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Brenden Pelkie


Huat Thart-Chiang


Karen Li


Maria Politi

UNIVERSITY of WASHINGTON

Integrating ML and AI with 'Open' Laboratory Automation

Prof. Lilo D. Pozzo

Chemical Engineering

University of Washington

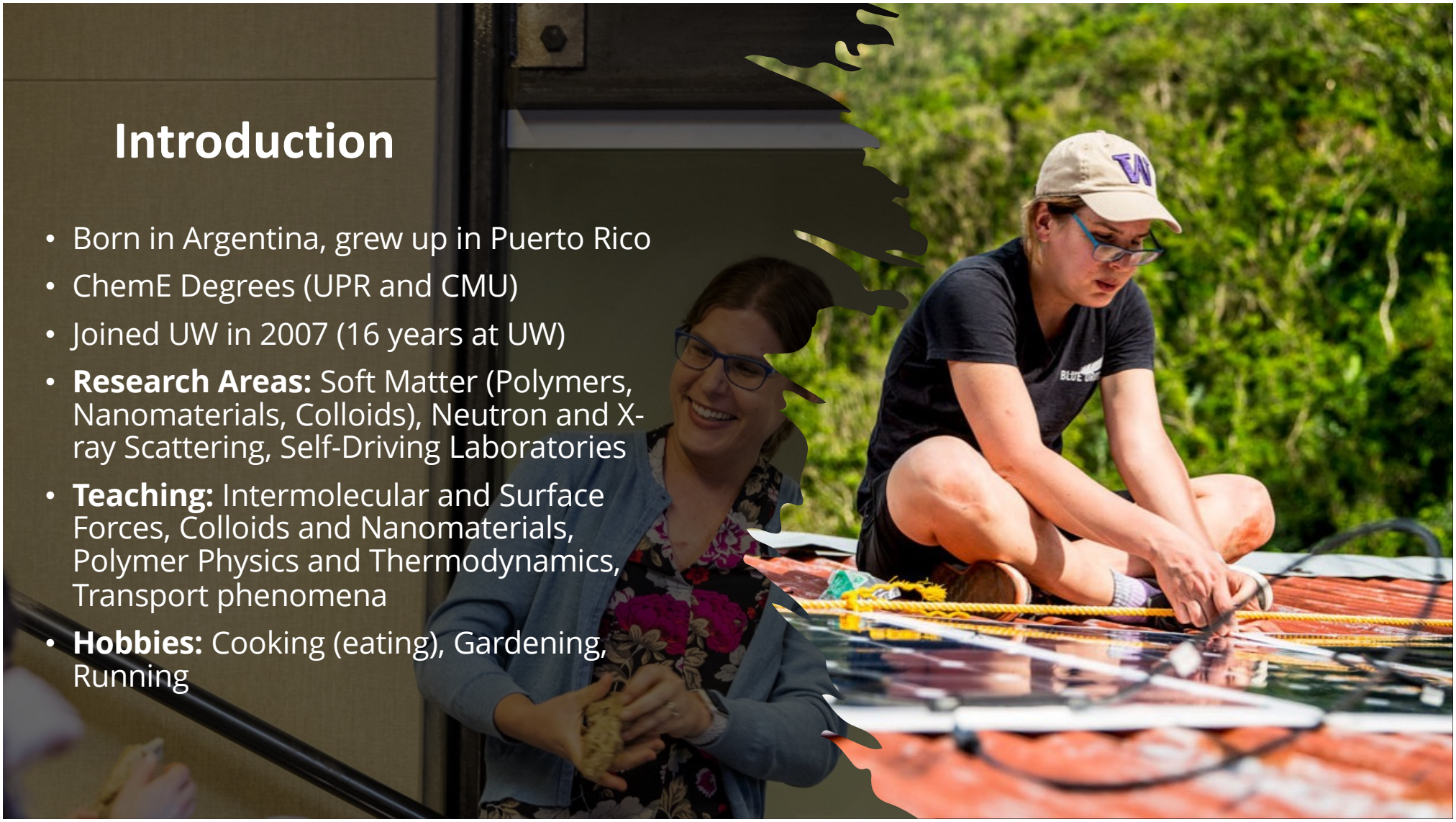
U.S. DEPARTMENT OF ENERGY | Office of Science

CSSAS Center for the Science of Synthesis Across Scales

NSF

Introduction

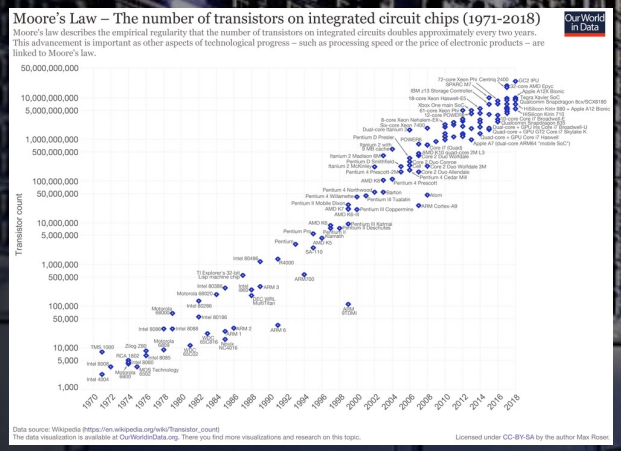
- Born in Argentina, grew up in Puerto Rico
- ChemE Degrees (UPR and CMU)
- Joined UW in 2007 (16 years at UW)
- **Research Areas:** Soft Matter (Polymers, Nanomaterials, Colloids), Neutron and X-ray Scattering, Self-Driving Laboratories
- **Teaching:** Intermolecular and Surface Forces, Colloids and Nanomaterials, Polymer Physics and Thermodynamics, Transport phenomena
- **Hobbies:** Cooking (eating), Gardening, Running



Modern-Day Materials Challenges

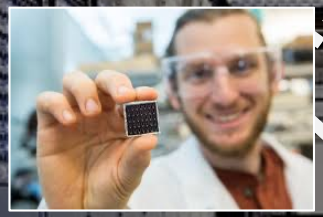
- Clean energy
  - Energy conversion
  - Energy storage
- Clean water
- Disease management
- Sustainability
  - Food
  - Polymers
  - Infrastructure

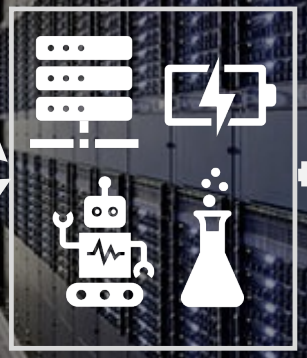
Can we achieve Moore's law for Materials Design?

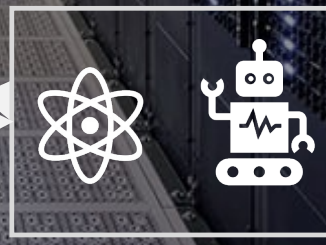


It takes 10-20 years to fully develop new materials

Way too slow…







MAP: Systems Integration

Automation
HTE Robotics

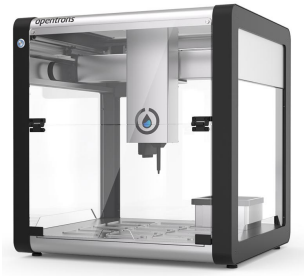
Human
Intuition
(Creativity)

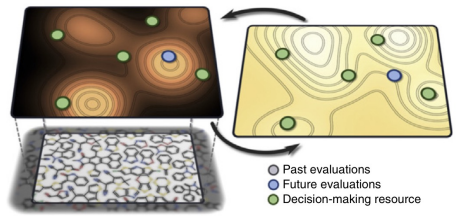
**Materials
Acceleration
Platforms
(MAPs)**

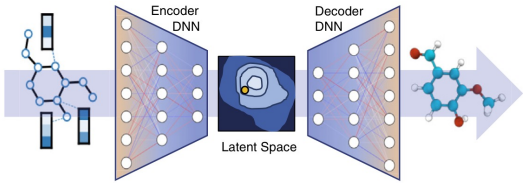
Artificial
Intelligence

Orchestration

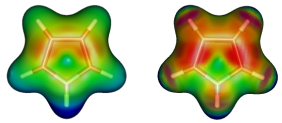
Databases







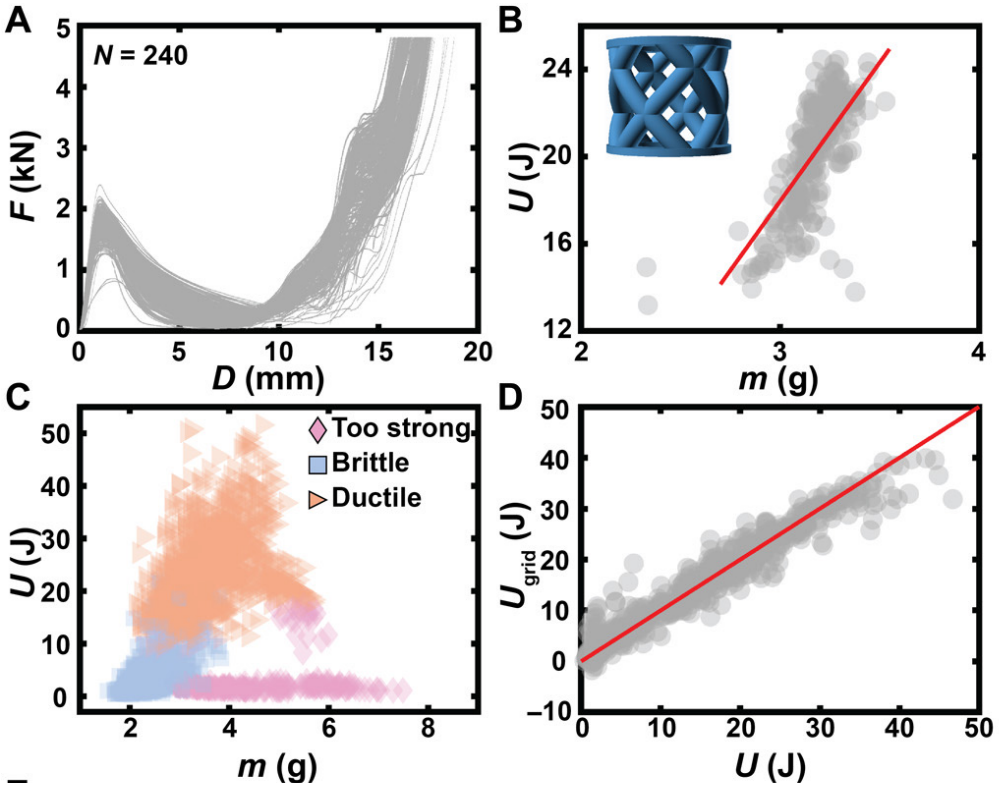
The Materials Project
materialsproject.org



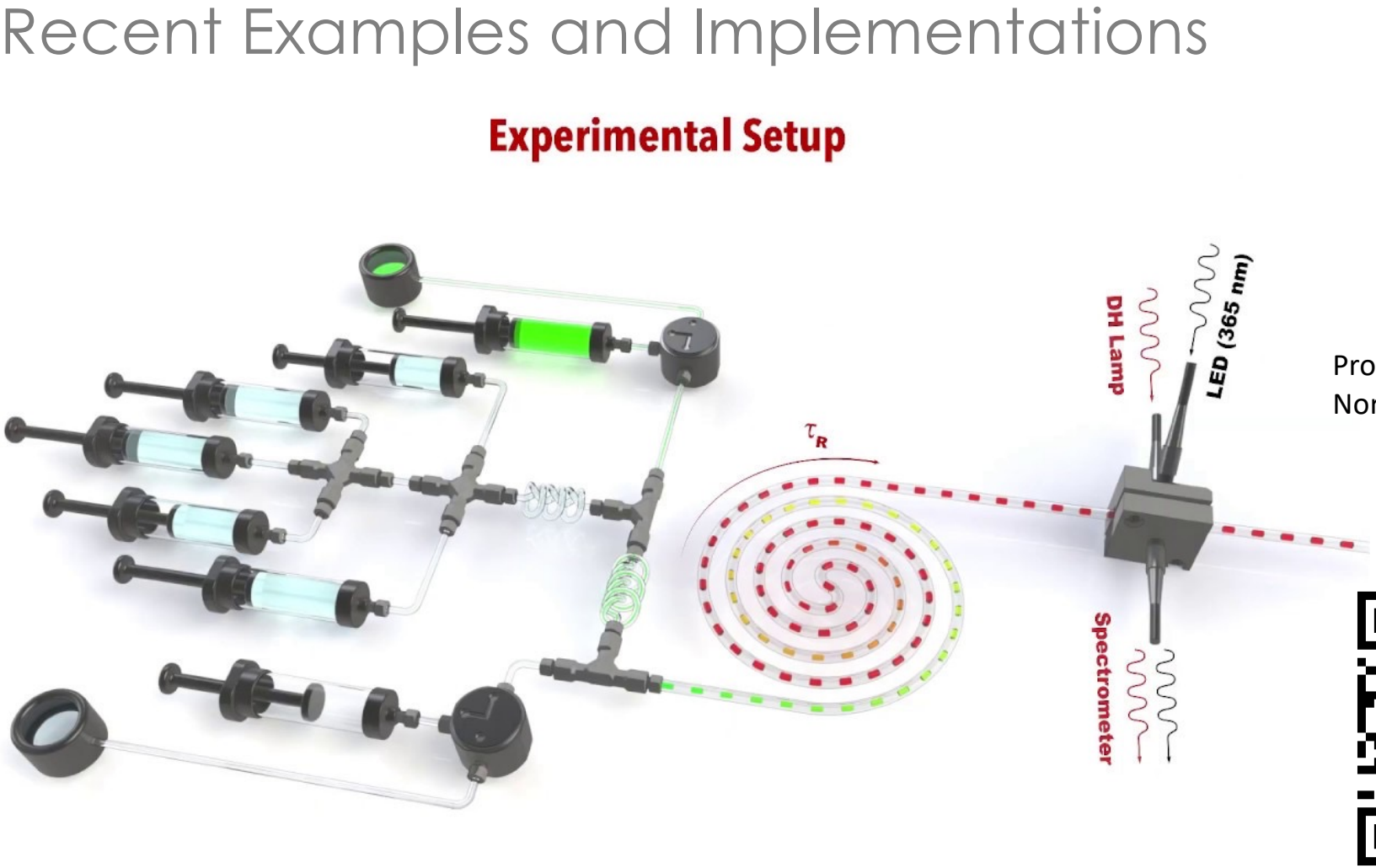
Martha M. Flores-Leonar, et.al. Current Opinion in Green and Sustainable Chemistry,100370, (2020)

