --> Substrate]

For the GaInP/Si system, the vectors of predicted 1D PhCs' structure are:

TAM2: [Incident--> TiO2: 12.78nm/Al2O3: 19.54nm/TiO2: 77.28nm/MgF2: 164.12nm/TiO2: 98.27nm/MgF2: 148.28nm/TiO2: 99.37nm/Al2O3: 15.45nm/TiO2: 12.77nm --> Substrate]
TA2: [Incident--> TiO2: 12.42nm/Al2O3: 17.95nm/TiO2: 78.03nm/Al2O3: 132.17nm/TiO2: 95.09nm/Al2O3: 132.93nm/TiO2: 105.88nm/Al2O3: 138.20nm/TiO2: 104.66nm --> Substrate]
TM2: [Incident--> TiO2: 11.54nm/MgF2: 42.18nm/TiO2: 82.44nm/MgF2: 165.02nm/TiO2: 98.81nm/MgF2: 137.74nm/TiO2: 103.36nm/MgF2: 147.27nm/TiO2: 93.19nm --> Substrate]
TSM2: [Incident--> TiO2: 11.14nm/SiO2: 34.54nm/TiO2: 73.11nm/MgF2: 167.51nm/TiO2: 100.31nm/MgF2: 146.64nm/TiO2: 103.94nm/SiO2: 149.85nm/TiO2: 85.78nm --> Substrate]
TS2: [Incident--> TiO2: 101.11nm/SiO2: 137.06nm/TiO2: 93.37nm/SiO2: 160.83nm/TiO2: 96.30nm/SiO2: 154.02nm/TiO2: 123.92nm/SiO2: 33.85nm/TiO2: 14.77nm --> Substrate]

Section S9: PV simulation methods

Single-diode model (for GaAs and Si cells)

The single-diode model is employed to describe the current-voltage (J-V) characteristics of GaAs and Si cells. The model consists of a current source representing photogenerated carriers, a diode accounting for recombination losses, series resistance (R_s), and shunt resistance (R_{sh}).

The fundamental equation of the single-diode model(Huang et al., 2021) is:

$$J = J_{ph} - J_0 \left[\exp \left(\frac{q(V + JR_s)}{nk_B T} \right) - 1 \right] - \frac{V + JR_s}{R_{sh}} \quad (S8)$$

where J and V are current density and voltage of the cell, respectively, J_{ph} is the photogenerated current density, J_0 denotes the reverse saturation current density, q is the elementary charge (1.6×10^{-19} C), n is the diode ideality factor, k_B is Boltzmann constant (1.380649×10^{-23} J/K), T is the cell temperature.

The bandgap energy E_g varies with temperature according to the Varshni equation(Singh and Ravindra, 2012):

$$E_g(T) = E_{g,0K} - \frac{\alpha T^2}{T + \beta} \quad (S9)$$

where $E_{g,0K}$ is the bandgap at 0 K, and α and β are material-specific constants which can be found in the following parameters section.

The photogenerated current density J_{ph} is calculated by integrating the product of the incident spectral irradiance $G(\lambda)$, the filter transmission/reflectance $T(\lambda)$ or $R(\lambda)$, and the external quantum efficiency $EQE(\lambda)$ over the wavelength range:

$$J_{ph} = \frac{1}{hc} \int_{\lambda_{min}}^{\lambda_c} q \cdot \lambda \cdot G(\lambda) \cdot \eta_{spectral}(\lambda) \cdot EQE(\lambda) d\lambda \quad (S10)$$

where h and c are Plank's constant and speed of light, respectively, λ_c is the cutoff wavelength determined by the bandgap ($\lambda_c = hc/E_g$), λ_{min} is the strat boundary of the response band which is fixed to 400 nm in this work, and the EQE in the response band from λ_{min} to λ_c is set to 0.9, the EQE outside the response band is 0, $\eta_{spectral}(\lambda)$ represents the filter transmission (for high-bandgap cell) or reflectance (for low-bandgap cell). The reverse current density is scaled(De Soto et al., 2006) with the temperature using:

$$J_0(T) = J_{0,ref} \left(\frac{T}{T_{ref}} \right)^3 \exp \left[\frac{E_g(T_{ref})}{k_B T_{ref}} - \frac{E_g(T)}{k_B T} \right] \quad (S11)$$

where $J_{0,ref}$ denotes the reverse current density under the reference cell temperature T_{ref} .

