Supporting information for "Genetic-algorithm-aided meta-atom multiplication for improved absorption and colouration in nanophotonics"

Changxu Liu,[1,2], Stefan A. Maier[2,3*], Guixin Li[1,4*]

[1]Department of Materials Science and Engineering,
Southern University of Science and Technology, Shenzhen 518055, China
[2]Chair in Hybrid Nanosystems, Nanoinstitute Munich, Faculty of Physics,
Ludwig Maximilian University of Munich, 80539 Munich, Germany
[3] Department of Physics, Imperial College London, London SW7 2AZ, United Kingdom
[4]Shenzhen Institute for Quantum Science and Engineering,
Southern University of Science and Technology, Shenzhen 518055, China

*To whom correspondence should be addressed:
ligx@sustc.edu.cn, stefan.maier@physik.uni-muenchen.de

number of pages: 11

number of figures: 4

number of tables: 13

1 Details of the simulations and genetic algorithm

All simulations are based on FDTD method by a commercialised software (LUMERICAL, FDTD Solution). The refractive index of Au is based on the data from ref (*1*) while the refractive index of dielectric (SiO_2) layer is selected as 1.45. A linear polarised light source is applied at the normal incidence. The direction of the polarisation is along x, as demonstrated in Fig.2b in the main text. A periodic boundary condition is applied along both x and y axes.

Genetic algorithm (GA) is a bio-inspired meta-heuristic optimisation technique. For the fitness function $F(\mu)$ parameterised by a real-number vector μ , the GA is able to seek the optimised such that the function is minimised. For the absorption, the fitness function is defined as $F(\mu) = 1 - \bar{A}$, with $\bar{A}$ the averaged absorption between 350nm and 800nm. For the colouration, the fitness function is defined as $F(\mu) = \Delta$, with Δ the distance between the aimed colour and generated colour in the CIE diagram. The population size P is 20 for unit cells with single meta-atom and 200 for extended unit cells with four meta-atoms, considering the different number of parameters in the two situations (4 vs 15). Individuals with the best values of fitness function in the current generation are guaranteed to survive to the next generation. These individuals are called elite children. The value of elite count is selected as 5% of the population size. The fraction of individuals in the next generation, other than elite children, are created by crossover. The crossover fraction is set to 0.8. All the parameter is discretised. And no mutation is implemented for this integer problem. The minimum step of the dielectric thickness t, the height of the disk H and the period of the unit cell T is 10nm while for rest parameters is 2.5nm. The thickness t ranges from 0nm to 100nm. The height H of the disk ranges from 10nm to 300nm. The period T varies from 80(160) nm to 400(800) nm for unmultiplied (multiplied) cases. The diameter of the disk ranges from 10% to 80% of the period T for unmultiplied cases and 5% to 40% of the period T for multiplied cases. A position constrain is made so that the overlap distance between nanodisks is within 15 nm, by adding constrain functions to GA (ref. 43 in the manuscript).

All simulations were run on a Dell workstation Precision Tower 7740 with Intel Xeon Bronze 3104 1,7 GHz, 6 Kerne/6 Threads. For absorption optimisation, 25 generations were implemented. For colouration optimisation, 20 generations were implemented. The time consumption is summarised in Table S1 and S2 for absorption and structural colours, respectively. The values listed are averaged ones.

Table S1: Computational time for absorption optimisation.

	Time consumption for one simulation (s)	Time consumption for one generation (min)	Total time consumption (min)
without multiplication	30	10	260
with multiplication	120	400	10400

Table S2: Computational time for structural colour optimsiation.

	Time consumption for one simulation (s)	Time consumption for one generation (min)	Total time consumption (min)
without multiplication	30	10	210
with multiplication	120	400	8400

In the unit cell with single meta-atom, 4 discretised variables were parameterised, providing the number of available configurations of $3 \cdot 10^5$. The number of single simulations through GA optimisation was on the order of 10^{-3} of a complete sweep. In the unit cell with four meta-atoms, 15 discretised variables were parameterised, providing the number of available configuration of $8.27 \cdot 10^{27}$. The number of single simulations through GA optimisation was on the order of 10^{-13} of a complete sweep. Despite the improvement of computation efficiency of GA compared with a parametric sweep, the global minimum is not guaranteed. Replacing GA with advanced AI algorithm may further improve the efficiency and increase the possibility to reach the global minimum.