Recent Examples and Implementations

Prof. Keith Brown, Boston University



Recent Examples and Implementations

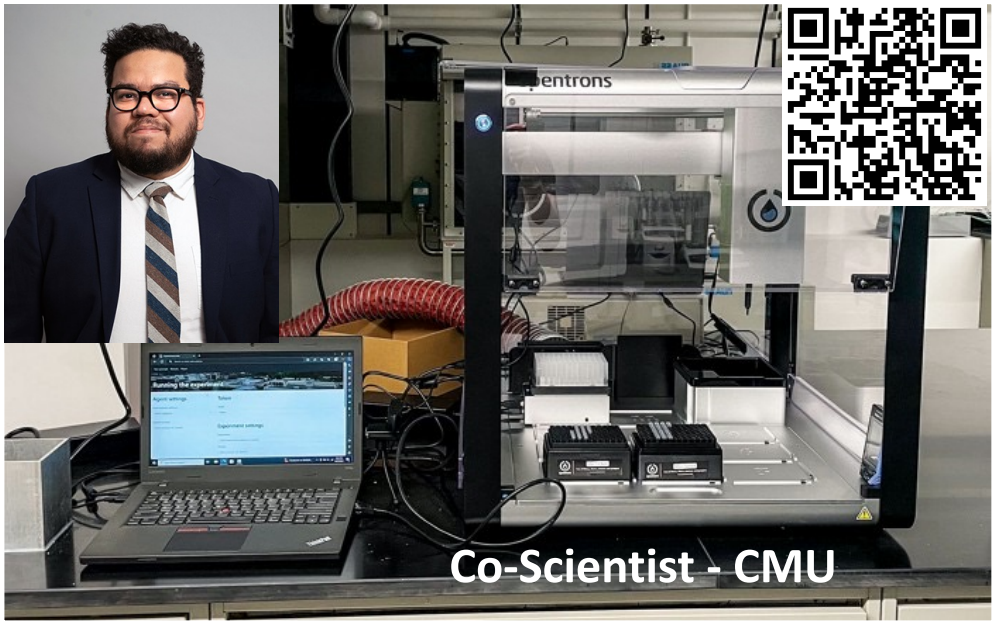


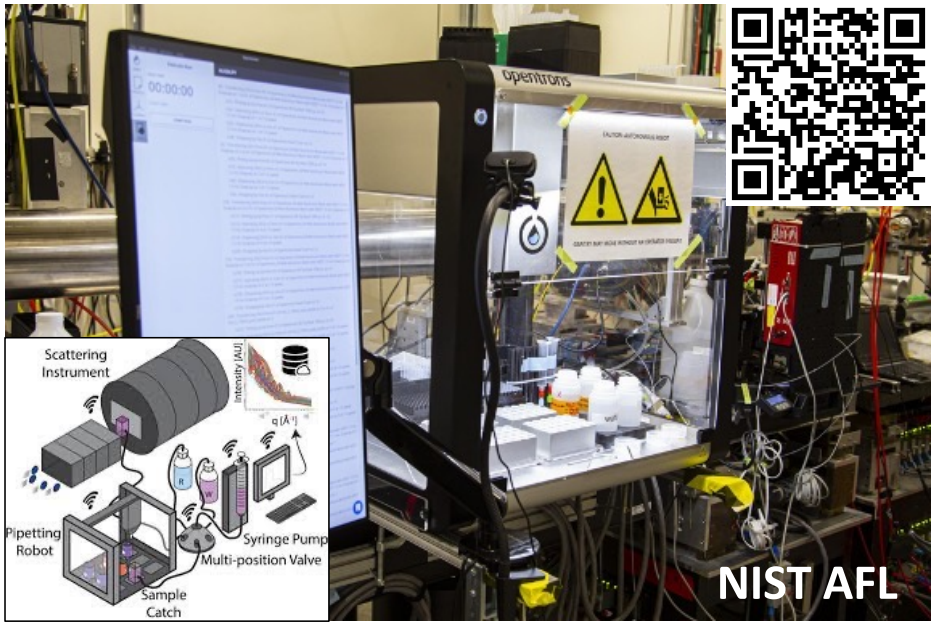
Prof. Milad Abolhasani
North Carolina State U.

OT2: A Success Story in Accessible SDL Platforms

- Low Cost Facilitates Adoption
- Open & Accessible (Python API)
- Adopted Standards (SLAS)

- Limited Capability (Move Liquids)
- Single Tool (Pipettes)
- Increasing Costs

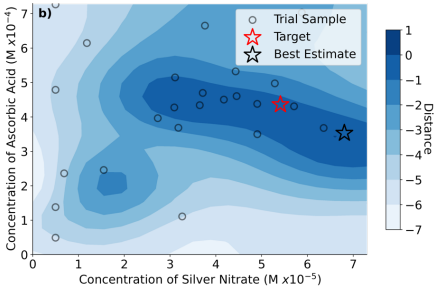




AI-Driven High-Throughput Materials Research

AI Orchestration

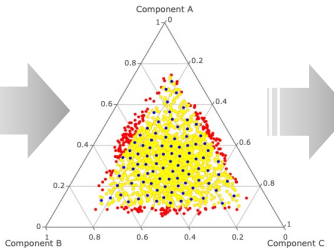
AI-Driven Materials Exploration



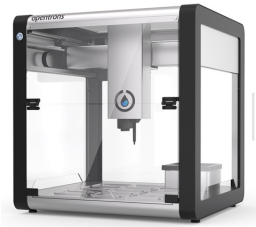
Iterative Exploration Campaigns

Prior Base Design Knowledge

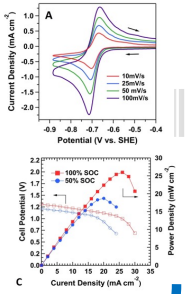
Design Of Experiments



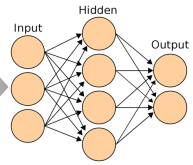
HT Sample Formulation



HT Characterization



Dimensionality Reduction
Feature Extraction
Machine Learning



Data / Metadata Stewardship

Optimized New Materials

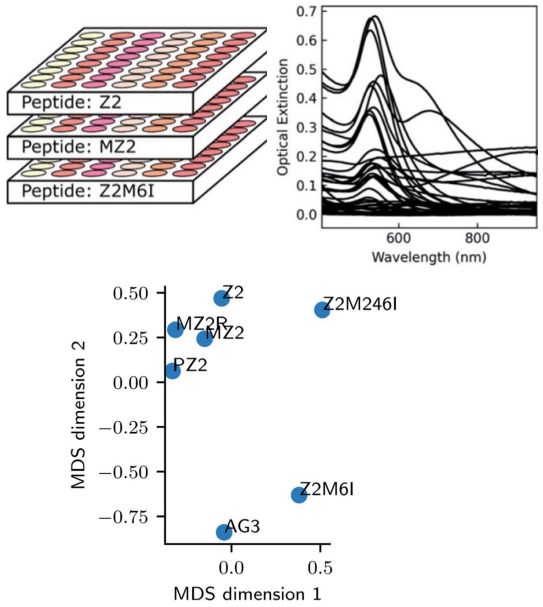
HT X-ray Characterization

@lilopozzo

GitHub Pozzo-Research-Group

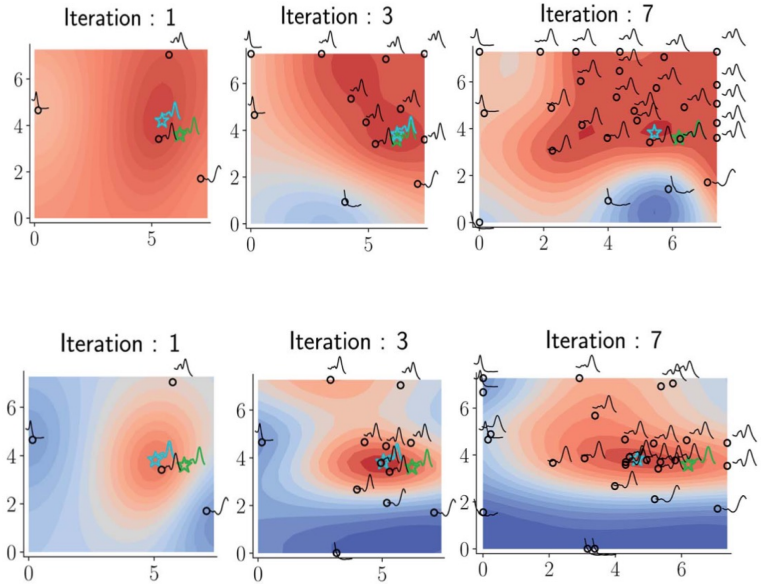
Examples of Materials Research Objectives

Multi-dimensional Correlations



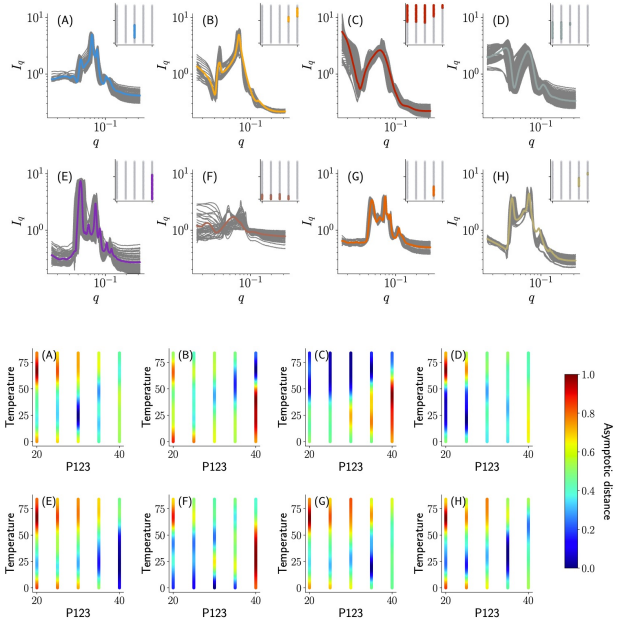
Lachowski, Kacper J., et al. "Multivariate analysis of peptide-driven nucleation and growth of Au nanoparticles." *Digital Discovery* (2022).

Retrosynthesis



Vaddi, Kiran, Huat Thart Chiang, and Lilo D. Pozzo. "Autonomous retrosynthesis of gold nanoparticles via spectral shape matching." *Digital Discovery* (2022).

Phase Mapping



K. Vaddi, K. Li, L. Pozzo,"Metric geometry tools for automatic structure phase map generation", Digital Discovery, 2, 1471-1483, (2023)

Open Questions

- How to know if target is ‘synthesizable’?
- Is the design space large enough? Too large?
- How to integrate established physical knowledge in AI?
- Synergistically use experiments and simulations?
- Can we discover new physical concepts?

Broadening Access

Democratizing MAPs and SDLs

How will the lab of the future look like?

