Supplementary material

Enhanced Circular Dichroism via Multilayer Weyl Semimetal Materials Structures Optimized with Runge-Kutta Algorithm

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1. 4′4 Transfer Matrix Method

In the case of incident circularly polarized waves, the propagation features of both handednesses can be readily calculated using the 4×4 TMM. Denoting the total matrix as **M**, the relationship between the fields before and after the MS can be expressed as [1, 2]:

$$\begin{pmatrix} E_+^i \\ E_+^r \\ E_-^i \\ E_-^r \end{pmatrix} = \mathbf{M} \begin{pmatrix} E_+^t \\ 0 \\ E_-^t \\ 0 \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} & 0 & 0 \\ M_{12} & M_{22} & 0 & 0 \\ 0 & 0 & M_{33} & M_{34} \\ 0 & 0 & M_{43} & M_{44} \end{pmatrix} \begin{pmatrix} E_+^t \\ 0 \\ E_-^t \\ 0 \end{pmatrix}, \tag{S1}$$

where the subscripts + and - represent LCP and RCP waves, respectively, while *i*, *r*, and *t* denote the incident, reflected, and transmitted components. For an MS with a total of *J* dielectric layers as shown in Eq.(2), the matrix **M** can be expressed as the product of the dynamical matrix **D**, which is related to the boundaries of the MS, and the characteristic matrices **S** of the dielectric layers [2]:

$$\mathbf{M} = \mathbf{D}_0^{-1} \left(\prod_{j=1}^{J} \mathbf{S}_j \right) \mathbf{D}_{J+1}. \tag{S2}$$

Here,

$$\mathbf{D}_j = \begin{pmatrix} 1 & 1 & 0 & 0 \\ N_+^{(j)} & -N_+^{(j)} & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & N_-^{(j)} & -N_-^{(j)} \end{pmatrix}, \tag{S3}$$

$$\mathbf{S}_j = \begin{pmatrix} \cos\beta_+^{(j)} & \frac{i}{N_+^{(j)}}\sin\beta_+^{(j)} & 0 & 0 \\ iN_+^{(j)}\sin\beta_+^{(j)} & \cos\beta_+^{(j)} & 0 & 0 \\ 0 & 0 & \cos\beta_-^{(j)} & \frac{i}{N_-^{(j)}}\sin\beta_-^{(j)} \\ 0 & 0 & N_-^{(j)}\sin\beta_-^{(j)} & \cos\beta_-^{(j)} \end{pmatrix}. \tag{S4}$$

For a layer of WSM, $N_\pm^{(j)} = \sqrt{\varepsilon_d \, \mathrm{m}\varepsilon_a}$, while for an isotropic dielectric medium with a relative permittivity of ε_j, $N_\pm^{(j)} = \sqrt{\varepsilon_j}$. $\beta_\pm^{(j)} = (\omega/c) N_\pm^{(j)} d_j$, with d_j representing the thickness of each dielectric layer and *c* denoting the speed of EM waves in a vacuum [2]. From this, the transmission (*t*) and reflection (*r*) coefficients for each component can be calculated as follows [2]:

$$t_+ = \frac{1}{M_{11}}, \quad t_- = \frac{1}{M_{33}}, \quad r_+ = \frac{M_{21}}{M_{11}}, \quad r_- = \frac{M_{43}}{M_{33}}. \tag{S5}$$

Where M_{ij} (i, j = 1, 2, 3, 4) denotes the element in the *i*-th row and *j*-th column of the matrix **M**. The transmittance (*T*), reflectance (*R*), and absorptance (*A*):

$$T_\pm = |t_\pm|^2, \tag{S6}$$

$$R_{\pm} = \left| r_{\pm} \right|^2 , \tag{S7}$$

$$A_{\pm} = 1 - T_{\pm} - R_{\pm} . \tag{S8}$$

2. The Runge-Kutta Optimization Algorithm

Over a century ago, Runge and Kutta introduced the Runge-Kutta method (RKM) for solving ordinary differential equations [3]. More than a hundred years later, in 2021, researchers developed a new swarm-based model incorporating stochastic components, inspired by the principles of RKM, and named it RUN optimizer [3].