Here, we implement colour optimisation using another algorithm, the particle swarm (PS) (*2*). The target colour is selected as green. The population size, number of generations and the range of parameters are identical to the ones used in GA. The inertia range is selected between 0.1 and 1.1. The minimum neighbour fraction is selected as 0.25. The self adjustment weight and social adjustment weight are selected as 1.49. Figure S1 provides a comparison between GA and PS algorithms. Figure S1a demonstrates the relationship between the generations and distance to target colour in CIE diagram (Δ). In this specific case, PS shows a slight better optimisation ability. But the optimised results are comparable, as verified by the reflection spectrum (R) and colour generated shown in Fig. S1b and Fig. S1c respectively. The optimised geometric parameters from PS can be found in Table S3. The comsuption of computational time is shown in Table S4. The time used for PS is the same compared to GA, since the time used for the algorithms is much less than the one used for solving the Maxwell equations based on the FDTD method. Systemic Comparisons between GA and some conventional optimisation algorithm can be found in ref (*3–6*).

Table S3: Parameters of extended unit cell for green colour generation from PS.

Generation	T(nm)	H(nm)	t(nm)	D_1(nm)	D_2(nm)	D_3(nm)	D_4(nm)	x_1(nm)	x_2(nm)	x_3(nm)	x_4(nm)	y_1(nm)	y_2(nm)	y_3(nm)	y_4(nm)
20	370	300	80	150	90	20	40	27.5	-65	-140	112.5	45	100	-140	-37.5

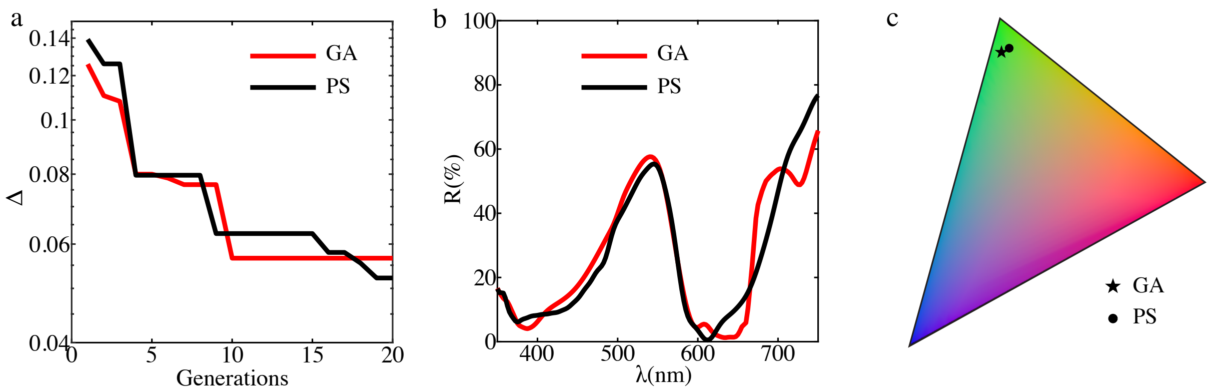

Fig. S1: A comparison between GA and PS algorithms. (a) The distance Δ between the target colour and the structural colour generated in the CIE diagram as a function of generations. (b) A comparison of optimised reflection spectra between GA and PS algorithms. (c) The generated colours in the CIE diagram, circle for PS and pentagram for GA.

Table S4: Computational time for green colour by PS algorithm.

	Time consumption for one simulation (s)	Time consumption for one generation (min)	Total time consumption (min)
with multiplication	120	400	8400

2 Geometric parameters for the structures shown in the main text

2.1 Unit cell with single meta-atom

The period of the unit cell (T), the height (H) and the diameter (D) of metal disk, the thickness (t) of the dielectric layer are parameters for an unextended unit cell.

The geometric parameters for broadband absorption are demonstrated in Table S5, while The geometric parameters for green colour are demonstrated in Table S6.

Table S5: Parameters of unextended unit cell for absorption.

Generation	T(nm)	H(nm)	D(nm)	t(nm)
0	200	100	100	30
3	120	55	80	10
10	100	55	70	10
25	100	60	70	10

Table S6: Parameters of unextended unit cell for green colour generation.

Generation	T(nm)	H(nm)	D(nm)	t(nm)
20	310	40	260	140

2.2 Extended unit cell with multiple meta-atoms

While definitions of T, H and t are the same for the unextended case, there are more parameters for the extended unit cell. D_i is the diameter of the disk and (x_i, y_i) is the position of the disk with $i = 1, 2, 3, 4$. The origin is at the centre of the unit cell.

The geometric parameters for broadband absorption are demonstrated in Table S7, while the geometric parameters for green colour are demonstrated in Table S8.

Table S7: Parameters of extended unit cell for absorption.