Prof. Andy Cooper

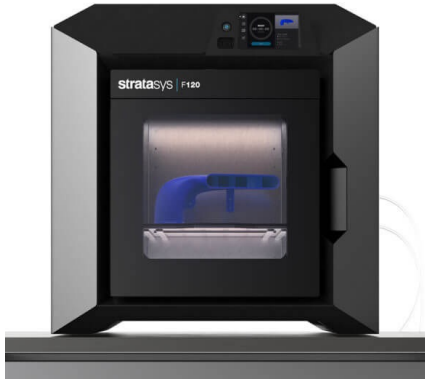
UNIVERSITY OF LIVERPOOL

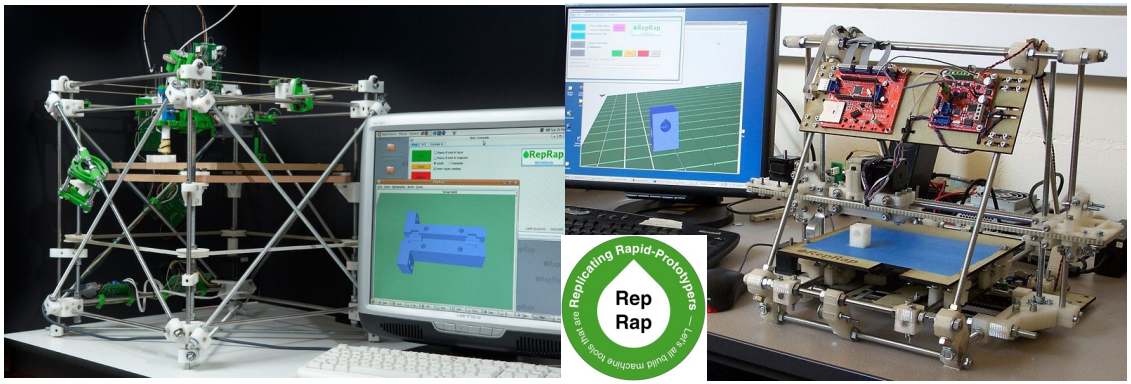
1. **Who can access these tools?**
2. **Who is trained to use them? … Who develops them?**
3. **Will they be broadly adopted?**
4. **Will SDLs revolutionize every field?**
5. **Who will they serve?**

Burger, B., Maffettone, P.M., Gusev, V.V. *et al. Nature* **583**, 237–241 (2020). https://doi.org/10.1038/s41586-020-2442-2

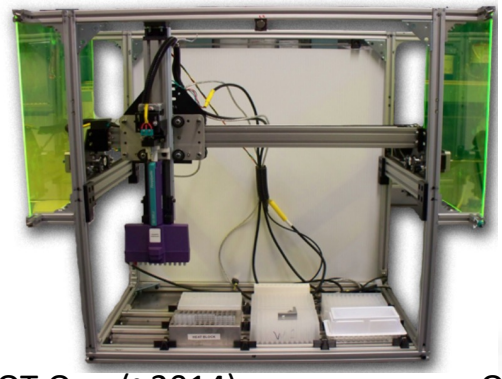
Accelerating Development and Access: Open Hardware

Open-Source RepRap Project (from 2005)

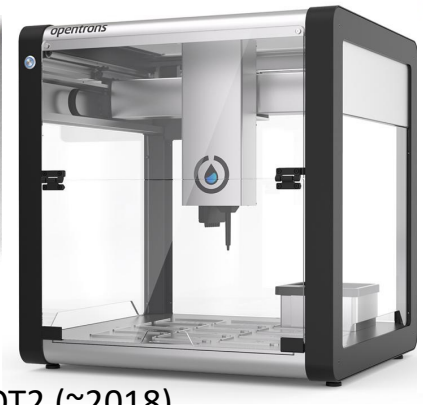




Commercial

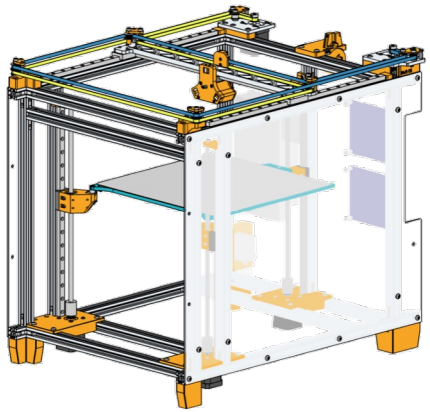


OT-One (~2014)



OT2 (~2018)

Jubilee: an open-source, multi-tool motion platform

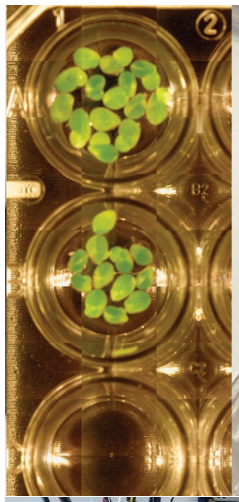


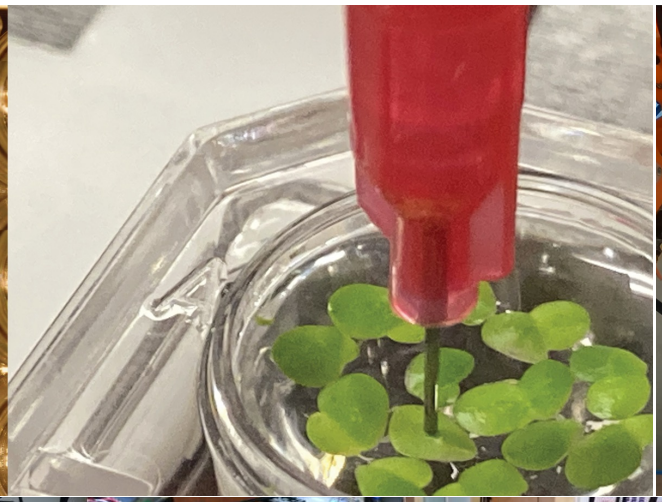
- Automatic tool change capabilities
- Stemming from the Maker Movement
- Open-hardware design- reconfigurable
- Affordable : ~$2000 USD (motion platform)

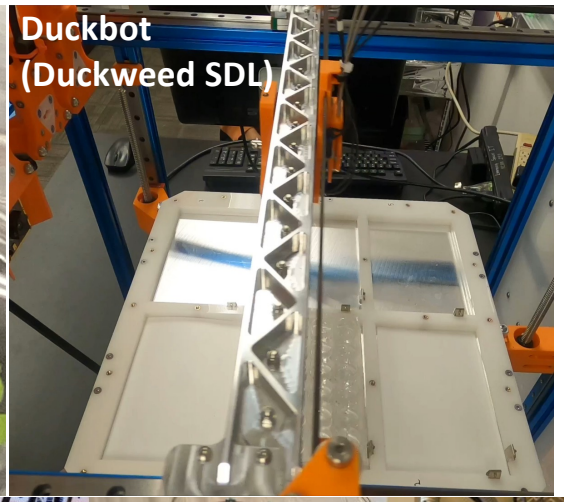
Prof. Nadya Peek
Machine Agency

- Accessible
- Allows creation of automation ecosystems
- Enables broader tool development/libraries

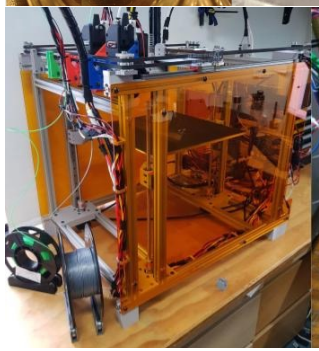
Opportunities for Open-Hardware in Lab Automation

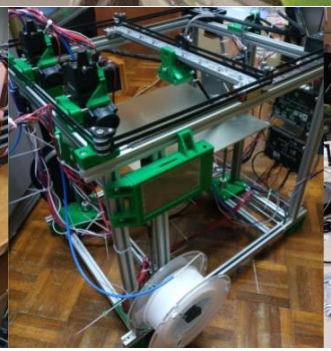


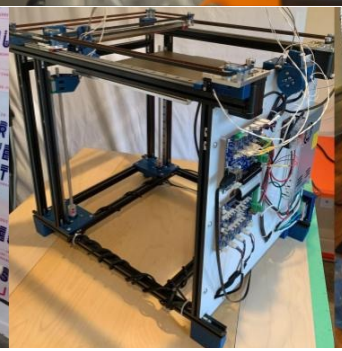


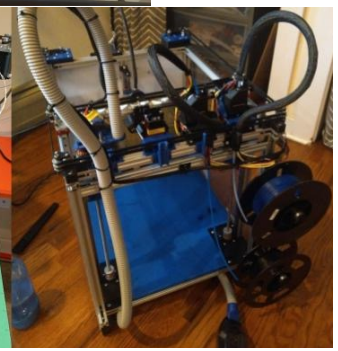


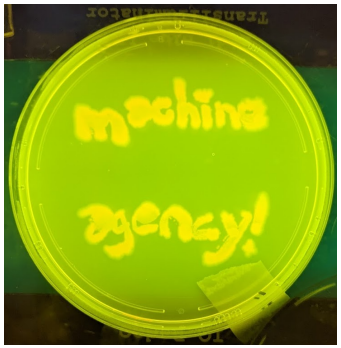
Jubilee for Science





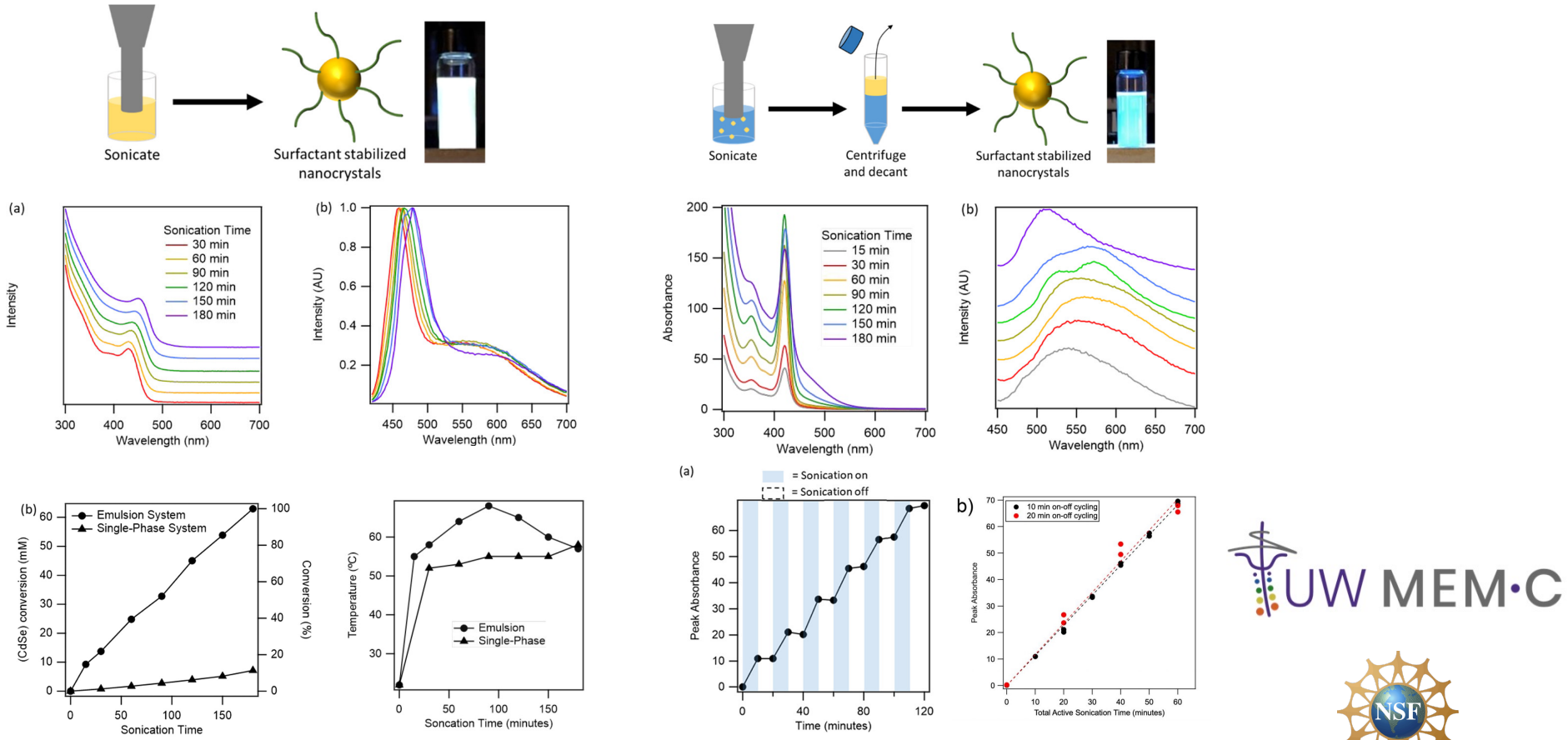






The Duckbot: A system for automated imaging and manipulation of duckweed B Subbaraman, O de Lange, S Ferguson, N Peek. Plos one 19 (1), e0296717 (2024)