The optimization process can be broadly divided into the following steps: First, N_p positions are randomly generated within a population of size N_p, which is referred to as the initialization step.

For a minimization problem, $x_b = x_n - \Delta x$ is defined as the optimal solution obtained from a single iteration, while $x_w = x_n + \Delta x$ is defined as the worst solution. The initial values of x_b and x_w are generated from three randomly selected solutions in the population, denoted as x_{r1}, x_{r2}, and x_{r3}, where $r_1 \neq r_2 \neq r_3 \neq n$.

Based on the RKM, k_1 can be defined as $k_1 = (x_b - x_w)/2\Delta x$, where Δx represents the position increment. In the RUN algorithm, however, to enhance exploration and introduce stochastic behavior, k_1 is redefined as:

$$k_1 = \frac{1}{2\Delta x}\left(rand \times x_w - u \times x_b \right) , \tag{S9}$$

where

$$u = round\left(1 + rand\right) \times \left(1 - rand\right) , \tag{S10}$$

rand is any number between [0,1], and *round*(1+*rand*) indicates selecting either 1 or 2 as an integer. Similarly, other coefficients can be defined (for a fourth-order RKM, these are k_2, k_3, and k_4):

$$k_2 = \frac{1}{2\Delta x}\left(rand.\left(x_w + rand_1.k_1.\Delta x \right) - \left(u.x_b + rand_2.k_1.\Delta x \right) \right) , \tag{S11}$$

$$k_3 = \frac{1}{2\Delta x}\left(rand.\left(x_w + rand_1.\left(\frac{1}{2}k_2 \right).\Delta x \right) - \left(u.x_b + rand_2.\left(\frac{1}{2}k_2 \right).\Delta x \right) \right) , \tag{S12}$$

$$k_4 = \frac{1}{2\Delta x}\left(rand.\left(x_w + rand_1.k_3.\Delta x \right) - \left(u.x_b + rand_2.k_3.\Delta x \right) \right) . \tag{S13}$$

Here, $rand_1$ and $rand_2$ are two additional random numbers within the range [0, 1]. For the optimization function $f(x)$, the initial values of x_b and x_w for the next iteration are determined by comparing $f(x_n)$ with the optimal values of the three initial solutions, denoted as $f(x_{bi})$. In this work, $f(x)$ consists of bandwidths under different CD conditions (definitions detailed in Section 3 in the main text). Since the RUN algorithm is more suitable for minimizing values, the bandwidth obtained in the calculations needs to be further converted to its opposite number. The core search mechanism of the RUN algorithm, based on the fourth-order RKM, is given as follows:

$$SM = \frac{1}{6}\left(x_{RK} \right)\Delta x , \tag{S14}$$

and

$$x_{RK} = k_1 + 2\left(k_2 + k_3\right) + k_4 . \tag{S15}$$

The search mechanism obtained in this step is used to guide the optimization algorithm in determining the direction for global and local searches during iterations. In addition to this, the RUN algorithm incorporates a series of complex mechanisms designed to update and improve solution quality. These mechanisms primarily depend on the value of the current iteration's *rand* to choose whether to conduct a local search (exploitation) around x_c or x_m, while simultaneously exploring potentially promising regions in the global space (exploration). The specific steps are as follows:

if $rand < 0.5$ (S16)