Generation	T(nm)	H(nm)	t(nm)	D_1(nm)	D_2(nm)	D_3(nm)	D_4(nm)	x_1(nm)	x_2(nm)	x_3(nm)	x_4(nm)	y_1(nm)	y_2(nm)	y_3(nm)	y_4(nm)
0	300	100	20	80	80	80	80	75	-75	-75	75	75	75	-75	-75
5	460	75	30	140	140	20	160	57.5	-80	-172.5	127.5	70	102.5	-57.5	-137.5
10	280	80	10	110	70	60	80	50	-85	-20	105	55	20	-27.5	-50
25	260	80	10	45	70	50	70	50	-77.5	-20	97.5	57.5	20	-20	-40

Table S8: Parameters of extended unit cell for green colour generation.

Generation	T(nm)	H(nm)	t(nm)	D_1(nm)	D_2(nm)	D_3(nm)	D_4(nm)	x_1(nm)	x_2(nm)	x_3(nm)	x_4(nm)	y_1(nm)	y_2(nm)	y_3(nm)	y_4(nm)
20	540	80	30	120	90	160	120	202.5	-202.5	-80	40	107.5	162.5	-107.5	-107.5

3 More details of the structural colour generation

Fig. S2 summarises the unit-cell design for a blue colour generation. Fig. S2a demonstrates the optimisation process. The extension of the unit cell leads to the enhanced absorption around 650nm, as shown in Fig. S2b. As a result, the colour generated from extended cell is closer to the desired colour (blue), as illustrated in both Fig. S2c and d.

Fig. S3 summarises the unit-cell design for a red colour generation. Due to the intrinsic optical properties of gold, it is feasible for both unextended and extended unit cell to produce standard red colour in sRGB (Fig. S3c and d.), in spite of the spectral difference shown in Fig.S3b. However, the colour generated from the unit cell with multiple meta-atoms is closer to the target colour, as verified by the value of Δ in Fig. S3a.

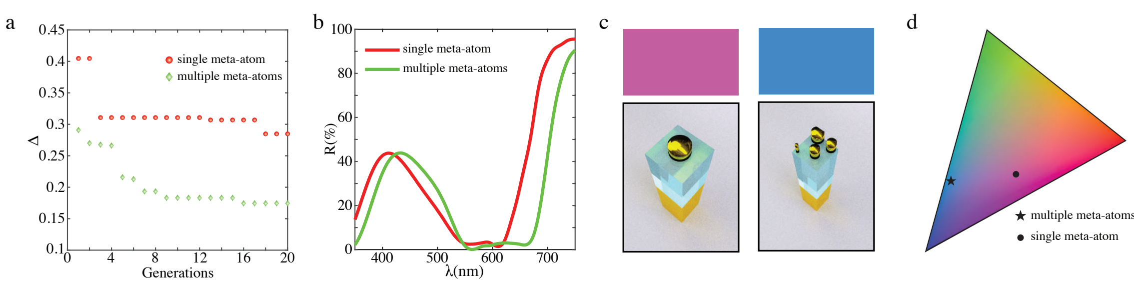

Fig. S2: GA based optimisation for the structural colour generation. The aim is the blue colour of sRGB. (a) The distance Δ between the target colour and the structural colour generated in the CIE diagram as a function of the number of generations. Green diamond represents the unextended unit cell while red circle represents the unit cell after meta-atom multiplication. (b) A comparison of reflection spectrum between the best samples of the unit cell with single meta-atom (green) and the unit cell with multiple meta-atoms (red). (c) A comparison of generated colours and corresponding configurations. Left column is for the unextended unit cell while right column is for the unextended unit cell. (d)The generated colours in the CIE diagram, circle for unextended case and pentagram for extended case.

For the red colour generation with meta-atom multiplication, the GA optimiser provides a configuration without a dielectric layer, which may introduce fabrication difficulties. By virtue of the enlarged parameter space, a configuration with dielectric layer can be readily found, as shown in Fig.S4a. Simultaneously, a better red colour is obtained, going beyond the red colour sRGB (Fig.S4c). The enhanced absorption around green (500nm) is the reason for the improved red colour.