Sonochemical Synthesis of CdSe Qdots and Magic-Sized Clusters

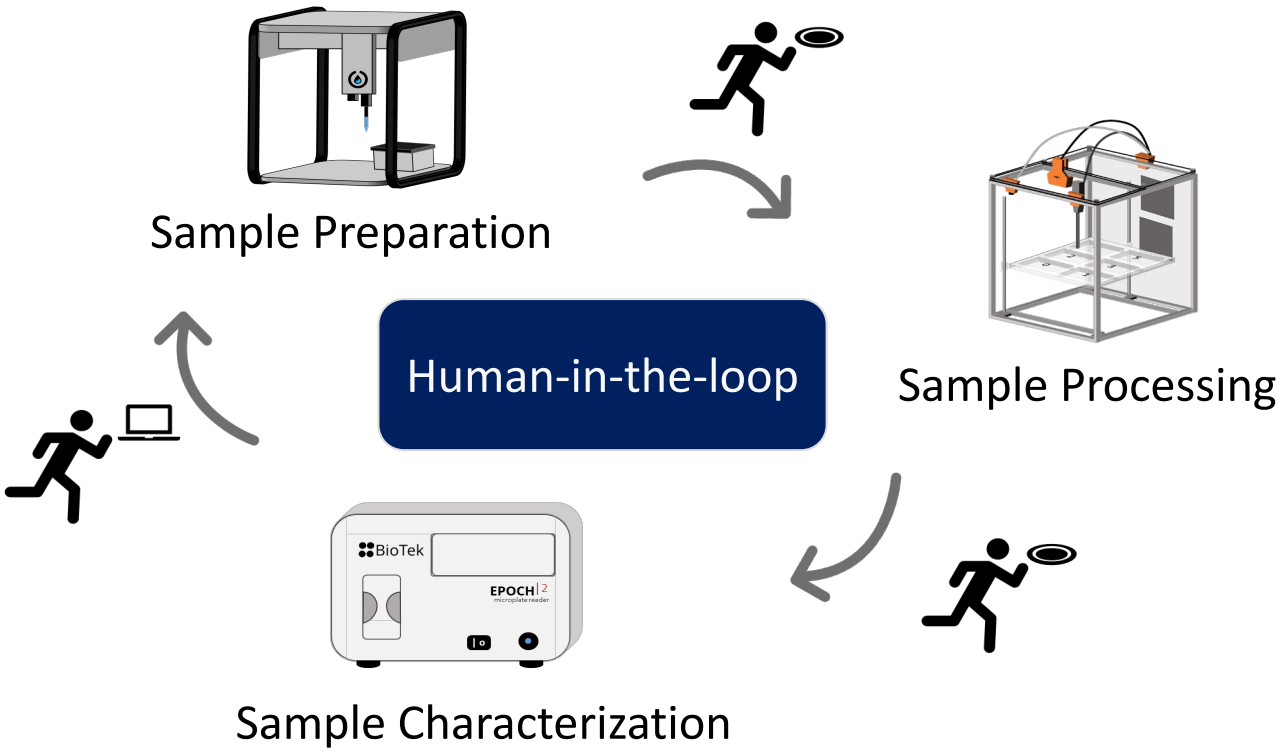


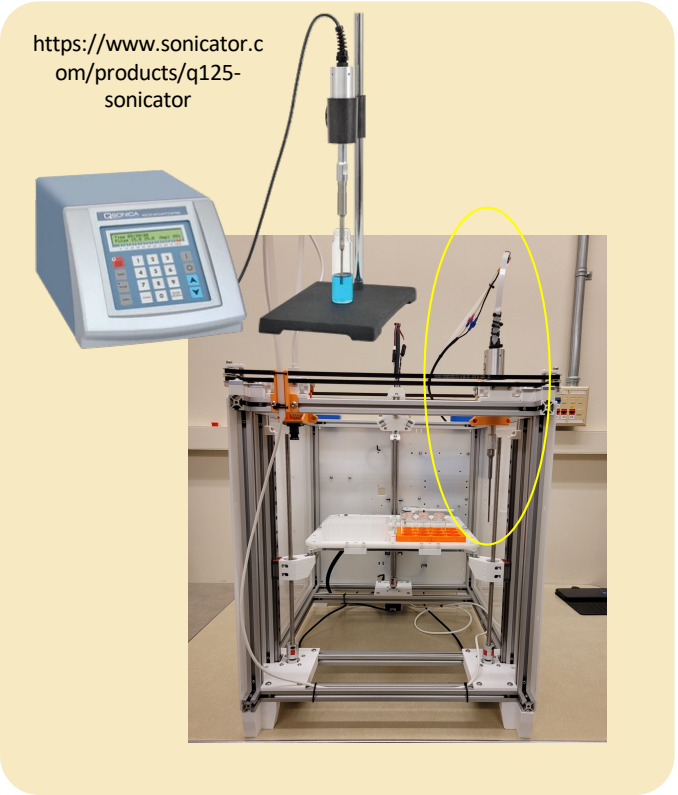
Kastilani, R.; Bishop, B. P.; Holmberg, V. C.; Pozzo, L. D., *Langmuir*, 2019, 35, 16583-16592.

UW MEM·C

NSF

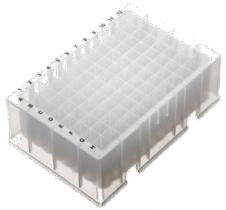
Jubilee for science – sonochemical CdSe QDs



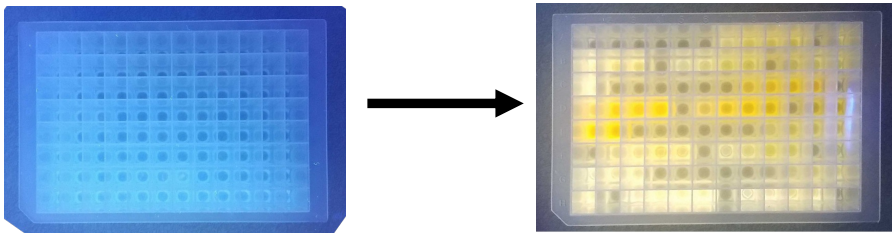


"A high-throughput workflow for the synthesis of CdSe nanocrystals using a sonochemical materials acceleration platform" M. Politi[2], F. Baum, K. Vaddi, E. Antonio[1], J. Vasquez, B. P Bishop, N. Peek, V. C Holmberg, LD Pozzo, Digital Discovery, 2, 1042-1057 (2023)

Preliminary Campaign for Colloidal CdSe



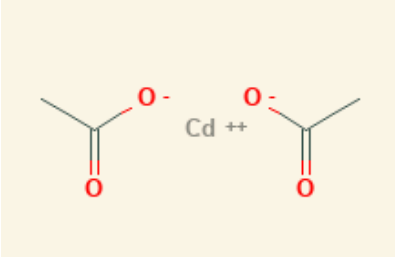
4 Different Components
5 Concentrations
625 samples (triplicate)
0.5 mL total volume/sample
5 minutes of (active) Sonication



In Octadecene

Metal Precursors

Cadmium Acetate



(Stock solution in TOP)

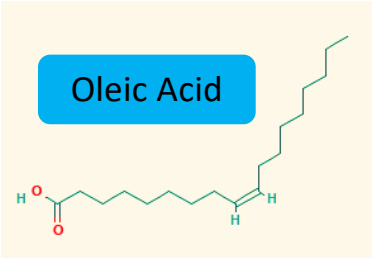
Selenium

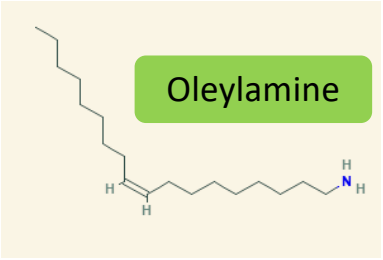
Se^{-2}

Anionic Selenide

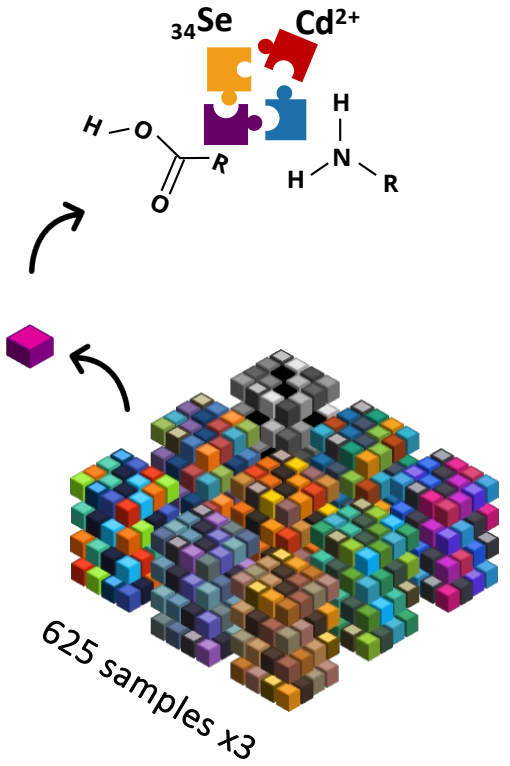
Ligands

(Pure Stocks)

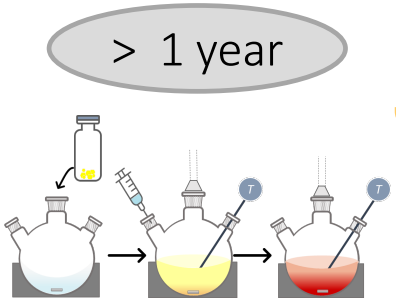




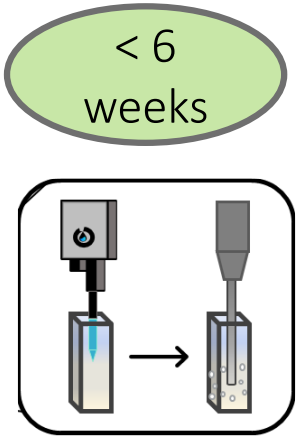
Experimental space explored in less than 6 weeks



Synthesize, Process, Characterize
1875 samples



Traditional Route

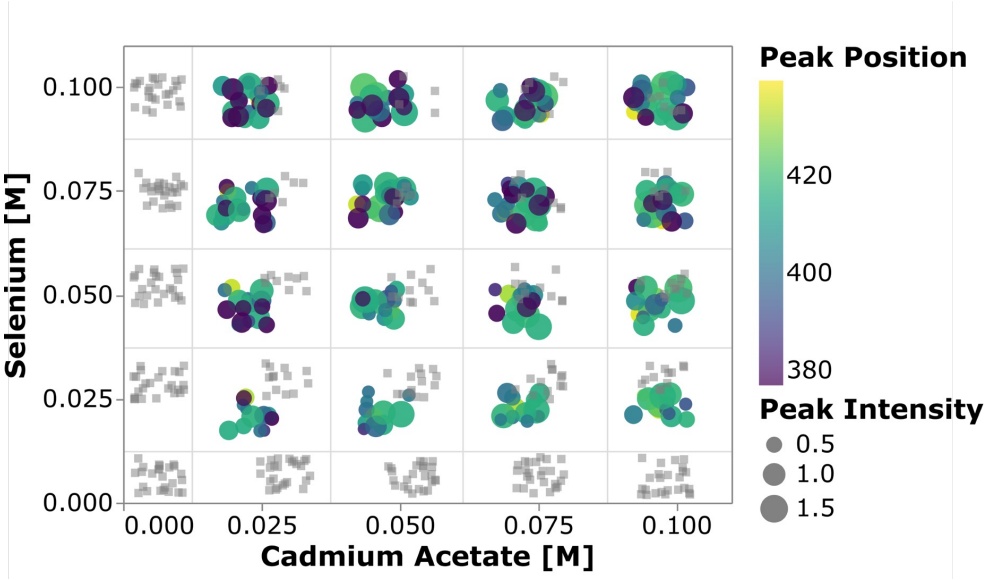


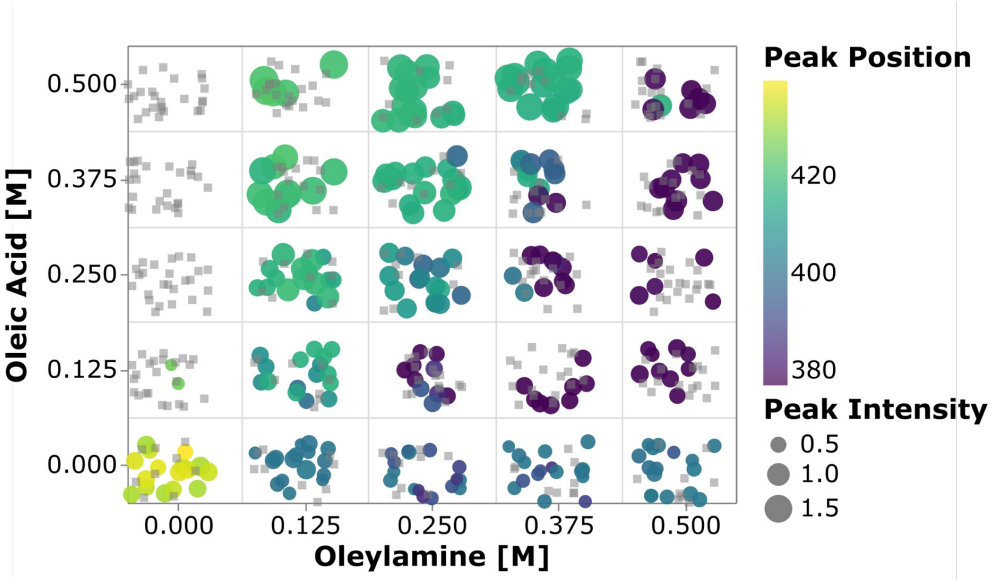
MAP

"A high-throughput workflow for the synthesis of CdSe nanocrystals using a sonochemical materials acceleration platform" M. Politi[2], F. Baum, K. Vaddi, E. Antonio[1], J. Vasquez, B. P Bishop, N. Peek, V. C Holmberg, LD Pozzo, Digital Discovery, 2, 1042-1057 (2023)

