Autonomous Mn-doped Perovskite Nanocrystals Synthesis by a Self-Driving Lab

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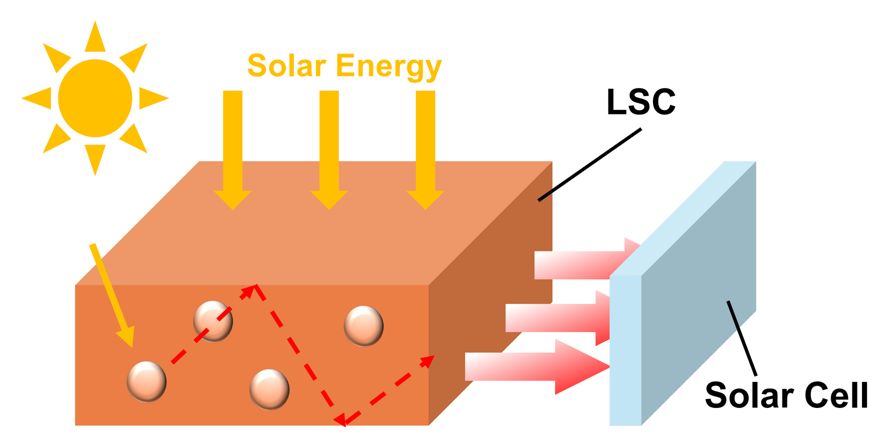
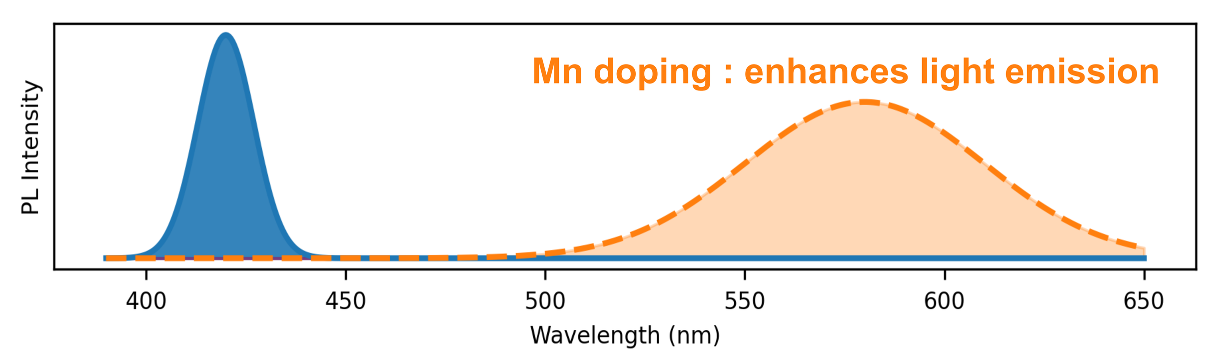
Luminescent Solar Concentrators

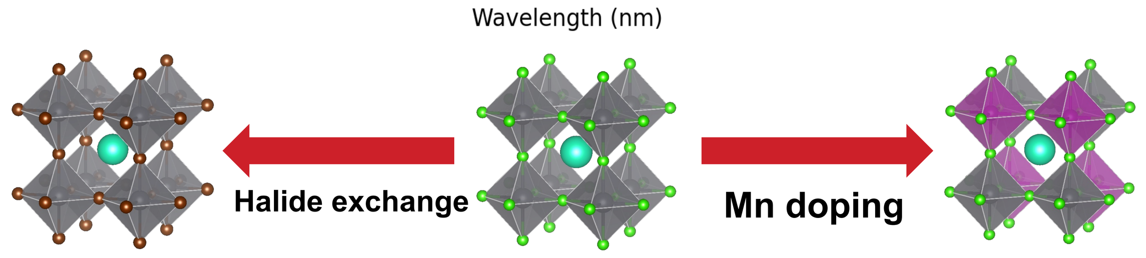
Luminescent Solar Concentrators (LSCs) are devices that **efficiently capture sunlight**. They are usually made from transparent plastic embedded with luminescent materials, such as **perovskites.**



Photoluminescence quantum yield (**PLQY**)= $\frac{\textit{Emitted Photons}}{\textit{Absorbed Photons}}$