For the GaInP cell, the double-diode model is employed to achieve higher accuracy, particularly accounting for both recombination in the quasi-neutral regions (diode 1) and recombination in the space-charge region (diode 2). The model equation is from literature(Barth et al., 2016):

$$J = J_{ph} - J_{01} \left[\exp \left(\frac{q(V + JR_s)}{n_1 k_B T} \right) - 1 \right] - J_{02} \left[\exp \left(\frac{q(V + JR_s)}{n_2 k_B T} \right) - 1 \right] - \frac{V + JR_s}{R_{sh}} \quad (S12)$$

where J_{01} and J_{02} are the reverse saturation current densities for diode 1 and diode 2, respectively, n_1 and n_2 are the ideality factors which are 1 and 2, respectively.

The reverse saturation current densities in the double-diode model can also be calculated by the scale law (Perl et al., 2016) which is similar with the one in the *S.Eq.11*.

$$J_{01}(T) = J_{01,ref} \left(\frac{T}{T_{ref}} \right)^3 \exp \left[\frac{E_g(T_{ref})}{k_B T_{ref}} - \frac{E_g(T)}{k_B T} \right] \quad (S13)$$

$$J_{02}(T) = J_{02,ref} \left(\frac{T}{T_{ref}} \right)^{1.5} \exp \left[\frac{E_g(T_{ref})}{2k_B T_{ref}} - \frac{E_g(T)}{2k_B T} \right] \quad (S14)$$

In the Python implementation, the J-V curve is obtained by solving the implicit diode equation numerically. A voltage array is created from 0 V to an estimated open-circuit voltage. For each voltage point V_i , the corresponding current density J_i is found by solving the transcendental diode equation using the fsolve function from the python library scipy.optimize. The solution from the previous voltage point is used as the initial guess for the next point to ensure convergence stability. The power density is calculated as $P = J \times V$, and the maximum power point (MPP) is identified as the peak of the P - V curve.

To be closer to the real condition of the system, the temperature dependence of the solar cells must be considered. Since the cell temperature T affects the electrical output (through E_g and J_0), and the electrical output affects the thermal balance (through heat dissipation), an iterative procedure is employed to achieve self-consistent solutions. First, an initial cell temperature is set as the ambient temperature plus 25 K. Second, calculate the incident thermal power by integrating the solar radiation spectrum that incident to the cell. Then calculate the electrical power at the MPP, P_{elec} , and solve the thermal balance equation for the new equilibrium temperature.

$$q_{conv} + q_{rad} = P_{in} - P_{elec} \quad (S15)$$

where q_{conv} denotes the convective heat loss, q_{rad} is the radiative heat loss. These losses can be calculated by

$$q_{conv} = 2h_{conv} (T - T_{amb}) \quad (S16)$$

$$q_{rad} = 2\sigma_{SB} (T^4 - T_{amb}^4) \quad (S17)$$

where h_{conv} is the passive convective heat transfer coefficient which is set to $15 \text{ Wm}^{-2}\text{K}^{-1}$, σ_{SB} is the Stefan-Boltzmann constant, T_{amb} is the environmental temperature which is 298 K in this work.

Section S10: Equations of forward TMM in PV system simulation

Since the incident angle should be considered in the system-level simulation, the forward TMM calculation has a little difference from the one which is applied as a part of loss function. Hence, the equations are attached in this supplementary materials.