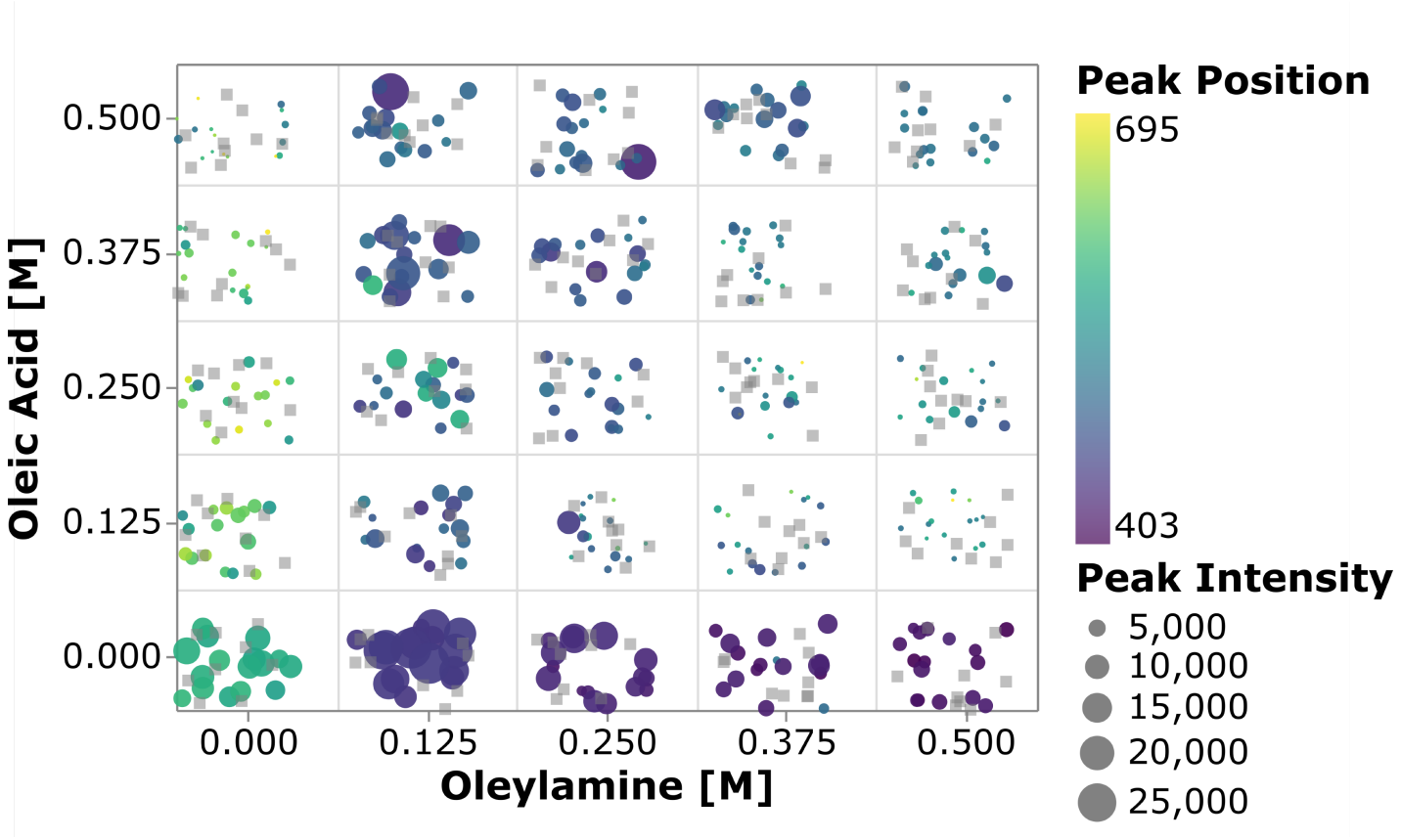
UV-Vis Extinction: Large Data Representation

Each box: experimental condition for the ligands
Circles are randomly shifted to avoid overlapping

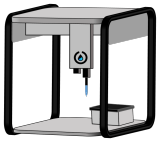




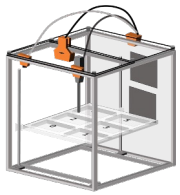
PL Spectroscopy Large Data Representation



Jubilee as a fully integrated self-driving lab



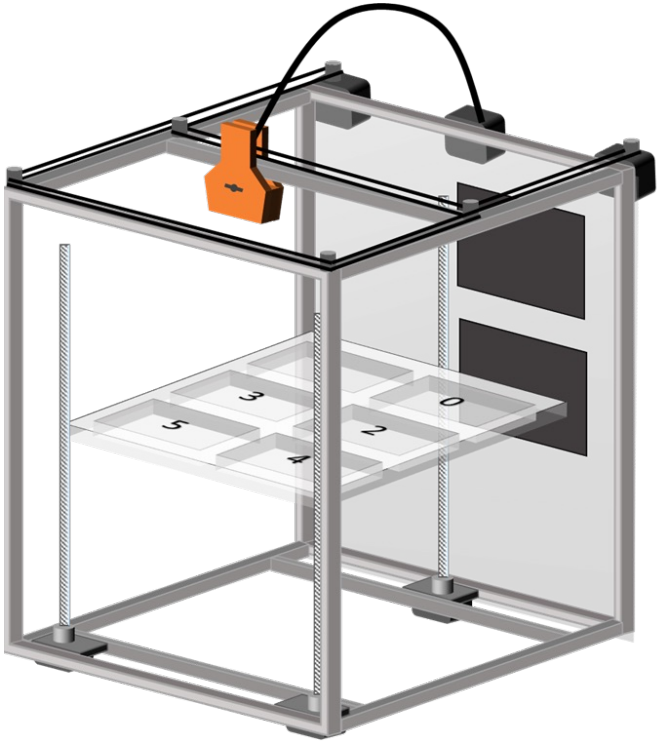
Sample Preparation



Sample Processing

Sample Characterization

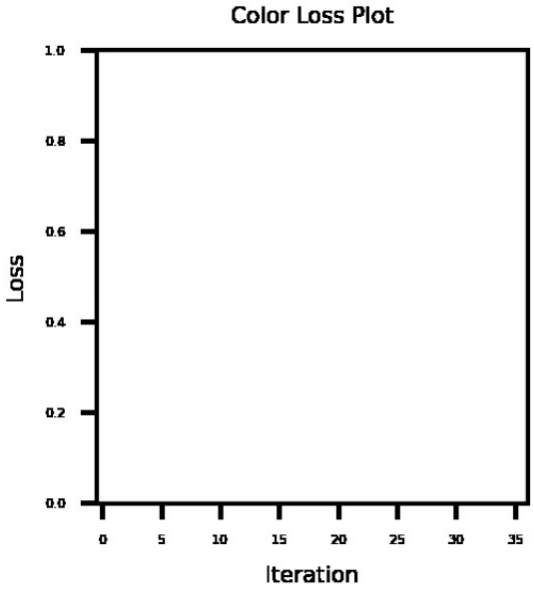
Decision Making Algorithm



SDL demonstration: color-matching campaign

Target Color: Train Data : 6 , Iterations: 30

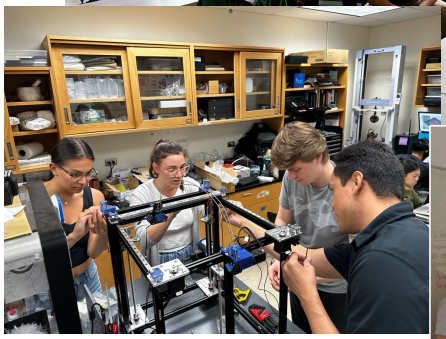
Most Recent Photo

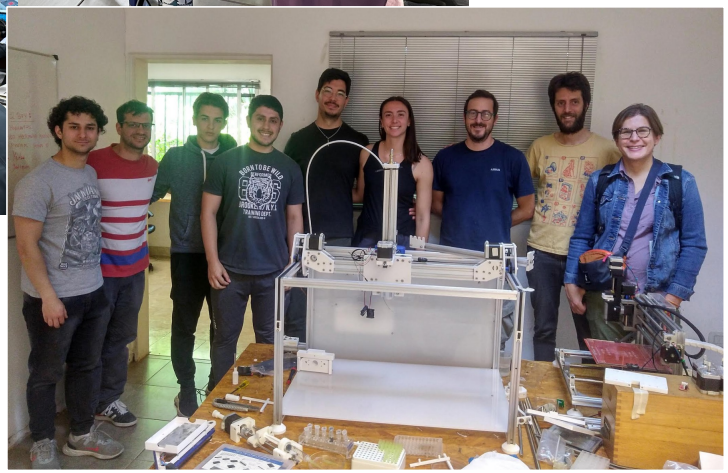


Increasing Access and Education on SDLs Across the World

Clubes de Ciencia,
Guadalajara,
Mexico

UNIVERSITY of HAWAI'I MĀNOA





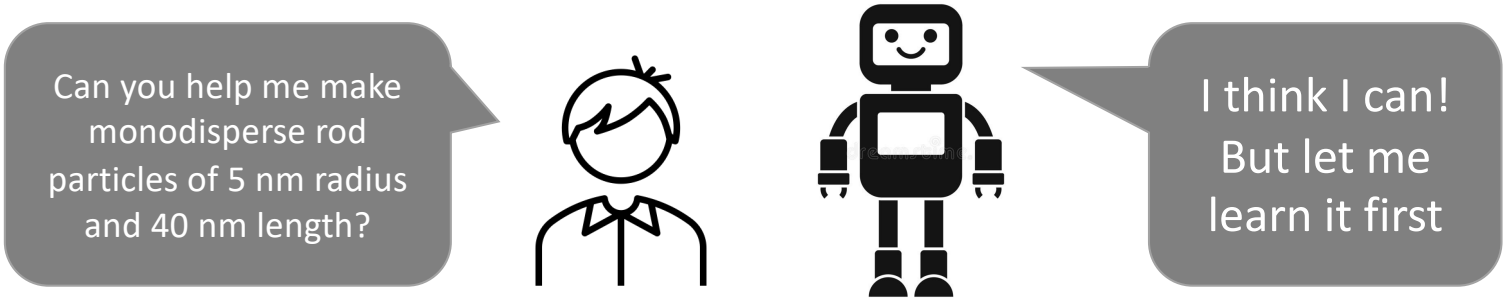
UNSAM Buenos Aires Argentina
Instituto de Nanosistemas
Gaston Corthei - Pipetin

Building Community Across the World

POSE Workshop
Seattle WA, April 2024

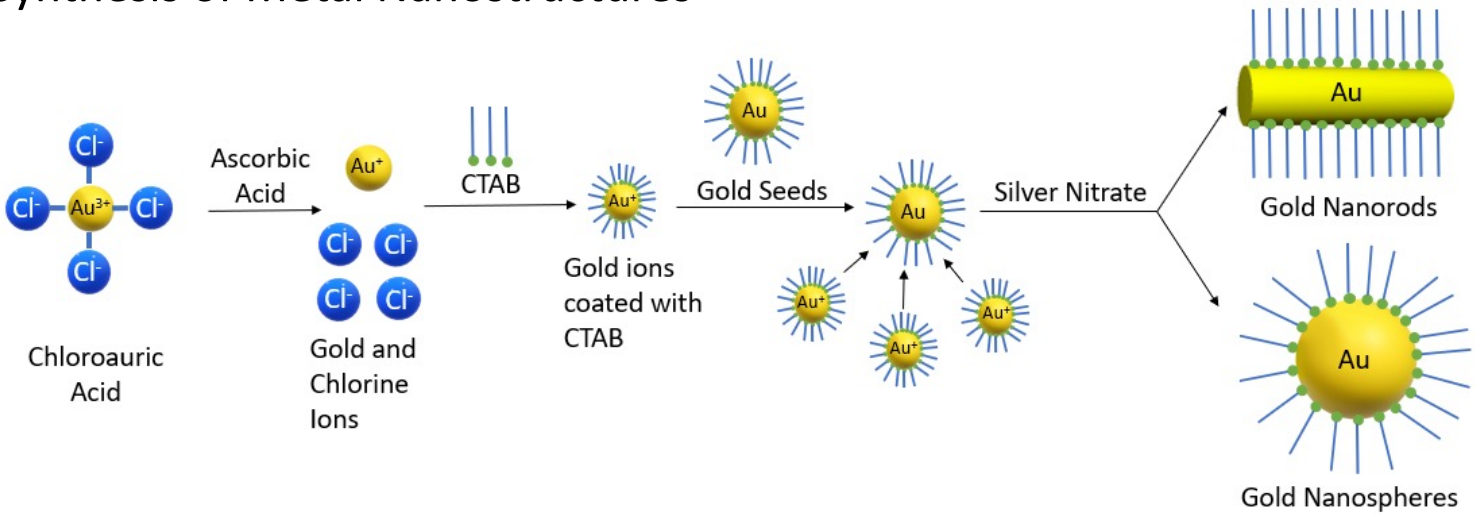
AI-Driven Retrosynthesis

Retrosynthesis: Solve Inverse Design Problems by Iterative Learning



'Fruit Fly' Problems: Synthesis of Metal Nanostructures

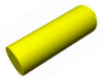
- Metal salt(s)
- Reducing Agent
- Surfactant (CTAB)
- Seeds
- Order of addition
- T, P



Automated Retrosynthesis

1. Pick Target

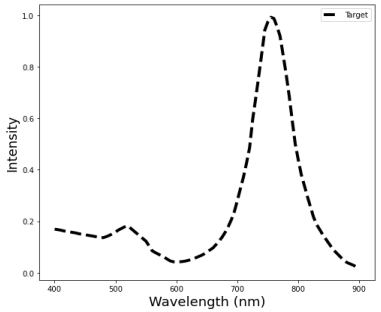
Gold Nanorod of 55nm in Length and 10nm in diameter



Spectra Scattering…

Forward Model

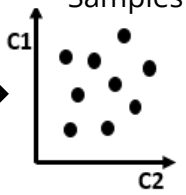
2. Simulate Target Data



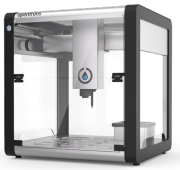
3. Perform Optimization

Bayesian Optimization

Composition of Samples



Robotic Synthesis

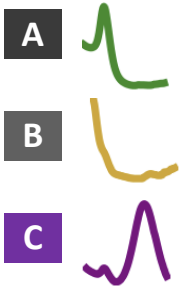


Sample A

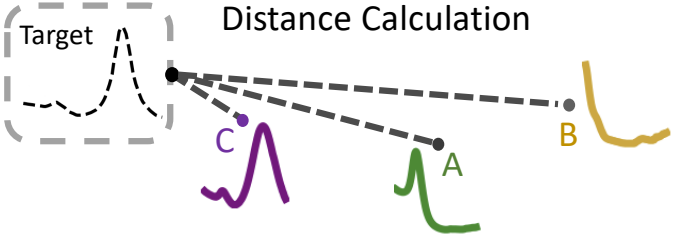
Sample B

Sample C

Characterization



Distance Calculation



Score

Comp. A	2
Comp. B	3
Comp. C	1

Stopping criteria

Stop After X Iterations

Converges within a Resolution

Cold, warm, warmer, hot… search game

Distance Metrics

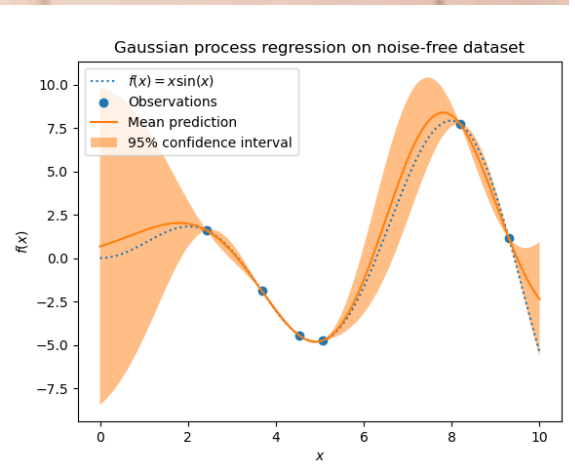
LIKELIHOOD
The probability of "B" being True, given "A" is True

PRIOR
The probability "A" being True. This is the knowledge.

$$P(A|B) = \frac{P(B|A).P(A)}{P(B)}$$

POSTERIOR
The probability of "A" being True, given "B" is True

MARGINALIZATION
The probability "B" being True.