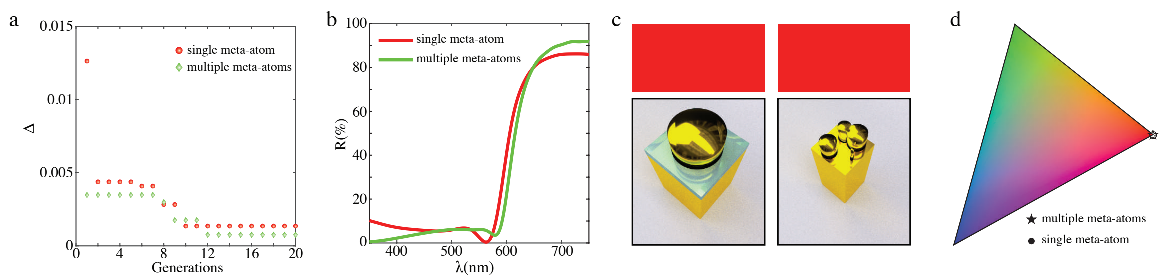

Fig. S3: GA based optimisation for the structural colour generation. The aim is the blue colour of sRGB. (a) The distance Δ between the target colour and the structural colour generated in the CIE diagram as a function of the number of generations. Green diamond represents the unextended unit cell while red circle represents the unit cell after meta-atom multiplication. (b) Reflection spectrum between the best samples of the unit cell with single meta-atom (green) and the unit cell with multiple meta-atoms (red). (c) A comparison of generated colours and corresponding configurations. Left column is for the unextended unit cell while right column is for the unextended unit cell. (d)The generated colours in the CIE diagram, circle for unextended case and pentagram for extended case.

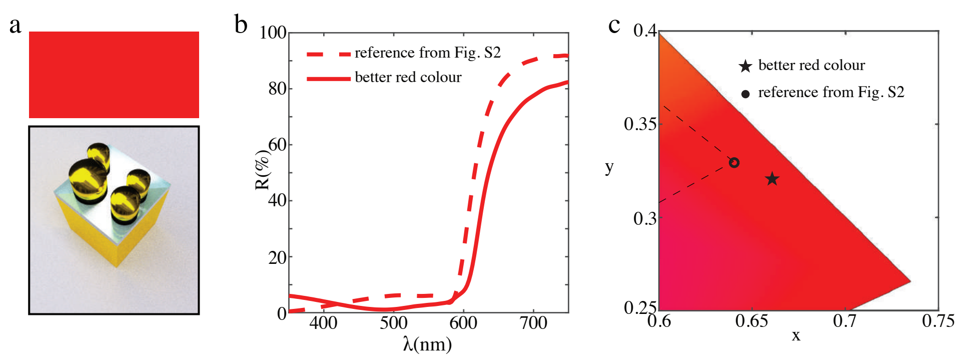

Fig. S4: A better configuration for red colour generation with extended until cell. (a) Generated colour (upper panel) and corresponding configurations (lower panel). (b) Reflection spectrum of the configuration in a). The dash line shows the spectrum of the configuration in Fig. S3 as a reference. (c)The generated colours in the CIE diagram, pentagram for the improved design in a) and circle for the configuration in Fig. S3.

The corresponding geometric parameters are demonstrated in Table S9-13.

Table S9: Parameters of unextended unit cell for blue colour generation.

Generation	T(nm)	H(nm)	D(nm)	t(nm)
20	150	35	67.5	250

Table S10: Parameters of unextended unit cell for red colour generation.

Generation	T(nm)	H(nm)	D(nm)	t(nm)
20	230	75	160	30

Table S11: Parameters of extended unit cell for blue colour generation.

Generation	T(nm)	H(nm)	t(nm)	D_1(nm)	D_2(nm)	D_3(nm)	D_4(nm)	x_1(nm)	x_2(nm)	x_3(nm)	x_4(nm)	y_1(nm)	y_2(nm)	y_3(nm)	y_4(nm)
20	100	35	260	30	40	10	30	32.5	-22.5	-37.5	10	35	37.5	-37.5	-12.5

Table S12: Parameters of extended unit cell for red colour generation.

Generation	T(nm)	H(nm)	t(nm)	D_1(nm)	D_2(nm)	D_3(nm)	D_4(nm)	x_1(nm)	x_2(nm)	x_3(nm)	x_4(nm)	y_1(nm)	y_2(nm)	y_3(nm)	y_4(nm)
20	140	55	0	60	40	50	10	25	-17.5	-17.5	50	35	27.5	-42.5	-17.5

Table S13: Parameters of extended unit cell for the purer red colour generation.

Generation	T(nm)	H(nm)	t(nm)	D_1(nm)	D_2(nm)	D_3(nm)	D_4(nm)	x_1(nm)	x_2(nm)	x_3(nm)	x_4(nm)	y_1(nm)	y_2(nm)	y_3(nm)	y_4(nm)
20	200	65	20	50	50	80	60	55	-60	-35	60	20	20	-40	-35

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