Optimization of UV LED design using evolutionary algorithms

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Motivation and objective

Motivation - nitride-based UV LED devices are used for:

- surface sterilization
- gas and disease detection
- water purification etc.

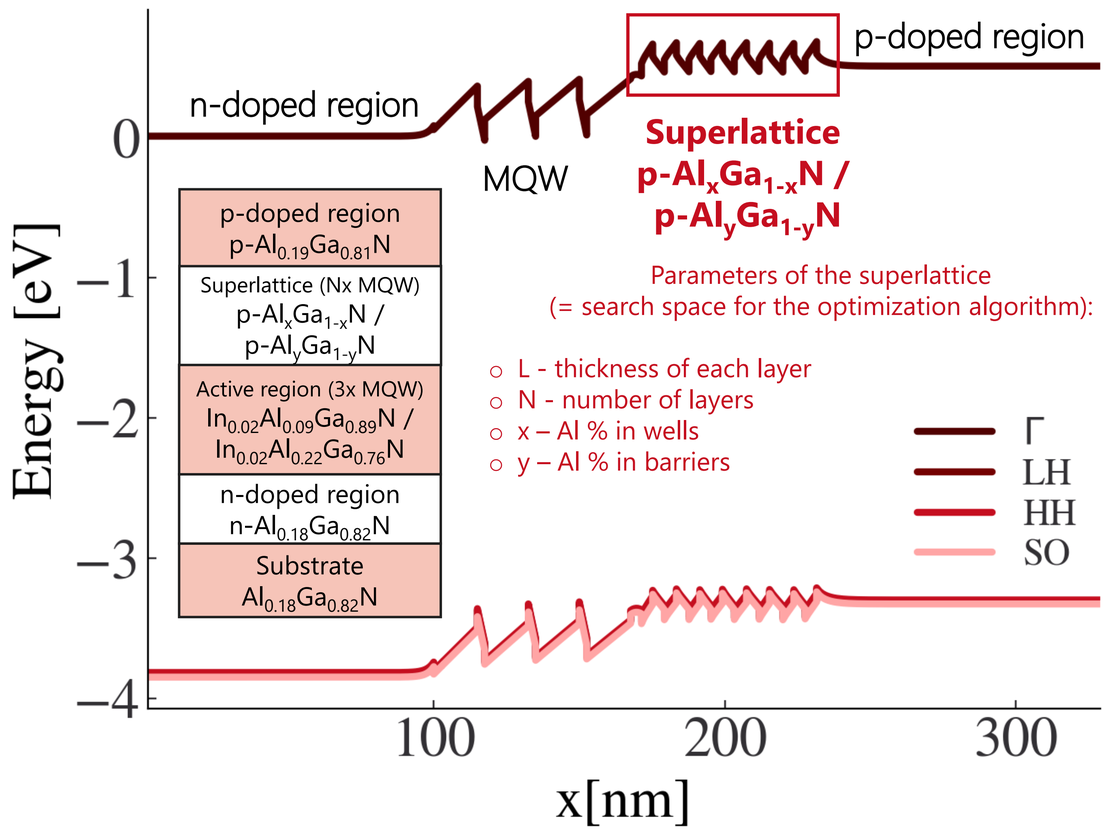
Objective - optimize the design of the device to enhance its performance and maximize its internal quantum efficiency.

Method - combine semiconductor calculation software **nextnano++** [1] with optimization algorithm based on **evolution strategies** [2].

[1] S. Birner *et al*, nextnano: General Purpose 3-D Simulations, IEEE Trans. Electron Dev. 54, 2137, 2007.

[2] H.G. Beyer and H.P. Schwefel, Evolution Strategies, Natural Computing 1: 3–52, 2002.