First, some new variables are introduced: θ_0 denotes the incident angle, $\tilde{\theta}_{j,\lambda}$ is the complex refractive angle in the j th layer at the wavelength of λ , $\sigma \in \{\text{TE}, \text{TM}\}$ represent the polarization state, the complex refractive index of j th layer at the wavelength of λ is $\tilde{n}_{j,\lambda} = n_{j,\lambda} - ik_{j,\lambda}$, n_0 and n_s are refractive index of the incident and substrate material, respectively. The other variables refer to the ‘‘Introduction of the differentiable transfer matrix method’’ section.

Snell’s law:

$$n_0 \sin \theta_0 = \tilde{n}_{j,\lambda} \sin \tilde{\theta}_{j,\lambda} \quad (S18)$$

$$\cos \tilde{\theta}_{j,\lambda} = \sqrt{1 - \left(\frac{n_0 \sin \theta_0}{\tilde{n}_{j,\lambda}} \right)^2} \quad (\text{S19})$$

$$\delta_{j,\lambda} = k_0 \tilde{n}_{j,\lambda} d_j \cos \tilde{\theta}_{j,\lambda} = \frac{2\pi}{\lambda} \tilde{n}_{j,\lambda} d_j \cos \tilde{\theta}_{j,\lambda} \quad (\text{S20})$$

where $\delta_{j,\lambda}$ is a complex number, the real part represents phase delay, while the imaginary part corresponds to amplitude attenuation.

Complex optical admittances for TM and TE polarization:

$$\tilde{Y}_{j,\lambda}^{\text{TE}} = \sqrt{\frac{\epsilon_0}{\mu_0}} \tilde{n}_{j,\lambda} \cos \tilde{\theta}_{j,\lambda} \quad (\text{S21a})$$

$$\tilde{Y}_{j,\lambda}^{\text{TM}} = \sqrt{\frac{\epsilon_0}{\mu_0}} \frac{\tilde{n}_{j,\lambda}}{\cos \tilde{\theta}_{j,\lambda}} \quad (\text{S21b})$$

$$\mathbf{M}_{j,\lambda}^{(\sigma)} = \begin{bmatrix} \cos \delta_{j,\lambda} & \frac{i \sin \delta_{j,\lambda}}{\tilde{Y}_{j,\delta}^{(\sigma)}} \\ \tilde{Y}_{j,\lambda}^{(\sigma)} i \sin \delta_{j,\lambda} & \cos \delta_{j,\lambda} \end{bmatrix} \quad (\text{S22})$$

$$\mathbf{M}_{\lambda}^{(\sigma)} = \prod_{j=1}^p \mathbf{M}_{j,\lambda}^{(\sigma)} = \begin{bmatrix} m_{11,\lambda} & m_{12,\lambda} \\ m_{21,\lambda} & m_{22,\lambda} \end{bmatrix} \quad (\text{S23})$$

$$r_{\lambda}^{(\sigma)} = \frac{\tilde{Y}_0^{(\sigma)} m_{11,\lambda} + \tilde{Y}_0^{(\sigma)} \tilde{Y}_s^{(\sigma)} m_{12,\lambda} - m_{21,\lambda} - \tilde{Y}_s^{(\sigma)} m_{22,\lambda}}{\tilde{Y}_0^{(\sigma)} m_{11,\lambda} + \tilde{Y}_0^{(\sigma)} \tilde{Y}_s^{(\sigma)} m_{12,\lambda} + m_{21,\lambda} + \tilde{Y}_s^{(\sigma)} m_{22,\lambda}} \quad (\text{S24})$$

$$t_{\lambda}^{(\sigma)} = \frac{2\tilde{Y}_0^{(\sigma)}}{\tilde{Y}_0^{(\sigma)} m_{11,\lambda} + \tilde{Y}_0^{(\sigma)} \tilde{Y}_s^{(\sigma)} m_{12,\lambda} + m_{21,\lambda} + \tilde{Y}_s^{(\sigma)} m_{22,\lambda}} \quad (\text{S25})$$

$$R_{\lambda}^{(\sigma)} = |r_{\lambda}^{(\sigma)}|^2 = r_{\lambda}^{(\sigma)} \cdot r_{\lambda}^{(\sigma)*} \quad (\text{S26})$$

$$T_{\lambda}^{(\sigma)} = \frac{\text{Re}(\tilde{Y}_s^{(\sigma)})}{\text{Re}(\tilde{Y}_0^{(\sigma)})} |t_{\lambda}^{(\sigma)}|^2 \quad (\text{S27})$$

