Real word examples of using Bayesian Optimization in Materials design and discovery

Lecture 20, Feb 24

Overview

- Bayesian optimization (BO) methods are relatively widely popular in terms of applications to materials design
- Mainly BO is used as a decision-maker to optimize a property/structure/synthesis process given a single or set of targets.
- On a side note, it is also fairly common to present a simple BO algorithm application to materials problems under fairly flashy acronyms 😂

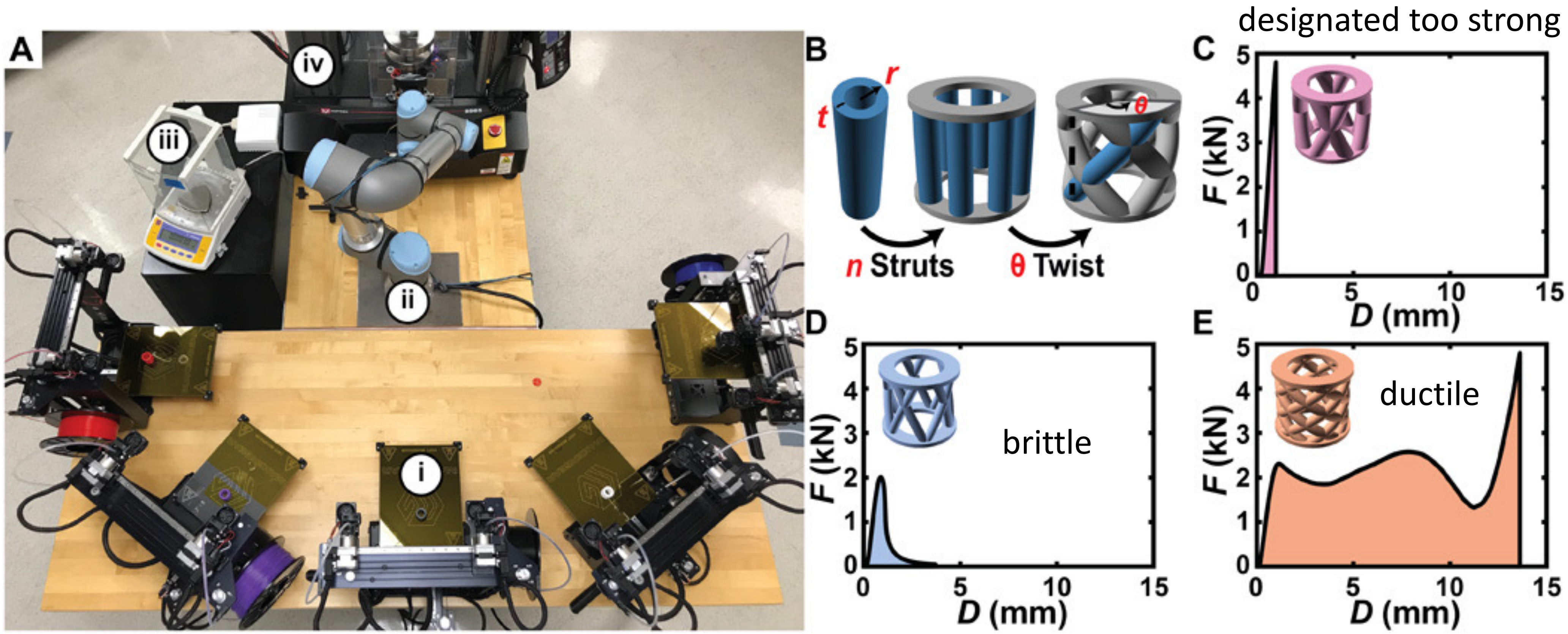
Bayesian experimental autonomous researcher (BEAR)

- Essentially uses BO in a high throughput experimental setting to optimize structures in additive manufacturing

- Optimizing the toughness of a 3D printed structure: requires maximizing a combination of two properties that tend to be inversely correlated, namely, strength and ductility

- Defined as the area under the force (F)–displacement (D) curve, toughness represents **how much energy a component can absorb before failure**, which makes it an important property to optimize in the context of design for safety and failure tolerance

