Supporting Information

for *Adv. Mater.*, DOI: 10.1002/adma.201905467

A Bidirectional Deep Neural Network for Accurate Silicon Color Design

Li Gao, Xiaozhong Li, Dianjing Liu, Lianhui Wang, and Zongfu Yu**

Supporting Information for

Bidirectional Deep Neural Network for Accurate Silicon Color Design

Li Gao,[1, *, †] Xiaozhong Li,[2, †] Dianjing Liu,[3] Lianhui Wang,[1] Zongfu Yu[3, *]

[1]Key Laboratory for Organic Electronics and Information Displays (KLOEID), Institute of Advanced Materials (IAM), School of Materials Science and Engineering, Nanjing University of Posts and Telecommunications, Nanjing 210023, China

[2]School of Electronic and Optical Engineering, Nanjing University of Science and Technology, Nanjing 210094, China

[3]School of Electrical and Computer Engineering, University of Wisconsin-Madison, Madison, WI 53706, USA

[†]These authors contributed equally to this work. [*]Corresponding author E-mail: iamlgao@njupt.edu.cn (L.G.); zyu54@wisc.edu (Z.Y.)

1. CIE 1931 color space and color matching functions.

CIE 1931 XYZ color space is created by the International Commission on Illumination (CIE) in 1931, of which XYZ represent the tristimulus values. The tristimulus values depend on the observer's field of view, so the color matching functions $\bar{x}(\lambda)$, $\bar{y}(\lambda)$, $\bar{z}(\lambda)$ (or called CIE standard observer) are further defined to eliminate the variable, as shown in **Figure S1**.

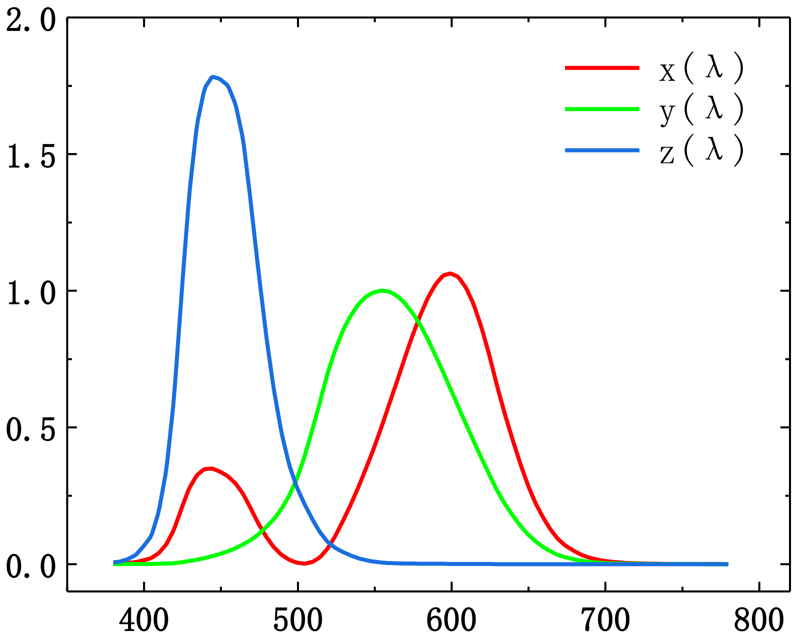

Figure S1. The color matching functions defined by CIE.[1]

With color matching functions, tristimulus values XYZ can be calculated from spectral data by:

$$X = \frac{\alpha}{K}\int_{\lambda 0}^{\lambda 1} I(\lambda)\cdot R(\lambda)\cdot \bar{x}(\lambda)d\lambda$$

$$Y = \frac{\alpha}{K}\int_{\lambda 0}^{\lambda 1} I(\lambda)\cdot R(\lambda)\cdot \bar{y}(\lambda)d\lambda$$

$$Z = \frac{\alpha}{K}\int_{\lambda 0}^{\lambda 1} I(\lambda)\cdot R(\lambda)\cdot \bar{z}(\lambda)d\lambda$$

In either reflective and transmissive case, where

$$K = \int_{\lambda 0}^{\lambda 1} I(\lambda)\ \cdot \bar{y}(\lambda)d\lambda$$

α is a scaling factor, whose magnitude can be set as 1 or 100 normally, and 1 is chosen in datasets of this work; λ is the wavelength of the illumination light, the standard limits of the integral are [380,780]; $I(\lambda)$ is the spectral power distribution of the illuminant, and $R(\lambda)$ is the corresponding reflectivity. In actual calculation, since there are limited spectrum data points, thus we approximate the integration as the sum of available data points.