(exploration phase)

$$x_{n+1} = \left(x_c + r \times SF \times g \times x_c\right) + SF \times SM + \mu \times x_s$$

else

(exploitation phase)

$$x_{n+1} = \left(x_m + r \times SF \times g \times x_m\right) + SF \times SM + \mu \times x_{s'}$$

end

in which

$$x_c = \varphi \times x_n + \left(1 - \varphi\right) \times x_{r1}, \tag{S17}$$

$$x_m = \varphi \times x_{best} + \left(1 - \varphi\right) \times x_{lbest}, \tag{S18}$$

$$x_s = randn.\left(x_m - x_c\right), \tag{S19}$$

$$x_{s'} = randn.\left(x_{r1} - x_{r2}\right), \tag{S20}$$

$$SF = 2.\left(0.5 - rand\right) \times f, \tag{S21}$$

$$f = a \times e^{-b \times rand \times \frac{i}{Maxi}}, \tag{S22}$$

$$\mu = 0.5 + 0.1 \times randn, \tag{S23}$$

φ represents a random number between (0,1), while *randn* denotes a value drawn from a standard normal distribution. x_{best} and x_{lbest} are used to indicate the best-so-far solution and the best solution of the current iteration, respectively. a and b are two constants. The variables i and $Maxi$ refer to the current iteration number and the set maximum number of iterations. r can be either 1 or -1, altering the search direction, and g is a random number within the range [0, 2].

To enable each solution to move towards a better position, the average of three random solutions (x_{avg}) is used in conjunction with the best solution (x_b) to generate a new solution (x_{new1}). Another new solution (x_{new2}) is generated using the following process:

if $rand < 0.5$ (S24)

if $w < 1$

$$x_{new2} = x_{new1} + r.w.\left|\left(x_{new1} - x_{avg}\right) + randn\right|$$

else

$$x_{new2} = \left(x_{new1} - x_{avg}\right) + r.w.\left|\left(u.x_{new1} - x_{avg}\right) + randn\right|$$

end

end

where

$$w = rand\left(0,2\right).e^{-c\frac{i}{Maxi}}, \tag{S25}$$

$$x_{avg} = \frac{x_{r1} + x_{r2} + x_{r3}}{3}, \tag{S26}$$

$$x_{new1} = \beta \times x_{avg} + \left(1-\beta\right) \times x_{best}, \tag{S27}$$

β is a random number selected from the interval [0,1], $c = 5 \times rand$, and r is randomly selected from the set {-1, 0, 1}.

However, the newly generated solution x_{new2} is not necessarily better than the existing solution x_n. Another new solution x_{new3} provides an additional opportunity to find a better position by:

if $rand < w$ (S28)

$$x_{new3} = \left(x_{new2} - rand.x_{new2}\right) + SF.\left[rand.x_{RK} + \left(v.x_b - x_{new2}\right)\right]$$

end

and $v = 2 \times rand$.

In summary, the pseudo-code for RUN is shown in Algorithm 1. For more details on the RUN process and a comprehensive explanation, please refer to Ref. [3].

Algorithm 1 The pseudo-code of the RUN algorithm

Input: N_p, $MaxIt$, D

Output: x_{best}

Stage 1. Initialization

Generate the RUN population X_n(n=1, 2..., N_p, including ε_j, d_j, and N)

Calculate the opposite number of the bandwidth (set as the objective function in this work) of each member of population

Determine the solutions x_w, x_b and x_{best}

Stage 2. RUN algorithm

while $it < MaxIt$ ***do***

for $i = 1 : N_p$ ***do***

if $rand < 0.5$ ***then***

exploration phase

else

exploitation phase

end if

Enhance the solution quality

if rand < 0.5 ***then***

Calculate position x_{new2} using Eq.(S24)

if f(x_{new2}) < $f(x_n)$ ***then***

Update x_n

else if $rand < w$ ***then***

Calculate position x_{new3} using Eq.(S28)

if $f(x_{new3}) < f(x_n)$ ***then***

Update x_n

end if

end if

end if

Update position x_w and x_b

end for

Update x_{best}

$it = it+1$

end while

Stage 3. return x_{best}

Reference

1 Š. Višňovský, K. Postava and T. Yamaguchi, *Czech J Phys*., 2001, **51**, 917–949.

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3 I. Ahmadianfar, A. A. Heidari, A. H. Gandomi, X. Chu and H. Chen, *Expert Syst. Appl.*, 2021, **181**, 115079.