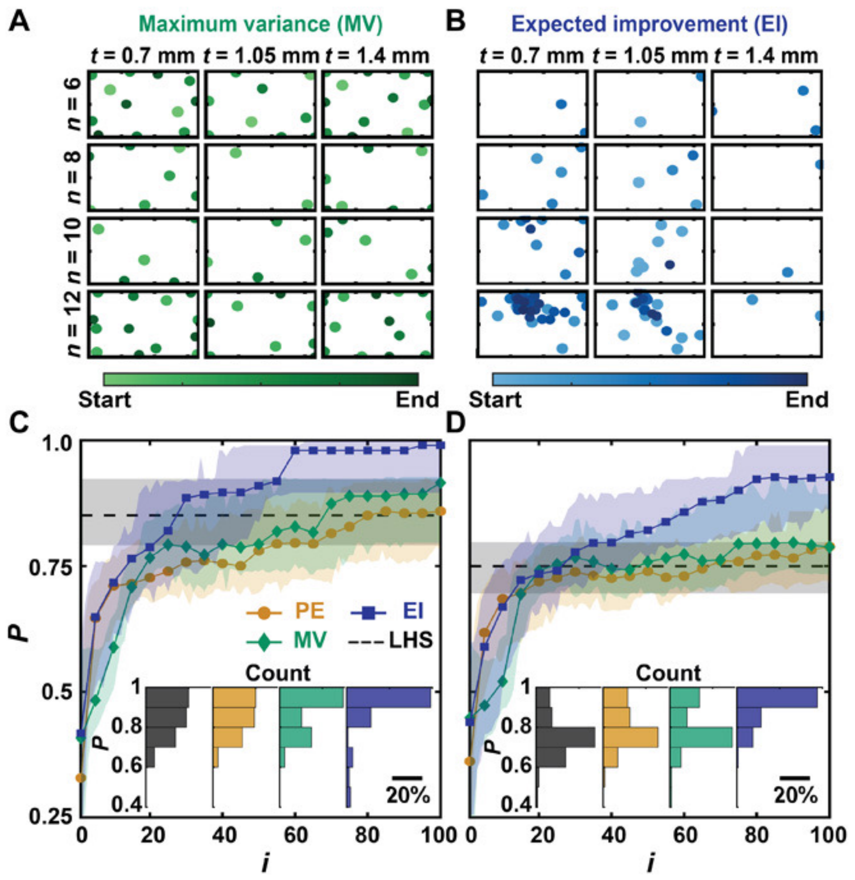
Bayesian experimental autonomous researcher (BEAR)



Design variables : n, θ, t, r

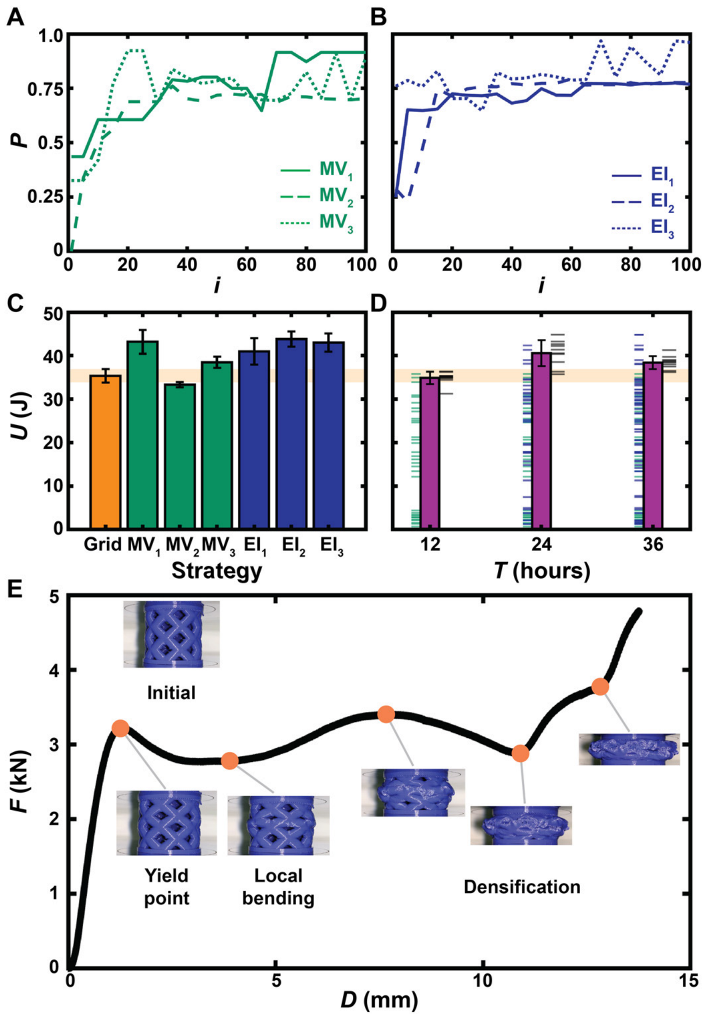
https://www.science.org/doi/10.1126/sciadv.aaz1708