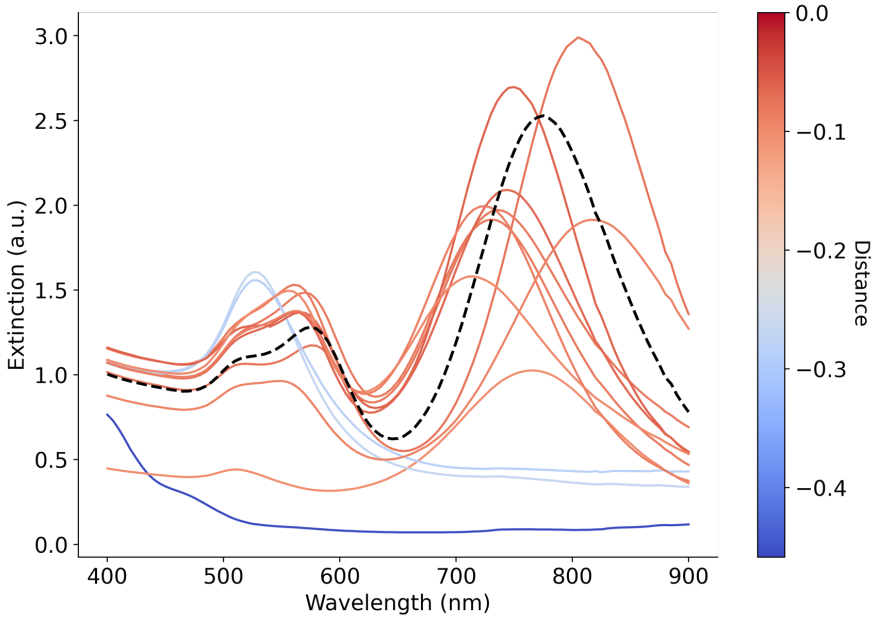


Bayesian Optimization

GP Regression

How to Meaningfully Compare Trials to Target?

- **Match in 'Expert' Parameters**
  - Peak Wavelength Intensity and Position (scalar values)
- **Euclidean Distance**
  - Mean squared difference of two spectra
- **Square Root Slope Function (SRSF)**
  - Compares the shape of spectra by taking derivatives
- **Amplitude-Phase Distance**
  - Accounts for variation along x-axis and y-axis after 'alignment' in function space



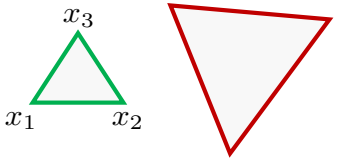
"Autonomous retrosynthesis of gold nanoparticles via spectral shape matching"
K. Vaddi, H. Chiang, L. Pozzo, Digital Discovery, 2022

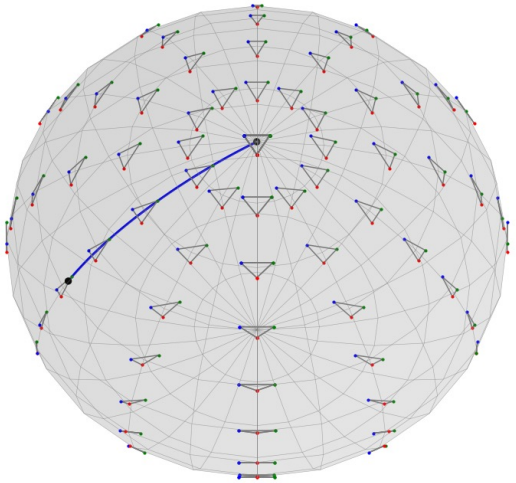
‘Distance’ in Function Shape Spaces

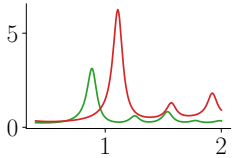
Kendall Shape Spaces

Function Shape Spaces

Original data

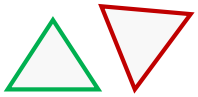




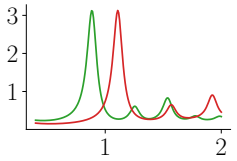


Remove scale

$\|x\| = 1$



$\int_0^1 f^2(t)\,\mathrm{d}t = 1$



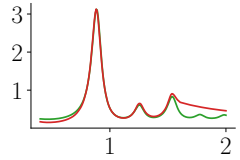
Group transformations

$\{[x] | x \in \mathcal{S}\} = \mathcal{S}/\mathrm{SO}(2)$

(rotations in 2D)

$\mathrm{Diff}^+(\Omega)$

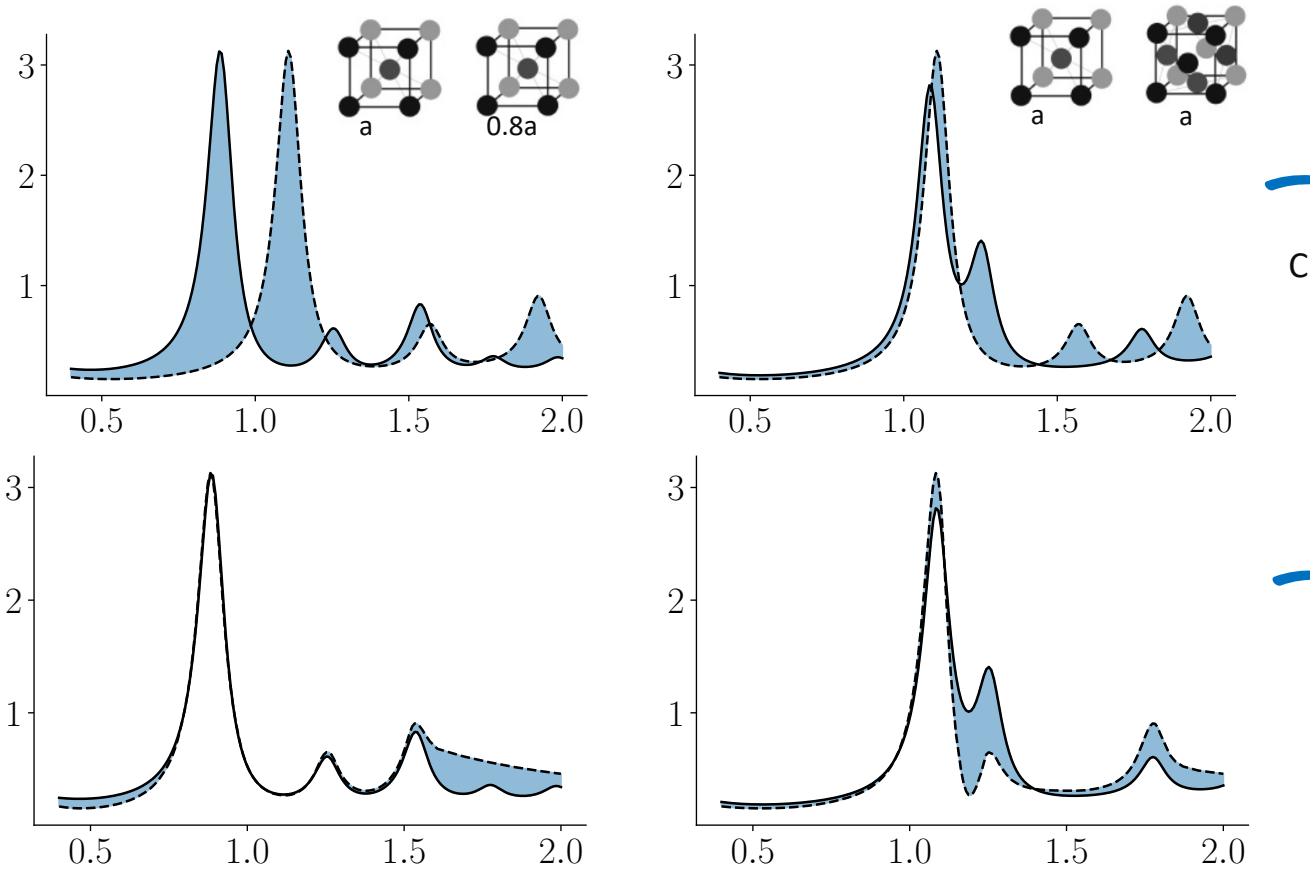
(diffeomorphism)



KENDALL, David G. et KENDALL, Wilfrid S. Alignments in two-dimensional random sets of points. Advances in Applied probability, 1980, p. 380-424.

https://geomstats.github.io

Shape-Based Similarity in Phase Identification



Conventional metrics select FCC and BCC to be similar

Shape metrics select BCC with different lattice values to be similar

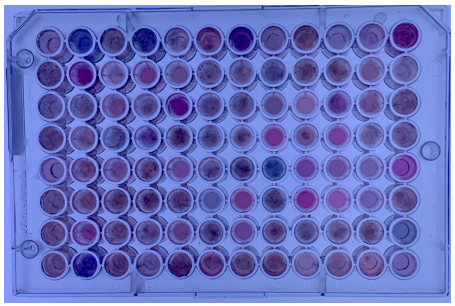
"Metric geometry tools for automatic structure phase map generation", K. Vaddi, K. Li, L. Pozzo, Digital Discovery, 2, 1471, (2023)

Seed-mediated growth of gold nanorods

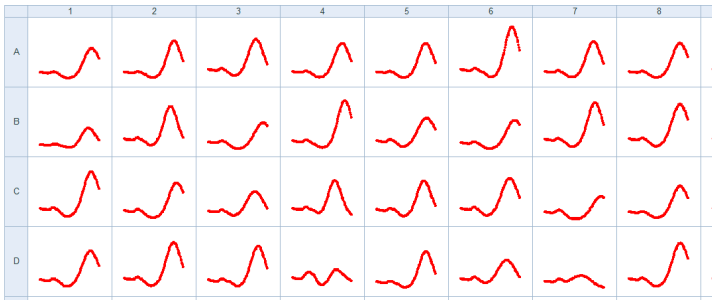
Reagent	Stock (M)	Target (M)	Range (M)
CTAB	2.0×10^{-1}	6.40×10^{-2}	6.40×10^{-2}
Gold (III) Chloride Trihydrate	1.0×10^{-3}	1.96×10^{-4}	1.96×10^{-4}
Silver Nitrate	6.4×10^{-4}	6.20×10^{-5}	$0 - 7.38 \times 10^{-5}$
Ascorbic Acid	6.3×10^{-3}	3.60×10^{-4}	$0 - 7.27 \times 10^{-4}$
Gold Seeds	1.8×10^{-5}	1.44×10^{-6}	1.44×10^{-6}

Two-dimensional design space

Sample preparation



Synthesized samples

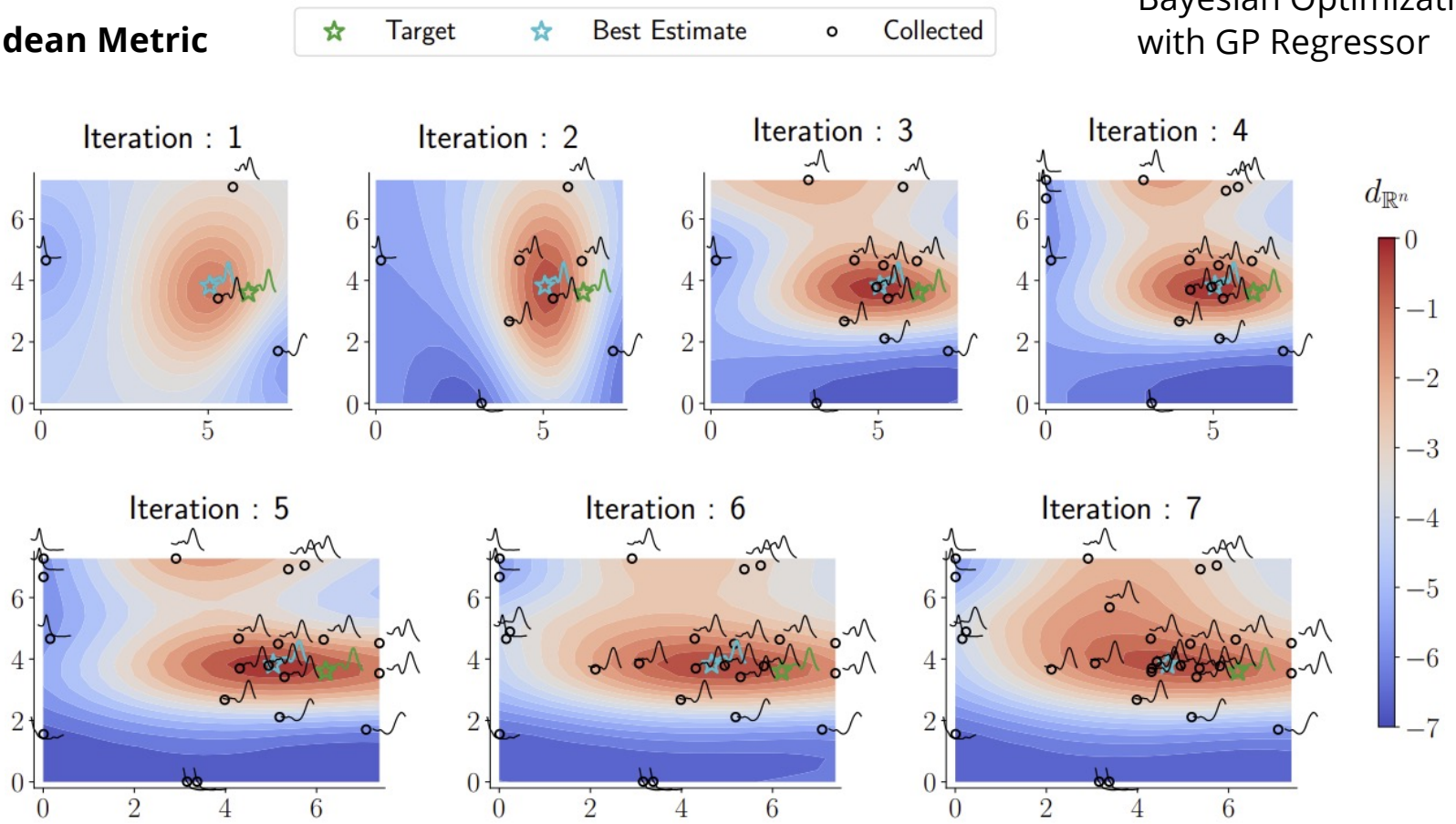


UV-Vis characterization

"Autonomous retrosynthesis of gold nanoparticles via spectral shape matching"
K. Vaddi, H. Chiang, L. Pozzo, Digital Discovery, 2022

