Machine Learning for Nanoparticle Synthesis

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In the field of advanced materials, AI has sparked transformative changes, primarily driven by the wealth of big data.[1,2] In particular, the combination of Bayesian Optimization (BO) and interpretable Machine Learning (ML) provide meaningful tools for optimizing the synthesis of nanoparticles and better understanding the mechanisms behind the nanocrystal's growth.
Here, we demonstrate a workflow where the combination of BO and ML can be exploited for revealing "missed knowledge" during the growth of gold nanorods and to accelerate the structural characterization of the nanoparticles during their growth.
Firstly, we show that by implementing BO algorithm guiding an experimentalist in the research laboratory, we could successfully demonstrate the existence of reaction conditions in which synergies between experimental conditions can be exploited to yield gold nanorods through different pathways but maintaining the quality of nanoparticles (Figure 1).[3] Specifically, we show the viable synthesis of gold nanorods in an uncharted territory (i.e., high concentration of reducing agent and high temperature) that goes against the intuition-guided conventional knowledge for growing of this type of nanoparticles. Thus, we uncovered previously unrecognized synergies between these two experimental parameters, wherein they can modulate each other's undesirable influences on the growth of gold nanorods. Thus, the accelerated production of high-quality gold nanorods serves as a promising avenue for the accelerated as well as large-scale production of nanorods.
Secondly, we show that simple neural network model can help assessing the structural parameters of growing gold nanorods in real time. The current workflow for the synthesis of plasmonic nanocrystals involves (1) colloidal synthesis, (2) spectroscopy analysis, and (3) electron microscopy (EM) characterization. The bottleneck of such a workflow is the need for the ex-situ EM analysis, which is cost-inefficient, time-consuming, and suffers from limited number of nanoparticles being analyzed (~1x10^3) as compared to a large number of nanoparticles in solution (~10x10^9). We show that a neural network model, trained on a small dataset of experimental extinction spectra (150 samples), is capable of assessing the shape and size of experimental gold nanoparticles (spheres, rods) in real-time during the nanocrystal growth (Figure 2). Our results open up possibilities for prescinding from the use of electron microscopy in nanoparticle characterization.
To close, while the insights garnered in this study are significant, this represents our preliminary investigation in our overarching objective of harnessing BO, interpretable ML, and high-throughput experimentation for generating new chemical knowledge in nanocrystal growth and accelerate their structural characterization.

References

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Figures

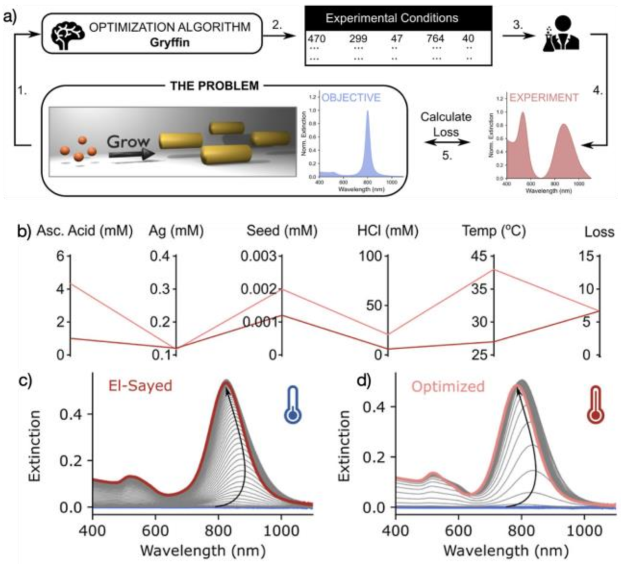

Figure 1. Open-loop exploration of chemical space in the synthesis of gold nanorods by Bayesian Optimization algorithm. a) Schematic illustrating the workflow utilized for the optimization of gold nanorods synthesis using BO algorithm. The calculated spectrum of nanorods (objective) was given to BO algorithm that generated experimental parameters to be later executed by human in the laboratory. The resulting optical spectra was compared with the objective one and calculated loss value send back to BO algorithm. b) Parallel coordinate graph showing experimental conditions for standard protocol and the one optimized by BO algorithm that suggested contra-intuitive high temperature conditions. c,d) Time-dependent UV−vis−NIR variation during the growth of gold nanorods under standard (left) and new (right) experimental conditions.

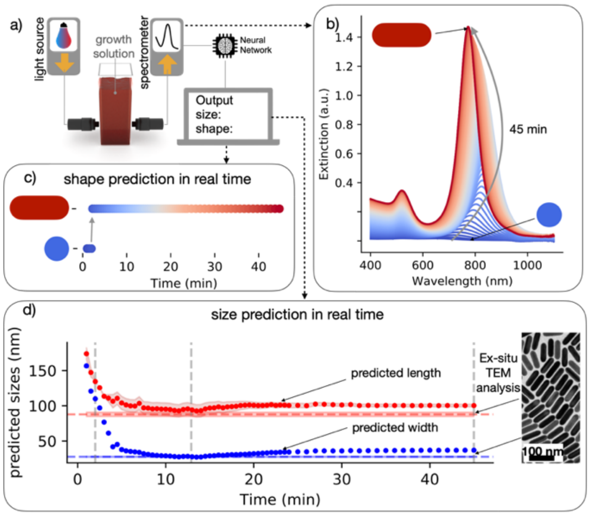

Figure 1. Prediction of structural parameters of gold nanorods. a) Schematic of experimental setup used to predict structural parameters in real-time. b) Time-resolved UV-Vis-NIR analysis during growth. c) Real-time shape prediction of gold nanocrystal during their d) Prediction of length and width of gold nanorods during the growth. Straight vertical lines correspond to the dimensions estimated by TEM analysis of the as-synthesized nanoparticles.