UV LED design



Simulation Software

|n⟩ nextnano++

- Poisson solver
- Quantum solver
- Self-consistent calculations
- Quantum optics
- Currents
- Strain considerations
- Effective mass approximation
- 8-band k.p model

$$-\nabla\varepsilon(\boldsymbol{x})\nabla\phi(\boldsymbol{x}) = \rho(\boldsymbol{x},\phi)$$

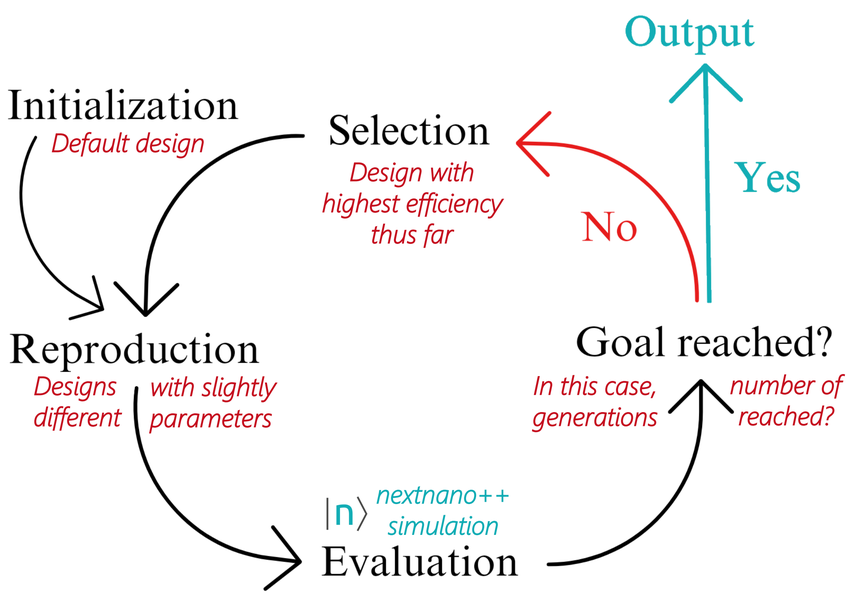
$$\left(\nabla\frac{1}{m^*(\boldsymbol{x})}\nabla + E_{\mathrm{c}}(\boldsymbol{x}) - \phi(\boldsymbol{x})\right)\Psi(\boldsymbol{x}) = E\Psi(\boldsymbol{x})$$

$$n(\boldsymbol{x}) = \sum_i |\Psi_i(\boldsymbol{x})|^2 f\left(\frac{E_i - E_{\mathrm{F}}(\boldsymbol{x})}{k_{\mathrm{B}}T}\right)$$

$$\boldsymbol{j}_n(\boldsymbol{x}) = \mu_n(\boldsymbol{x})n(\boldsymbol{x})\nabla E_{\mathrm{F}}(\boldsymbol{x})$$

Optimization algorithm

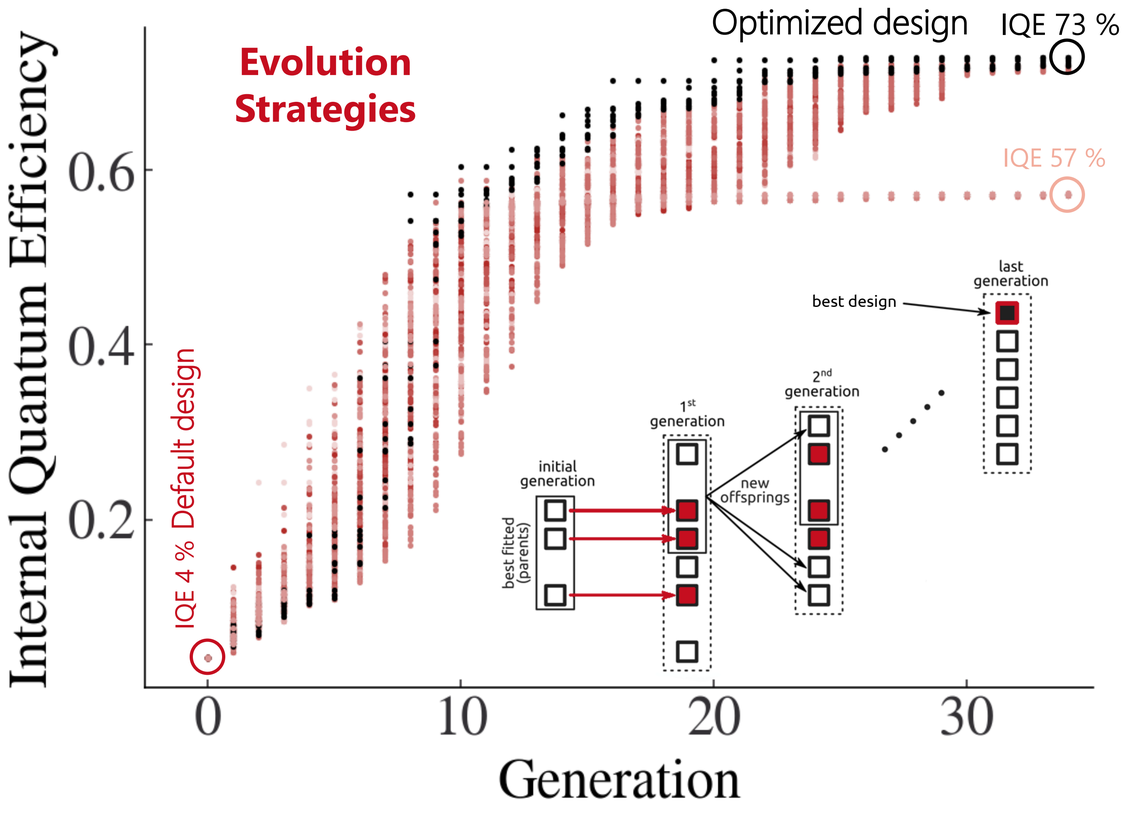
Evolution strategies employ biological processes such as selection and reproduction to find the best solutions to an optimization problem.