Amplitude Phase Metric Helps Agent Learn the Phase Diagram

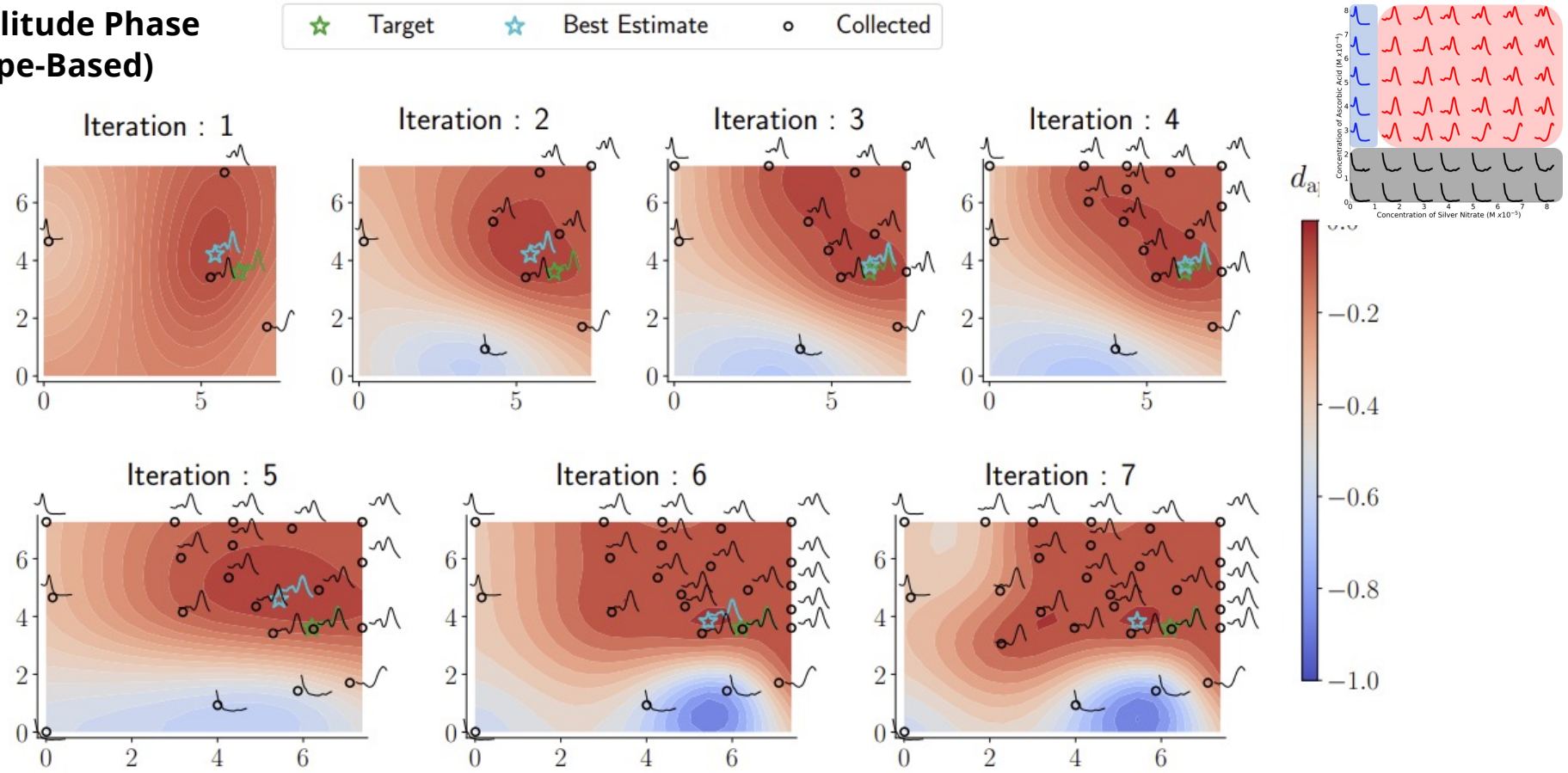
Euclidean Metric



Bayesian Optimization
with GP Regressor

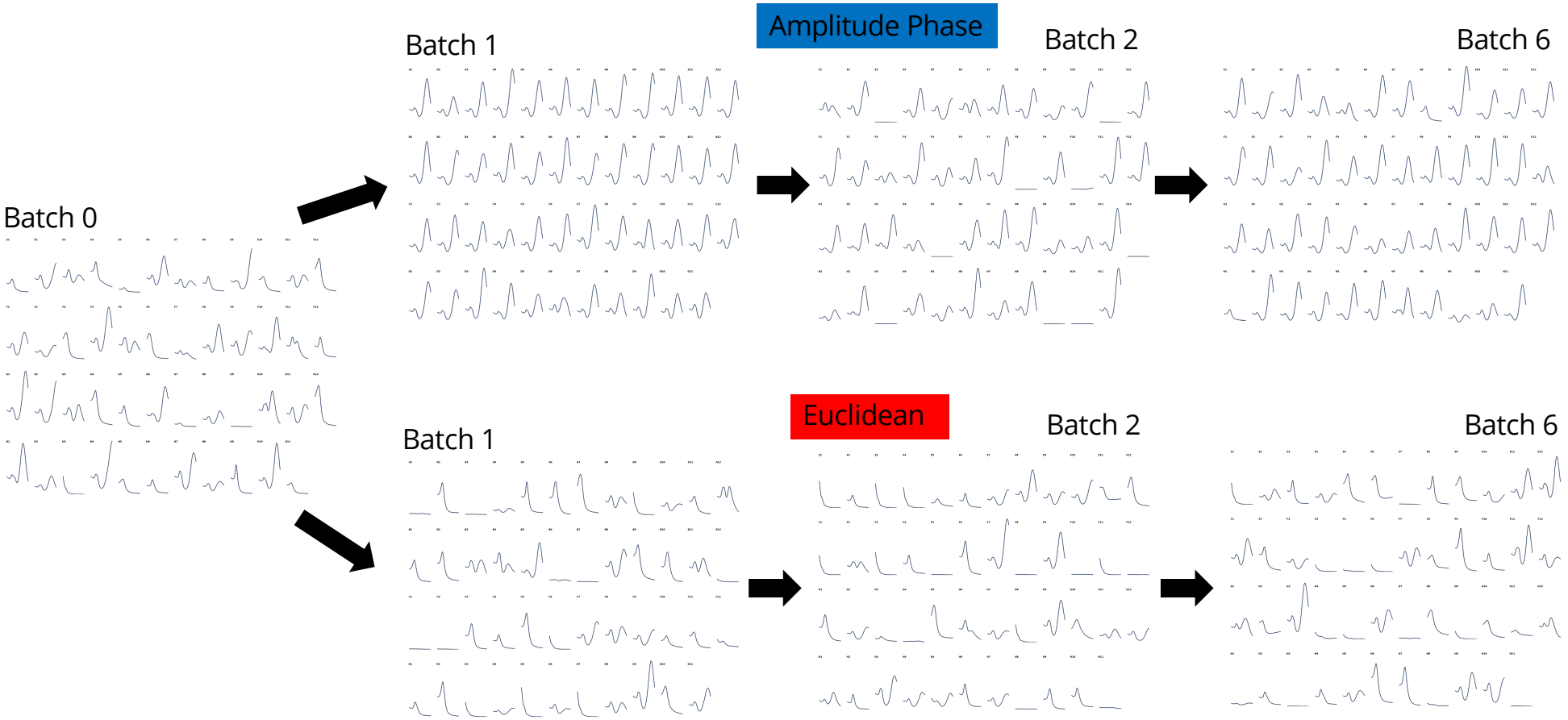
Amplitude Phase Metric Helps Agent Learn the Phase Diagram

Amplitude Phase (Shape-Based)

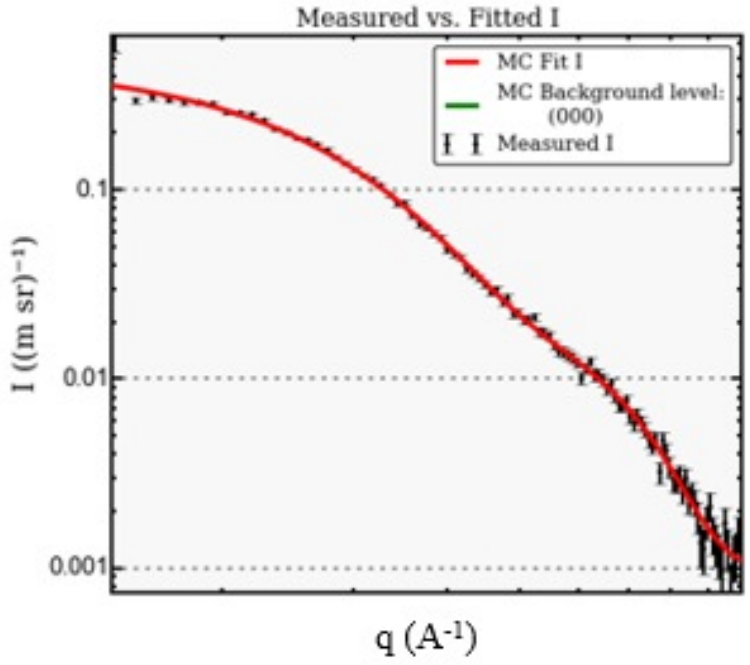


"Autonomous retrosynthesis of gold nanoparticles via spectral shape matching" K. Vaddi, H. Chiang, L. Pozzo, Digital Discovery, 2022

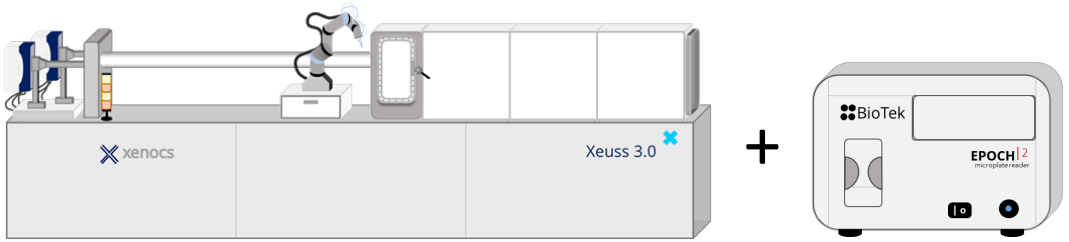
Amplitude Phase Metric Helps AI Identify Nano-Rod Space

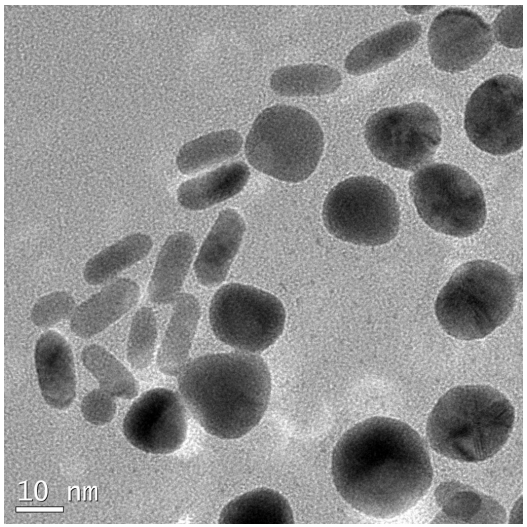


Did it work out?... Not as Expected



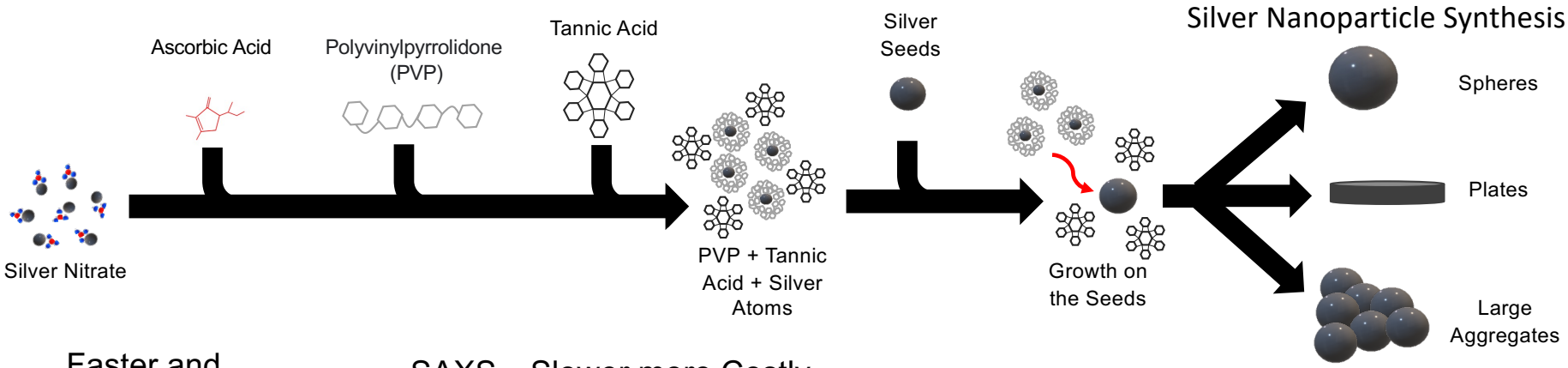
SAXS: nanorods of 8 nm in diameter and 15 nm in length and nanospheres of 16 nm in diameter



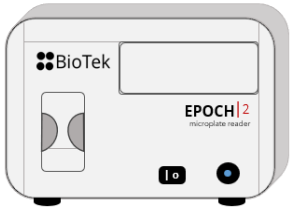


Need Multi-Fidelity Models!!