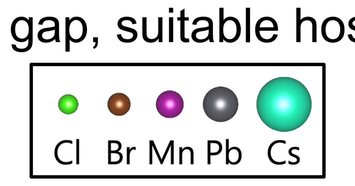
→ In this work, **absorption** and **emission peak area** were used to evaluate PLQY



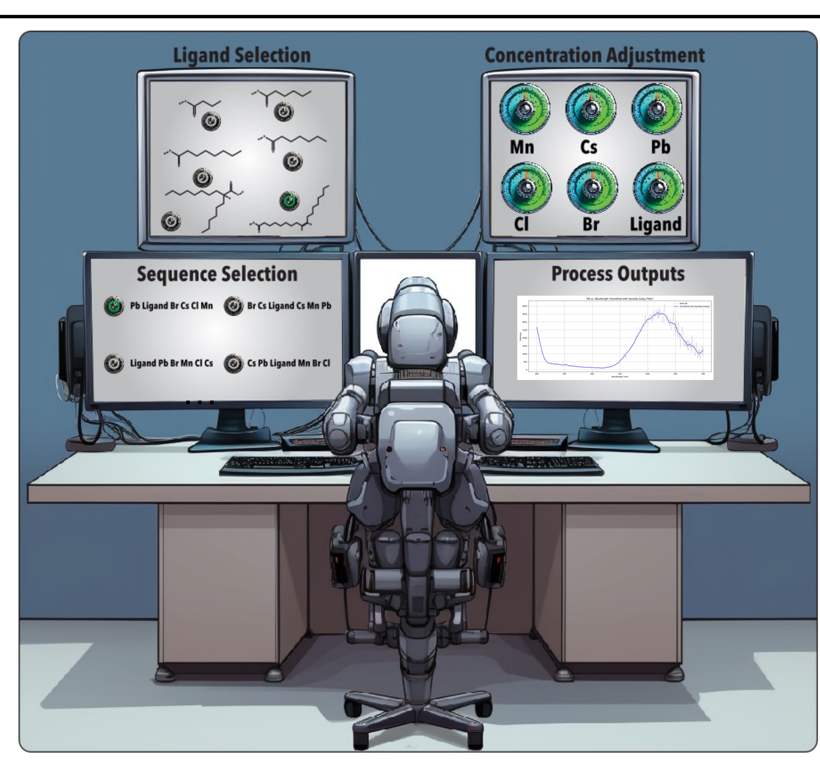


- Mn^{2+} : dual emission, easy to integrate into NCs
- Cl^- : effective Mn doping site, higher band gap, suitable host
- Br^- : suppress surface defects, stability