Overall reflectance:

$$R_{\lambda} = \frac{1}{2} (R_{\lambda}^{\text{TE}} + R_{\lambda}^{\text{TM}}) \quad (\text{S28})$$

Overall transmittance:

$$T_{\lambda} = \frac{1}{2} (T_{\lambda}^{\text{TE}} + T_{\lambda}^{\text{TM}}) \quad (\text{S29})$$

Overall absorbance:

$$A_{\lambda} = 1 - R_{\lambda} - T_{\lambda} \quad (\text{S30})$$

Section S11: Model parameters of solar cells

The parameters of the solar cells utilized in the single or double-diode model is summarized in this section. The single diode parameters of the Si cell is extracted from IV curves of a 9 cm² commercial Si cell, the Varshni parameters of Si and GaAs cells refer to literature (Singh and Ravindra, 2012), the single diode parameters of

GaAs is from reference(Li et al., 2017), the double-diode and Varshni parameters of GaInP cell are from literatures(Nuñez et al., 2023; Shu et al., 2011), respectively.

Table S2 The model parameters of solar cells in case 3

Parameter	Si	GaAs	GaInP
n	1.44	2	-
n_1	-	-	1
n_2	-	-	2
$R_s (\Omega \cdot \text{cm}^2)$	0.157	2.07	2.7
$R_{sh} (\Omega \cdot \text{cm}^2)$	7272	8986.2	2.1×10^6
$J_{0,\text{ref}} (\text{A}/\text{cm}^2)$	1.16×10^{-9}	1.0×10^{-7}	-
$J_{01,\text{ref}} (\text{A}/\text{cm}^2)$	-	-	3.33×10^{-13}
$J_{02,\text{ref}} (\text{A}/\text{cm}^2)$	-	-	1×10^{-8}
$T_{\text{ref}} (\text{K})$	298	298	443
$E_{g,0\text{K}} (\text{eV})$	1.1557	1.5216	1.9
$\alpha (\text{eV}/\text{K})$	7.021×10^{-4}	8.871×10^{-4}	3.7×10^{-4}
$\beta (\text{K})$	1108	572	160

Section S12: Case 3 results with 45 degree incident angle

To evaluate the angular robustness of the designed filters, we extended our analysis to 45° incidence. The predicted reflectance spectra at 45° (Fig. S7) show similar overall characteristics to those at 0°, with slightly reduced peak reflectance values due to the angle-dependent shift in the Bragg condition. The corresponding J-V curves at 45° incidence (Fig. S8) demonstrate that all five filter configurations maintain excellent performance under oblique illumination. Remarkably, the TS1 configuration still achieves the highest total power density of 0.0204 W/cm² at 45° incidence, which is relatively 22.4% higher than standalone GaAs cell (0.0166 W/cm²) and 24.1% higher than standalone Si cell (0.0164 W/cm²). This result unequivocally demonstrates that the spectral-splitting approach maintains its efficiency advantage even at practical operating angles.