Bayesian experimental autonomous researcher (BEAR)



- BO with pure exploitation (random choice after each iteration) and Maximum variance (based on a GP surrogate) compared with a Latin Hypercube Sampling (LHS)
- Performance $P(i) = U_{grid}(x_i)/\max(U_{grid})$.
- The output U values are simulated from a surrogate built from a grid design with $C)\ \sigma = 0.1, D)\ \sigma = 5$
- Fair to say that results from EI (or BO in general) dominate those coming from LHS or random search

Bayesian experimental autonomous researcher (BEAR)



- When combined with an experimental setup to run a BO guided experiment, the research found: in five instances—including all three based on the EI decision-making policy—100 well-chosen experiments were superior to 1800 experiments chosen on a grid.
- From a learning perspective, realizing a BEAR required advancing several facets including the development of modifications to standard EI algorithms and facile processes for performing BO in batch

Artificial Chemist/Robot Scientist

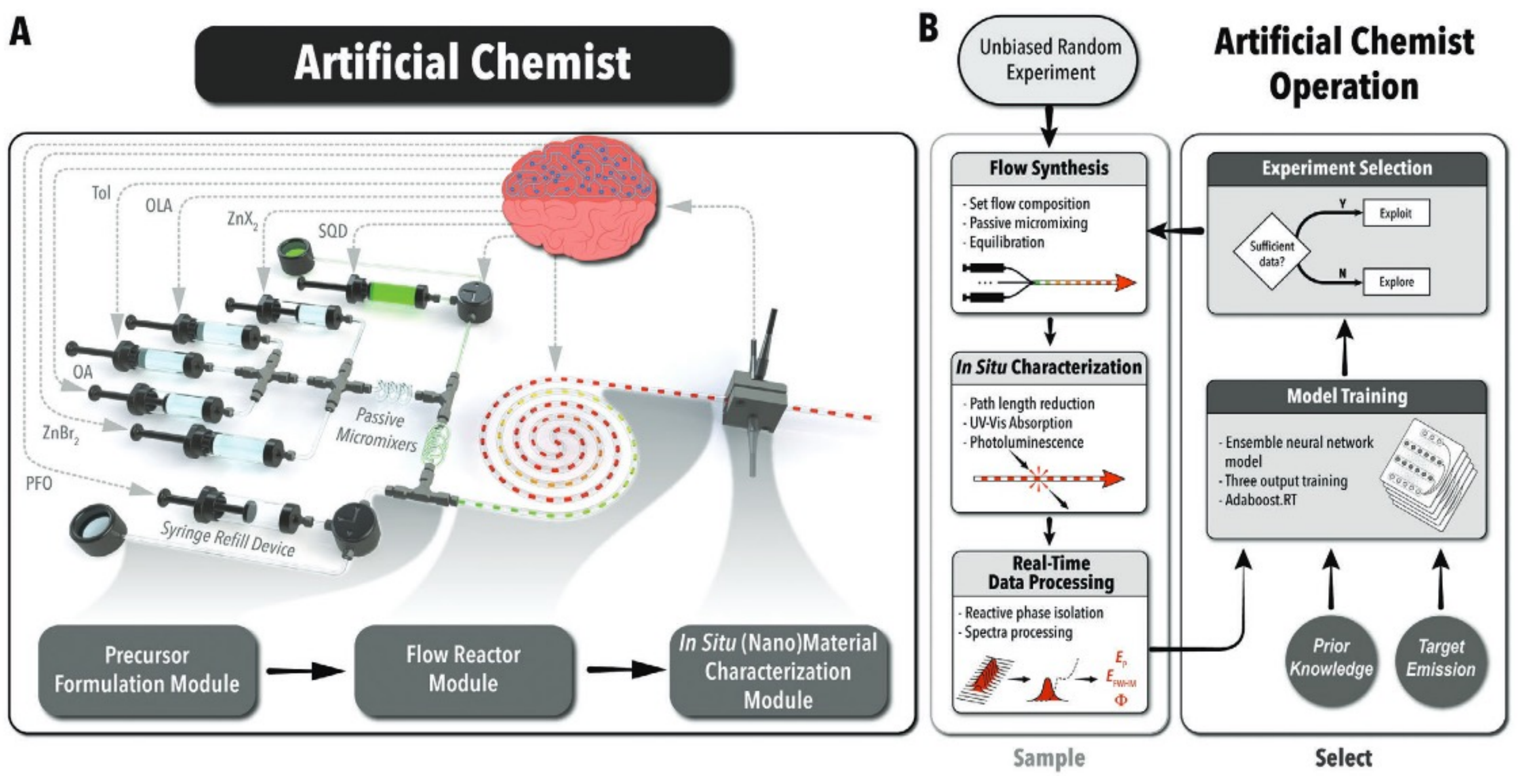


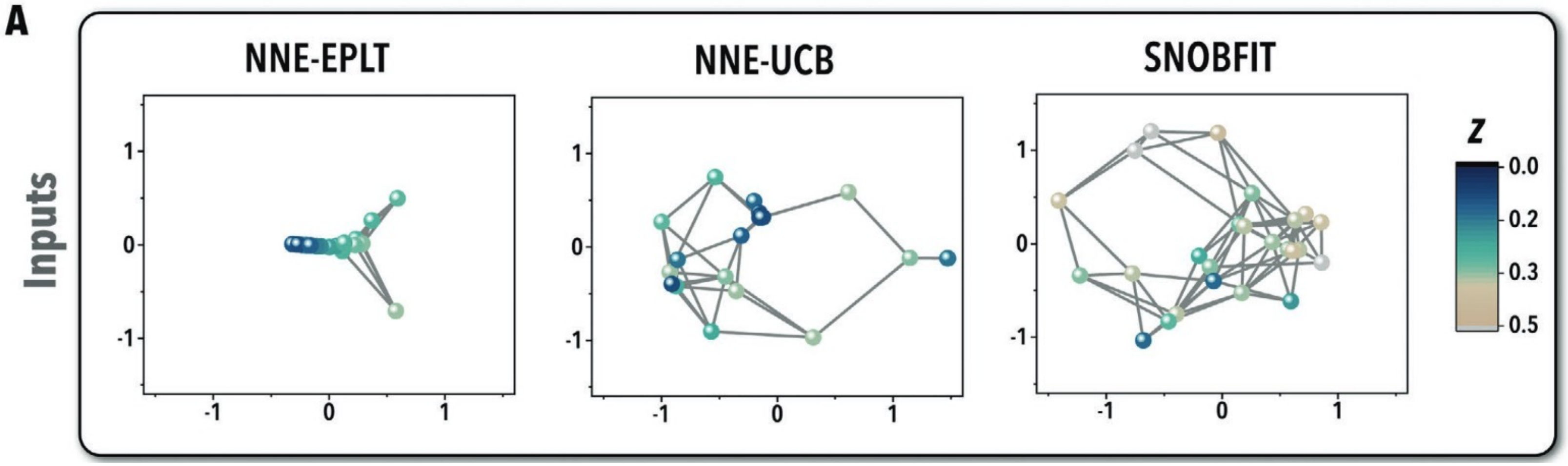
Figure 1. Design and operation of the Artificial Chemist. A) Schematic of the developed smart modular fluidic microprocessor for autonomous synthetic path discovery and optimization of colloidal QDs and B) the process flow diagram detailing its operation.

studied the bandgap tuning of metal halide perovskite QDs through halide exchange reactions using flow-synthesized cesium lead bromide (CsPbBr3) QDs as the starting quantum dots (SQDs)