→ **How to maximize PLQY?**

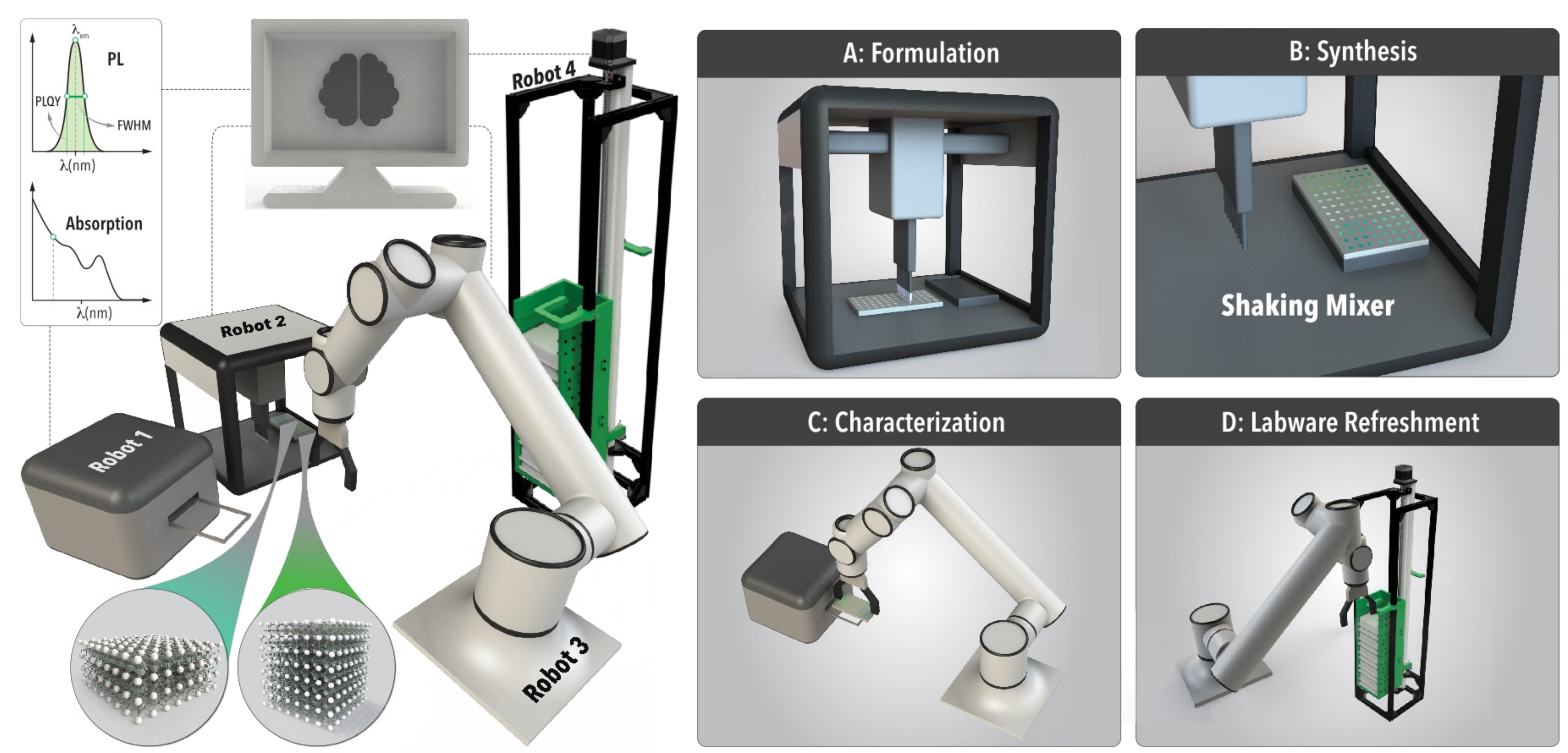


Vast Parameter Space



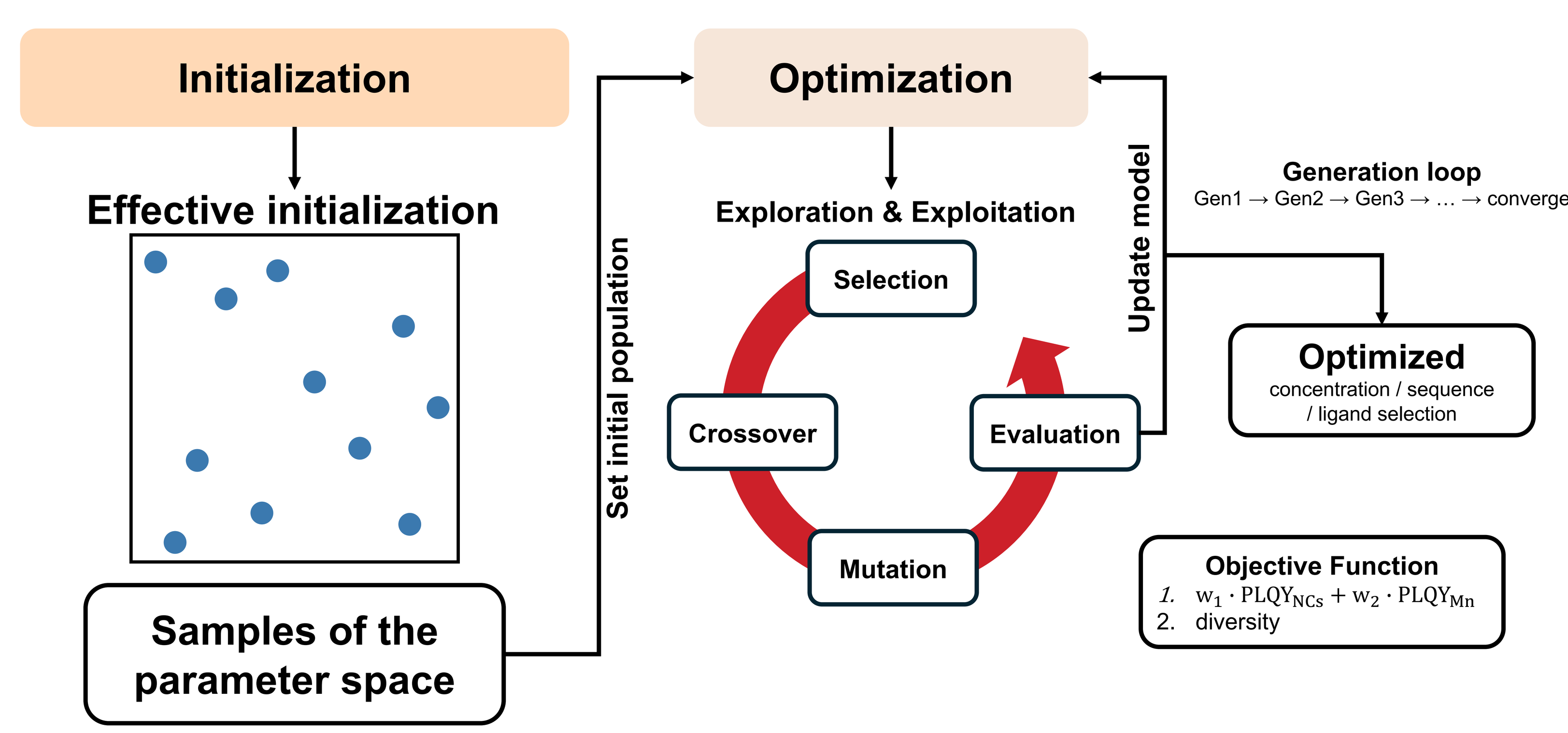
By independently adjusting a diverse set of parameters—including discrete variables (e.g., ligand type), continuous variables (e.g., precursor concentration), and sequential factors (e.g., injection order)—the system explores a **mixed-variable** and **high-dimensional parameter space**. Feedback from photoluminescence spectra guides the next decision, enabling efficient and interpretable optimization.