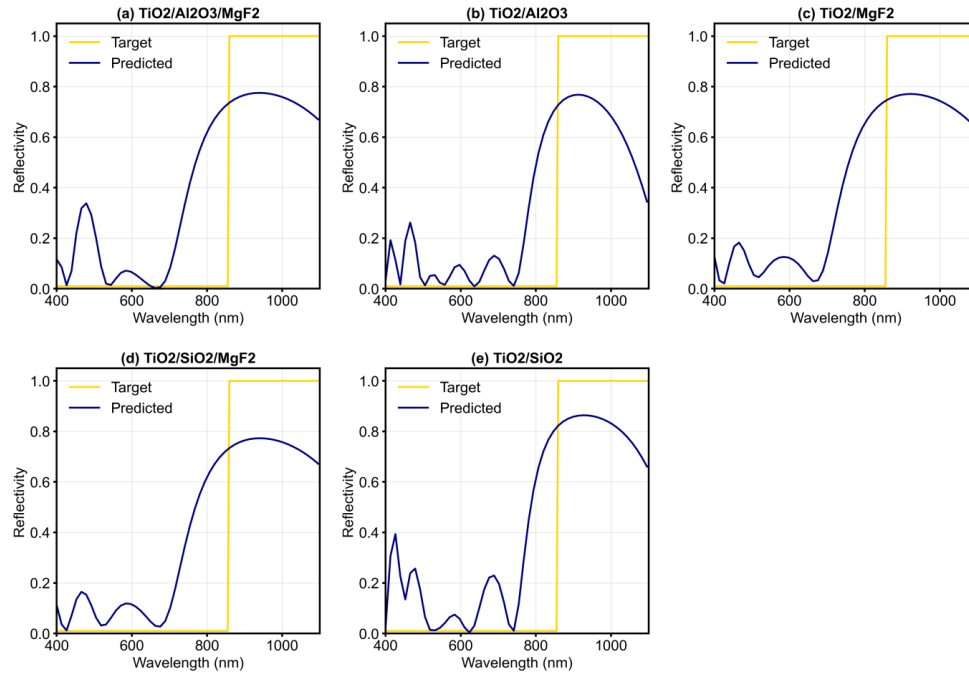


Fig. S7. Performance comparison of five models trained with distinct material configurations: GaAs/Si system. The reflectance spectra at 45 degree incident angle of: (a) TiO₂-Al₂O₃-MgF₂ (TAM1) (b) TiO₂-Al₂O₃ (TA1) (c) TiO₂-MgF₂ (TM1) (d) TiO₂-SiO₂-MgF₂ (TSM1) (e) TiO₂-SiO₂ (TS1).