https://doi.org/10.1002/adma.202001626

Artificial Chemist/Robot Scientist

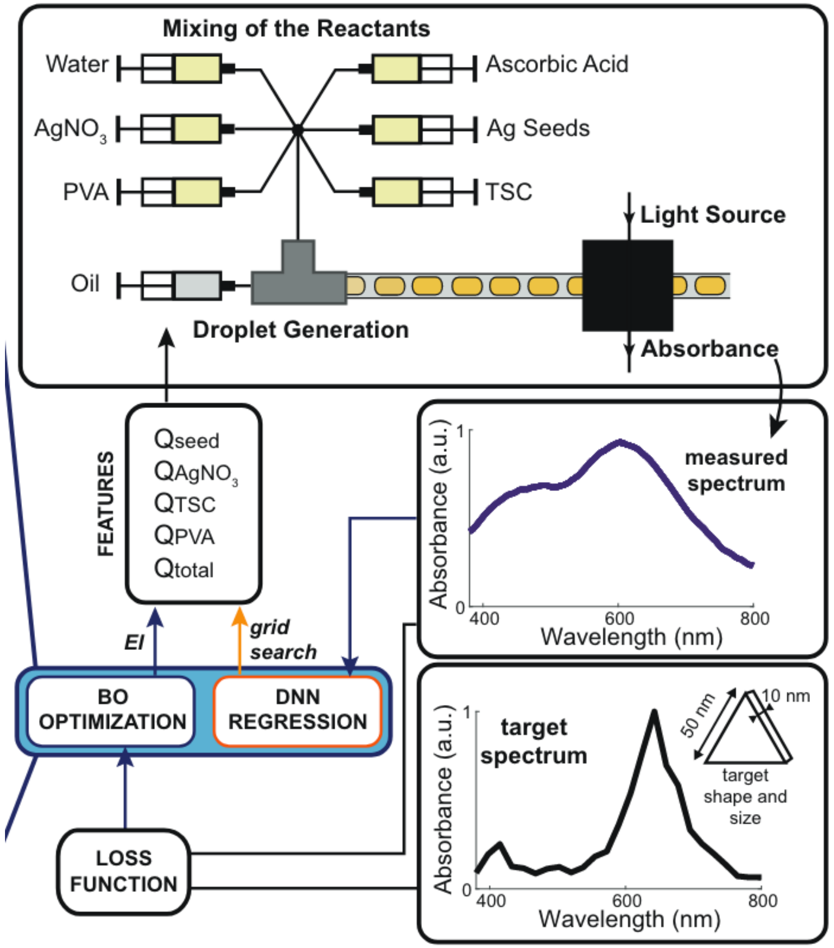
- Optimize for photoluminescence quantum yield (PLQY)-- a vital component in predicting the potential performance of as-synthesized QD samples in targeted optoelectronic device applications, such as solar cells and light emitting diodes.
- Many prior studies have applied Gaussian processes (GPs) to model these predictions and uncertainty estimates. However, it is difficult to impose complex structures on the GPs, which often simply encode continuity, smoothness, or periodicity.



This is an interesting way of showing whether your policy got the balance between exploration and exploitation right. The lower dimensional representations using **IsoMap** are used to look for the spread