A Multi-Robotic Platform for Autonomous Experimentation



- End-to-end closed-loop experiments
- Perform 256 experiments per day, 850μL chemical consumption per reaction
- Reliable and reproducible synthesis of MHP nanocrystals
- Modular multi-robotic platform controlled by Python, facile to reconfigure for specific tasks
- Rapid exploration through vast chemical space and accelerated material discovery

AI-assisted decision making

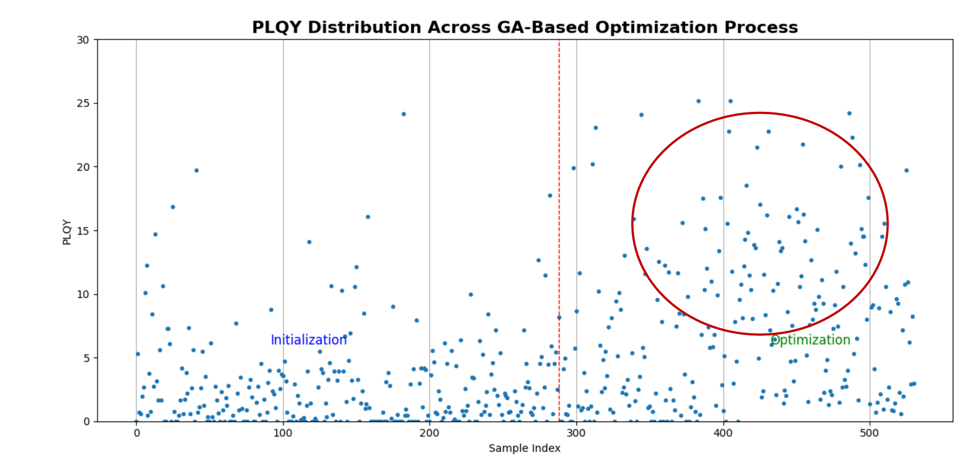


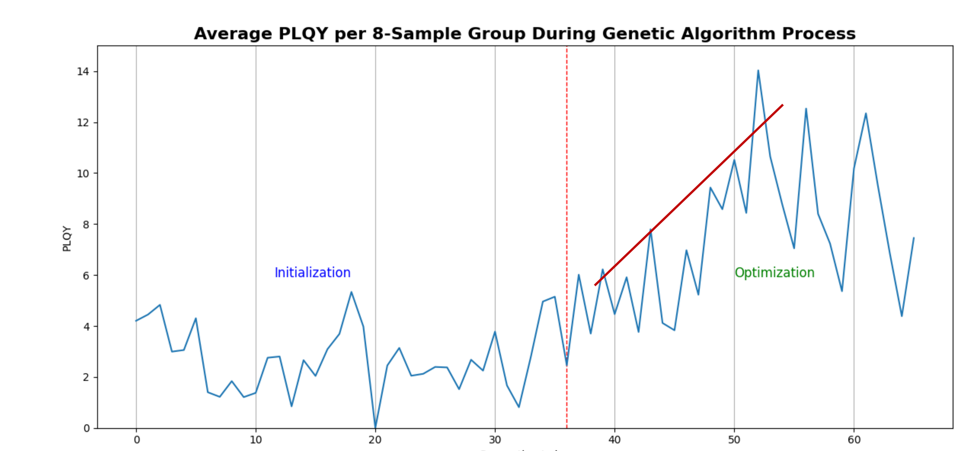
To optimize the synthesis of Mn-doped $CsPb(Cl/Br)_3$ nanocrystals, we employed a **Genetic Algorithm (GA)** for both the initialization and iterative refinement of synthesis conditions. GA was first used to broadly and evenly explore the parameter space, generating **diverse initial conditions** across precursor concentrations, injection sequences, and reaction times. These initial samples served as the starting population for GA, which iteratively refined them through selection, crossover, mutation, and evaluation.

The optimization process was guided by **maximizing PLQY** and the **spectral balance between Mn and $CsPb(Cl/Br)_3$ emission peaks**, ensuring not only high brightness but also dopant–host integration quality. This strategy enabled efficient convergence toward high-performing synthesis conditions with minimized experimental cost and maximized spectral performance.

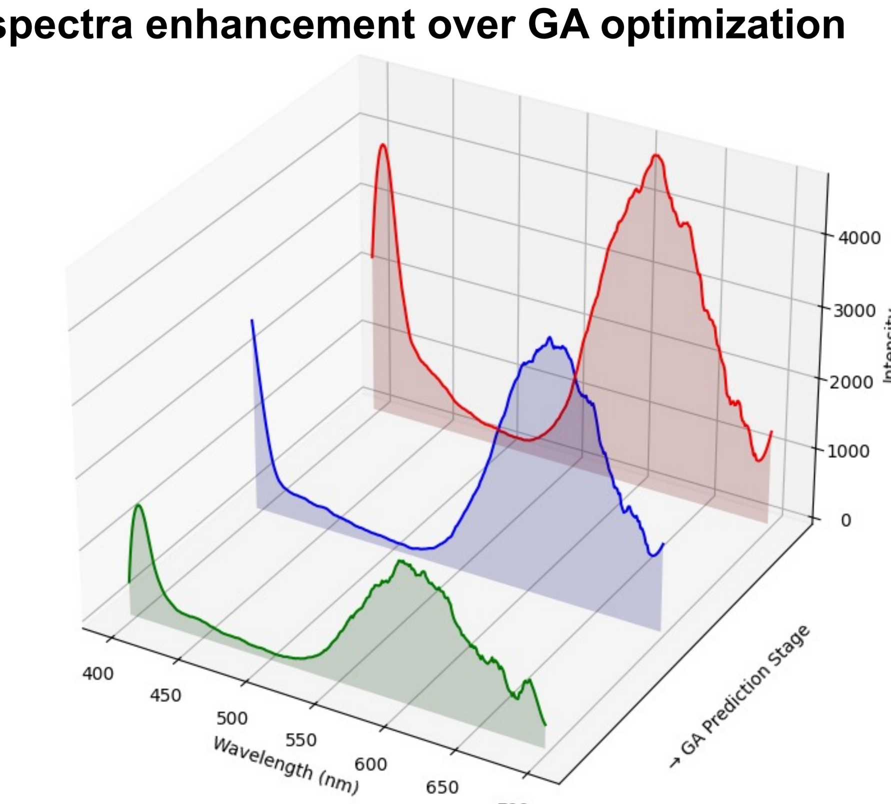
Results

PLQY enhancement over GA optimization





PL spectra enhancement over GA optimization



Conclusion / Future work

- Successfully demonstrated an autonomous approach for optimizing Mn-doped $CsPb(Cl/Br)_3$ nanocrystal synthesis.
- Achieved significant enhancement in PLQY and spectral intensity through GA-driven iterative refinement.
- Structural characterization (via TEM/EDS/EELS) of GA-evolved generations will be conducted to correlate optical improvement with doping distribution and halide composition evolution.