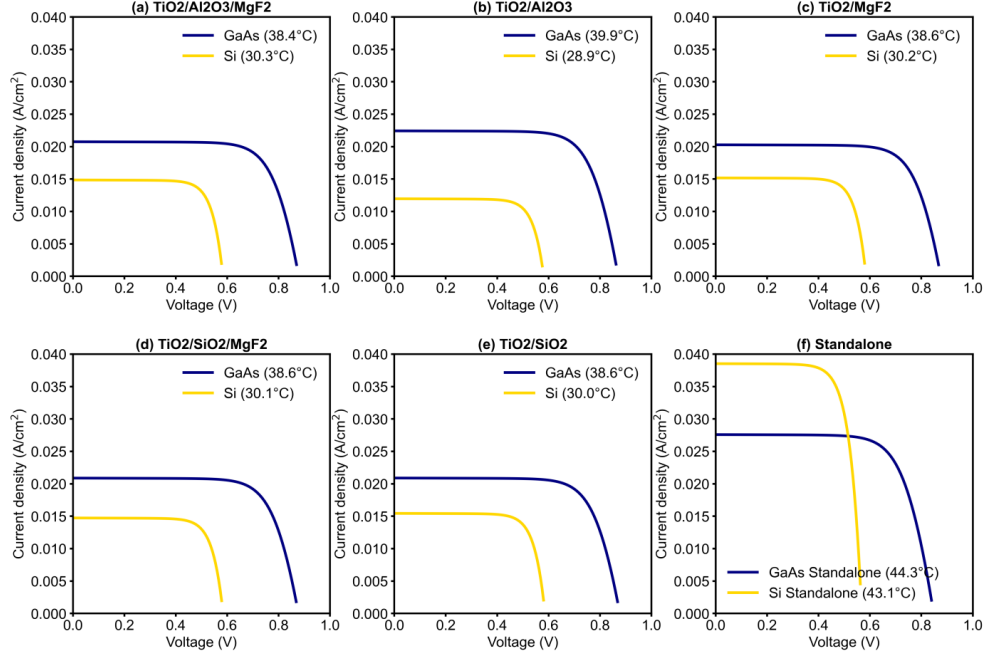


Fig. S8. J-V Curves of GaAs/Si combined solar cells under AM1.5G condition using different spectrum splitters with 45 degree solar incident angle to the splitters: (a) $\text{TiO}_2\text{-Al}_2\text{O}_3\text{-MgF}_2$ (TAM1) (b) $\text{TiO}_2\text{-Al}_2\text{O}_3$ (TA1) (c) $\text{TiO}_2\text{-MgF}_2$ (TM1) (d) $\text{TiO}_2\text{-SiO}_2\text{-MgF}_2$ (TSM1) (e) $\text{TiO}_2\text{-SiO}_2$ (TS1) (f) Standalone J-V curves of GaAs and Si as reference.

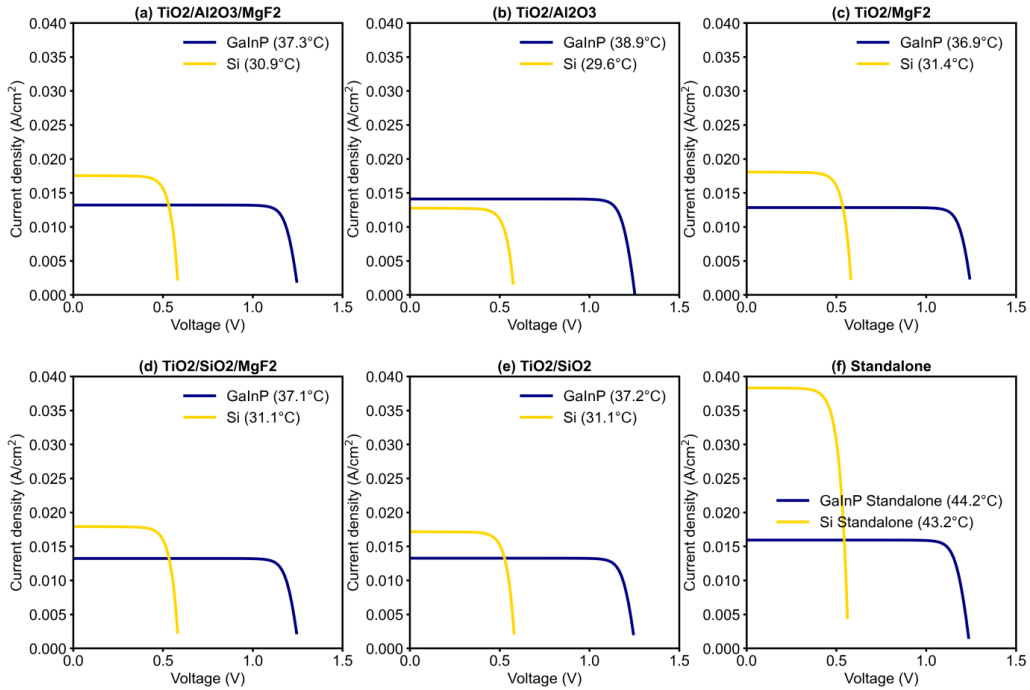


Fig. S9. J-V Curves of GaInP/Si combined solar cells under AM1.5G condition using different spectrum splitters with 45 degree solar incident angle to the splitters: (a) $\text{TiO}_2\text{-Al}_2\text{O}_3\text{-MgF}_2$ (TAM2) (b) $\text{TiO}_2\text{-Al}_2\text{O}_3$ (TA2) (c) $\text{TiO}_2\text{-MgF}_2$ (TM2) (d) $\text{TiO}_2\text{-SiO}_2\text{-MgF}_2$ (TSM2) (e) $\text{TiO}_2\text{-SiO}_2$ (TS2) (f) Standalone J-V curves of GaInP and Si as reference.

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