$$X = \frac{\alpha}{K}\sum_{i=1}^{n} I(\lambda_i)\cdot R(\lambda_i)\cdot \bar{x}(\lambda_i)\cdot \Delta\lambda$$

$$Y = \frac{\alpha}{K}\sum_{i=1}^{n} I(\lambda_i)\cdot R(\lambda_i)\cdot \bar{y}(\lambda_i)\cdot \Delta\lambda$$

$$Z = \frac{\alpha}{K}\sum_{i=1}^{n} I(\lambda_i)\cdot R(\lambda_i)\cdot \bar{z}(\lambda_i)\cdot \Delta\lambda$$

To correspond to a certain color, XYZ need another transformation:

$$x = \frac{X}{X+Y+Z}$$

$$y = \frac{Y}{X+Y+Z}$$

$$z = \frac{Z}{X+Y+Z} = 1 - x - y$$

Where x, y can define a CIE chromaticity diagram, and Y is used to measure the brightness of the color. The three parameters together form the CIE xyY color space.

2. The estimation of training data area coverage on the CIE chromaticity diagram.

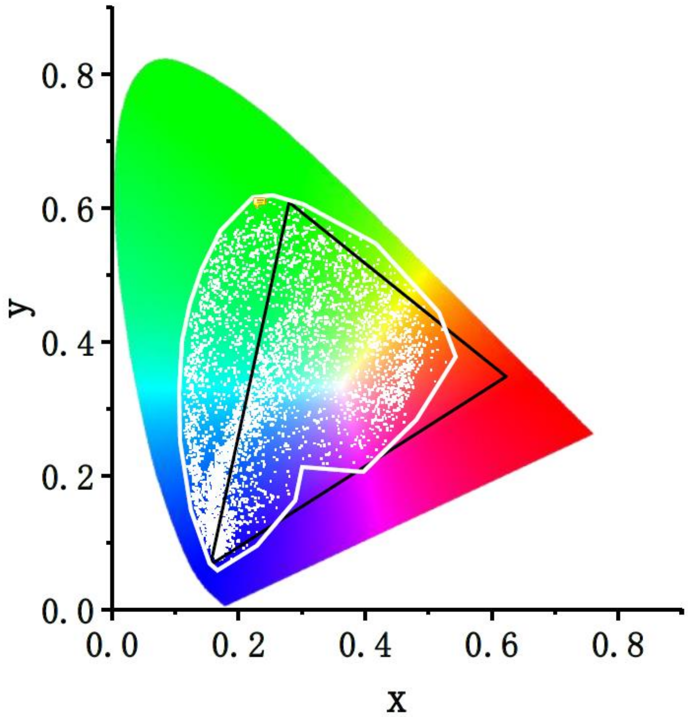

Figure S2. Area of the simulated silicon colors of the datasets (surrounded by the white line) in the CIE chromaticity diagram. The area of the sRGB in the CIE (area of the black triangle) is 0.11205, with the three vertices of (0.6400, 0.3300), (0.3000, 0.6000), and (0.1500, 0.0600). The area of the datasets is calculated to be 0.160, which is 143% of the sRGB area.

3. The impact of device geometry changes on color values.

P(nm)	G (nm)	D (nm)	H (nm)	x	y	Y
500	240	100	40	0.16364	0.17598	0.05931
500	240	100	80	0.19057	0.1616	0.041939
500	240	100	120	0.12718	0.20248	0.056121
500	240	100	160	0.13926	0.48332	0.16089
500	240	80	80	0.16376	0.22534	0.023332
500	240	100	80	0.19057	0.1616	0.041939
500	240	120	80	0.21305	0.24879	0.089783
500	240	140	80	0.26476	0.41033	0.1785
500	200	100	80	0.19159	0.16043	0.04123
500	240	100	80	0.19057	0.1616	0.041939
500	280	100	80	0.19087	0.1609	0.041632
500	320	100	80	0.19277	0.16035	0.04078
400	240	100	80	0.21179	0.15272	0.061628
500	240	100	80	0.19057	0.1616	0.041939
600	240	100	80	0.18551	0.18743	0.034513
700	240	100	80	0.19011	0.16433	0.029552

4. The choice of hyperparameters and representative training results.

The training results of the neural network is largely determined by the structure of the network and every hyperparameter. After various tests with the same training data sets, some of the hyperparameters can be fixed for the three networks, which are shown in **Table S1**. Others need to be further tested for each individual network to yield the best results, such as the number of hidden layers, the numbers of nodes in hidden layers, and the batch size of the datasets.

Table S1. Optimal settings of some hyperparameters.

