Electronic Supplementary Material (ESI) for Energy & Environmental Science

Genetic Algorithm Implementation

In order to provide a control over the variables during the optimization, four energy constraints are considered as an input for the GA implementation:

Minimum and maximum band-gap energy ($E_{g,min}$, $E_{g,max}$)
Minimum and maximum ΔE_S ($\Delta E_{S,min}$,$\Delta E_{S,max}$)
Minimum and maximum ΔE_e ($\Delta E_{e,min}$, $\Delta E_{e,max}$)
Minimum and maximum energy solar spectrum limit ($E_{G,min}$, $E_{G,max}$)

where
ΔE_e is the difference between the emission peak and the band gap energy
ΔE_a is the difference between the absorption peak and the emission peak

$$\Delta E_S = \Delta E_e + \Delta E_a \qquad (1)$$

First genetic algorithm population

The first GA population is generated by dividing the band-gap energy domain by the number of runs per generation n, variable equivalent to the number of individuals in the population. Each run simulates a different luminescent material configuration in a parallel fashion. The band-gap energy for the individual *i* in the population *n* is given by:

$$E_{g,i} = E_{g,min} + \Delta E_{g,i} * (i-1)/n \qquad (2)$$

To be used during mutation, the increment in band-gap energy is calculated and memory allocated, for the first population this value remains constant for all the individuals:

$$\Delta E_{g,i} = (E_{g,max} - E_{g,min})/n \qquad (3)$$

The rest of the variables are uniformly sampled using a random number ξ between (0,1) and given by equations (4) to (7)

$$\Delta E_{S,i} = \Delta E_{S,min} + \left(\Delta E_{S,max} - \Delta E_{S,min}\right)\xi, \quad \text{if } E_{g,i} + \Delta E_{S,i} < E_{G,max} \qquad (4)$$

$$\Delta E_{e,i} = \Delta E_{e,min} + \left(\Delta E_{e,max} - \Delta E_{e,min}\right)\xi \qquad (5)$$

$$\Delta E_{a,i} = \Delta E_{S,i} - \Delta E_{e,i} \qquad (6)$$

$$\Delta E_{x,i} = \Delta E_{a,i}\xi \qquad (7)$$

$\Delta E_{x,i}$ is the difference between the cross over point and emission peak.

Crossover and K-S optimization parameters

Mainly during crossover, in order to avoid degeneracy between two coding variables (for example, in the worst situation, when the crossover is dealing with a band-gap greater than the energy point of the absorption peak), the energy difference between the emission peak and the band-gap energy is stored as an additional variable as well as the energy difference between the absorption peak and the crossover point. The original values of absorption peak, emission peak and cross-over energy for a new individual that help to construct the absorption and emission spectrum by using the K-S theory can differ with respect to their predecessors during a given crossover. However, the proportions with respect to the band-gap energy and the K-S relationship are conserved and transmitted to future generations. With this consideration in mind, two indirect parameters are calculated to complement the genes space search:

$$k_e = \Delta E_e / \Delta E_S \qquad (8)$$

$$k_x = \Delta E_x / \Delta E_a \qquad (9)$$

The number of variables of each predecessor that will be inherited by the new individual will be randomly selected from a multi-point crossover chain for an individual *i* as a function of the number of layers, *l*, is given by

$$(\Delta E_{S,i}, E_{g,i}, k_{e,i}, k_{x,i}, \Delta E_{e,i}, \Delta E_{x,i}, \Delta E_{a,i}, \; i = 1, l)$$

A Boltzmann selection procedure was adapted to sigma scaling selection during crossover:[1]

$$Expected\ value\ (i,t) = \left.\frac{e^{-\frac{f(i)}{T}}}{\sum_i e^{-\frac{f(i)}{T}}}\right|_t \qquad (10)$$

where the expected value of an individual *i* in a generation *t* is given by the fraction of the individual fitness function *f(i)*, the numerator contains the Boltzmann weighting term and the denominator is a normalization factor that counts for the total number of individuals in the population. *T* is the Boltzmann temperature. Initially *T* is relatively high and the system visits more phase space, allowing a slow rate of good selection and fewer fit individuals to reproduce, but as the parameter *T* decreases gradually, the selection pressure does not allow fewer fit individuals to reproduce; the Boltzmann selection has been demonstrated to be more effective than other selection techniques such as Russian roulette.[2] The parameters of each individual that belongs to each layer of the next generation will be composed by a random selection of two predecessors of the current generation and selected by applying equation (10).

Mutation

Uniform operators were applied during mutation. The number of variables to mutate at each calculation was chosen in a random manner operating over the next mutation chain:

$$(\Delta E_{g,i}, E_{g,i}, k_{e,i}, k_{x,i}, \; i = 1, l)$$

The genetic algorithm stops after a maximum number of generations (input value in the code) is reached or when the global maximum difference between two consecutive generations is less than or equal to a user defined value.

References

1 M., de la Maza. *The Boltzmann Selection Procedure*, L. Chambers, editor. Practical Handbook of Genetic Algorithms. New Frontiers, Volume II, CRC Press, 1995, 111-138.

2 J. Li and H. Tsukamoto, *J. of Thermal Science*, 2001, **10**, 4.