As in natural selection, the design of the UV LED is modified over and over through the generations to find the one that yields the highest performance.

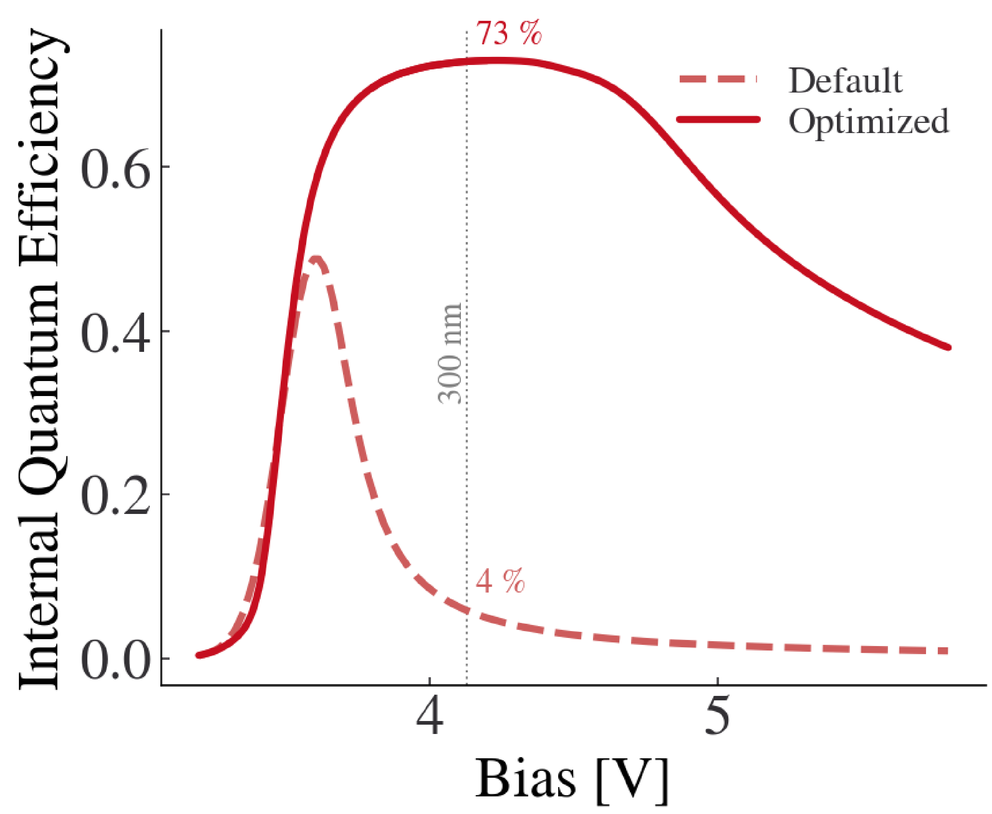
Optimization process

Multiple runs were performed all starting from the same default design. The different results illustrate the randomness of the optimization algorithm.



IQE improvement

The theoretical efficiency at the desired wavelength of 300 nm was improved by almost 70 % using the optimization algorithm.



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