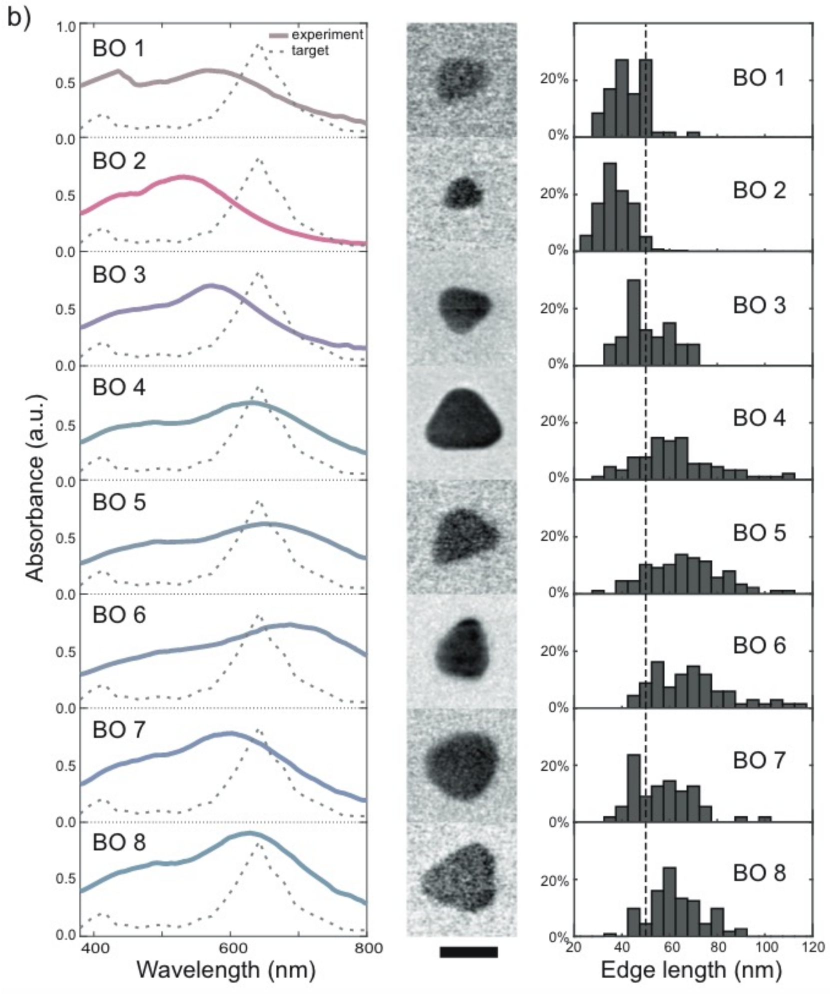
Material retrosynthesis

- algorithmic framework efficiently optimizes the nanomaterial synthesis to get the desired plasmon resonance
- You define a structural target and want the algorithm to provide you with the synthesis recipe that can make a particular morphology
- Directly optimizes for the plasmonic response shape of a nanoparticle to UV-Vis

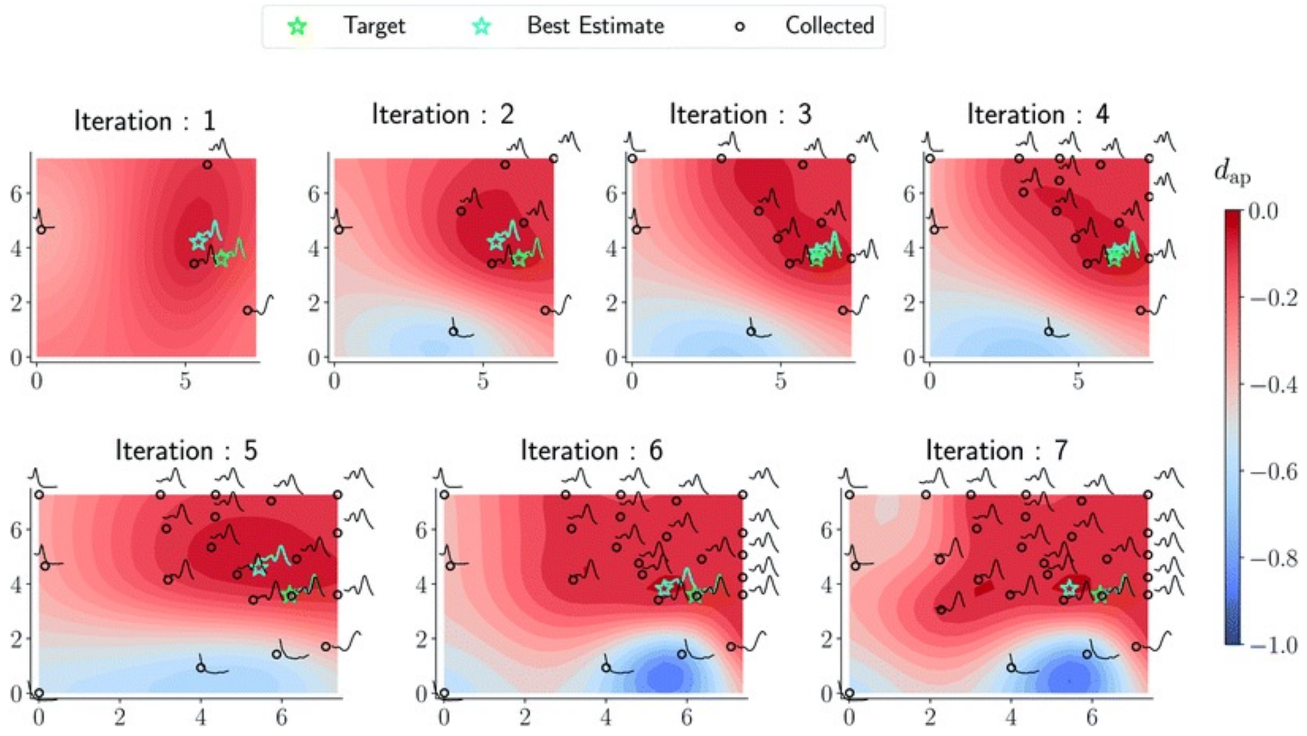


10.1038/s41524-021-00520-w

Material retrosynthesis



BO gradually synthesizes the target triangle-shaped nanoparticles



Using the right metrics for comparison between spectra, we can achieve optimization even when the sampled space is much more diverse. Here the algorithm essentially only samples in the region where nanorods can be synthesized.

(https://doi.org/10.1039/D2DD00025C)