Parameters of network	**Optimal settings**
Initializers	W: uniform; b: zeros
Activation function	Relu
Loss	MSE (mean squared error)
Optimizer	RMSPropOptimizer
Learning rate	0.001
Decay rate	0.99

Some of the test results for different network structures are shown in **Table S2, S3, S4**. Taking the forward modeling network as an example, dozens of groups are tested, and results of 7 groups are shown in table S2. The mean square errors (MSE) of training loss, validation loss and test loss determine the accuracy of a network, and in general, network performs better with lower losses, but it is vital that the training loss must not be too small compared to the validation loss, otherwise it means an overfitting result. Meanwhile, a smaller validation loss may be more significant than a smaller training loss. We comparethe results from group 5 and 6 which have the smallest validation loss and training loss, respectively. After comparing large amount of test data, network structure of group 5 shows better performance with higher accuracy, thus 320 nodes in 4 hidden layers with a batch size of 10 data points is chosen for the forward network. Hyperparameters of inverse network and tandem network is chosen by the same procedure and the best group is marked in **Table S3 and S4**.

Table S2. Representative training results for forward network.

Num	**Nodes**	**Batch**	**Training loss**	**Validation loss**	**Test loss**
①	250	25	1.02×10^{-6}	1.47×10^{-5}	1.94×10^{-5}
②	250	20	9.31×10^{-7}	1.38×10^{-5}	1.61×10^{-5}
③	250	15	8.36×10^{-7}	1.28×10^{-5}	1.50×10^{-5}
	…	…	…	…	…
④	300	10	7.1×10^{-7}	1.15×10^{-5}	1.31×10^{-5}
⑤	320	10	7.05×10^{-7}	1.03×10^{-5}	1.36×10^{-5}
⑥	350	10	6.81×10^{-7}	1.07×10^{-5}	1.36×10^{-5}
⑦	330	10	7.27×10^{-7}	1.21×10^{-5}	1.62×10^{-5}
	…	…	…	…	…

Table S3. Representative training results for inverse network.

Num	**Nodes**	**Batch**	**Training loss**	**Validation loss**	**Test loss**
①	250	20	0.021	0.036	0.036
②	275	20	0.021	0.034	0.036

③	300	20	0.019	0.034	0.036
	…	…	…	…	…
④	300	15	0.020	0.037	0.036
⑤	300	12	0.019	0.036	0.035
⑥	300	10	0.022	0.039	0.038
⑦	350	10	0.022	0.041	0.039
	…	…	…	…	…

Table S4. Representative training results for tandem network.

Num	nodes	batch	Training loss	Validation loss	Test loss
①	300	15	2.28×10^{-5}	5.10×10^{-5}	4.62×10^{-5}
②	250	15	2.07×10^{-5}	3.96×10^{-5}	5.5×10^{-5}
③	250	12	2.07×10^{-5}	3.93×10^{-5}	4.68×10^{-5}
	…	…	…	…	…
④	300	12	1.91×10^{-5}	3.88×10^{-5}	4.32×10^{-5}
⑤	300	10	2.27×10^{-5}	4.55×10^{-5}	4.83×10^{-5}
⑥	280	10	2.17×10^{-5}	5.3×10^{-5}	4.92×10^{-5}
⑦	320	10	2.52×10^{-5}	5.41×10^{-5}	5.43×10^{-5}
	…	…	…	…	…

5. The accuracy test for inverse designed color values as shown in Figure 5e.

Group		**x**	**y**	**Y**
1	Target	0.15707	0.089949	0.031531
	Designed	0.15615	0.091648	0.031434
	Relative error	0.59%	1.89%	0.31%
2	Target	0.14996	0.18166	0.078814
	Designed	0.14933	0.1819	0.081161
	Relative error	0.42%	0.13%	2.98%
3	Target	0.19537	0.55537	0.30709
	Designed	0.19728	0.55453	0.30855
	Relative error	0.98%	0.15%	0.48%
4	Target	0.43943	0.45744	0.40521
	Designed	0.44036	0.45679	0.3988
	Relative error	0.21%	0.14%	1.58%
5	Target	0.3627	0.5436	0.3678
	Designed	0.36231	0.54267	0.36477
	Relative error	0.11%	0.17%	0.82%

6	Target	0.5253	0.3847	0.1724
	Designed	0.51558	0.38925	0.17032
	Relative error	1.85%	1.18%	1.21%
7	Target	0.2452	0.1637	0.1355
	Designed	0.24857	0.16815	0.1379
	Relative error	1.37%	2.72%	1.77%
8	Target	0.3272	0.3243	0.2366
	Designed	0.33242	0.31747	0.23513
	Relative error	1.60%	2.11%	0.62%

Reference

[1] CIE (1932). Commission internationale de l'Eclairage proceedings, 1931. Cambridge: Cambridge University Press.