Hierarchical Multifidelity Analysis of Silver Nanoplates

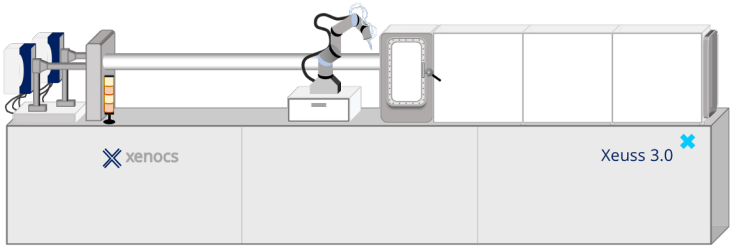


Faster and Cheaper



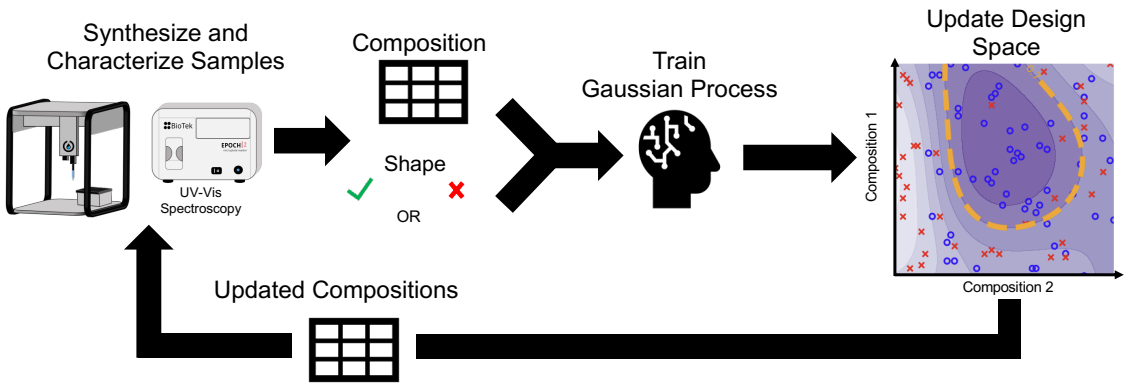
UV-Vis Spectroscopy

SAXS Slower more Costly

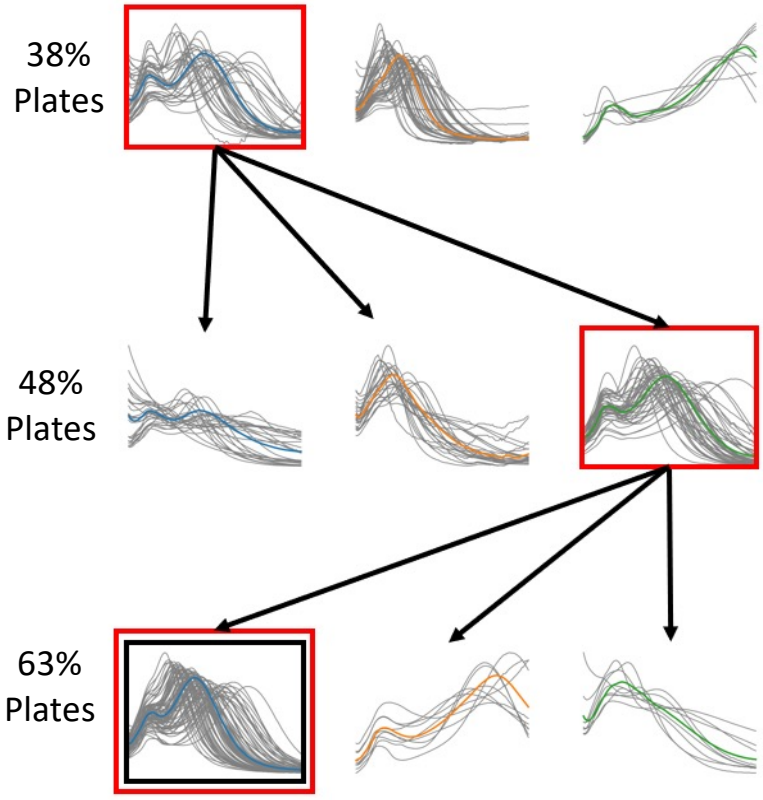


TEM Slowest and Costliest

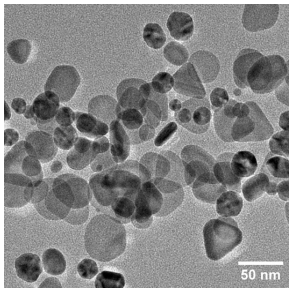
Hierarchical and Multi-Modal Analysis

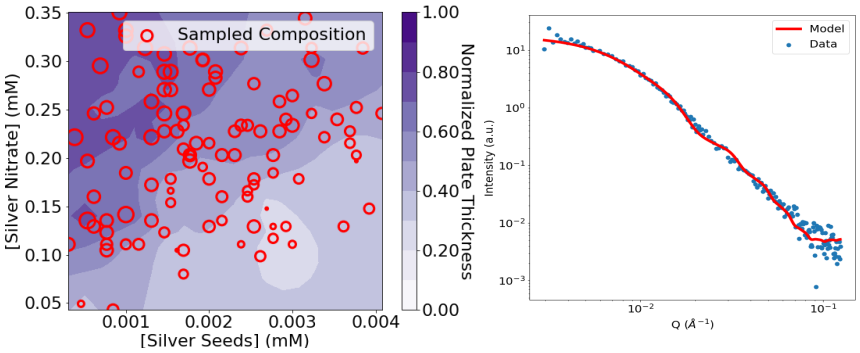


Autonomous Classification of Spectroscopic Curves Based on Shape



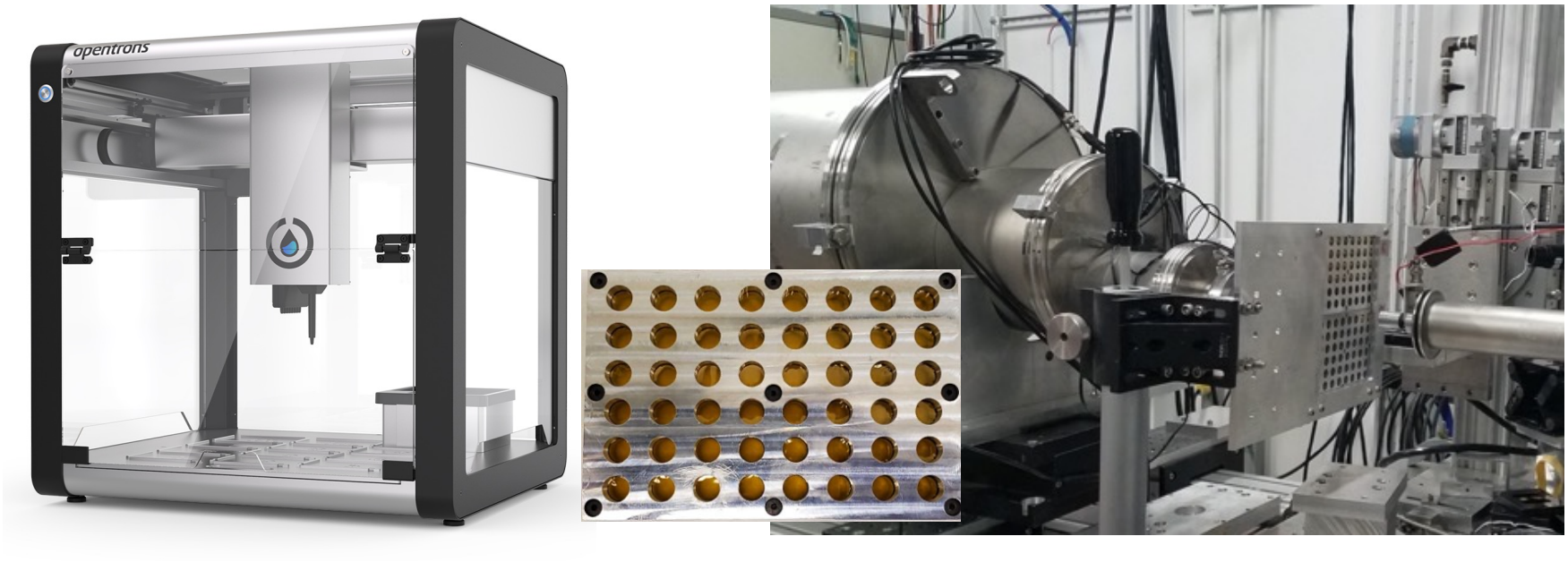
Optimized sampling to observe plate formation





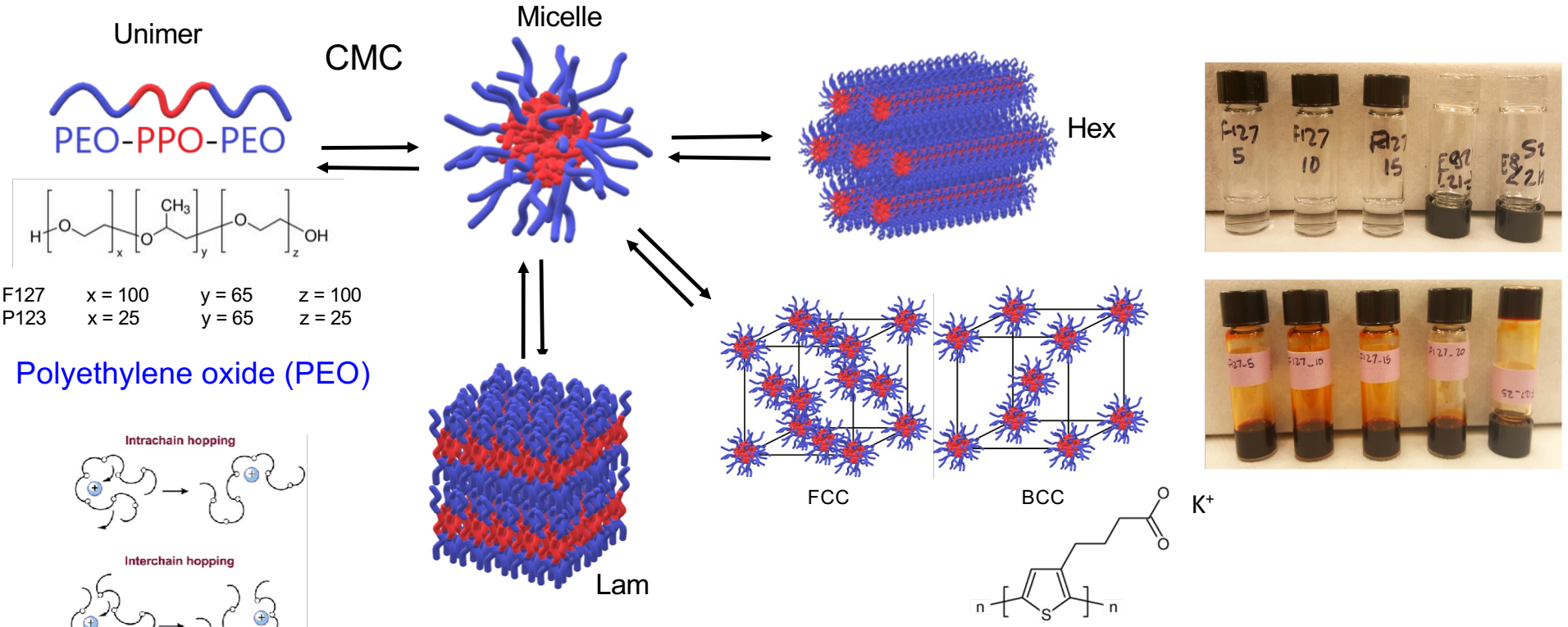
Autonomous Phase Mapping

Integration of automation and high-throughput analysis for SANS and SAXS

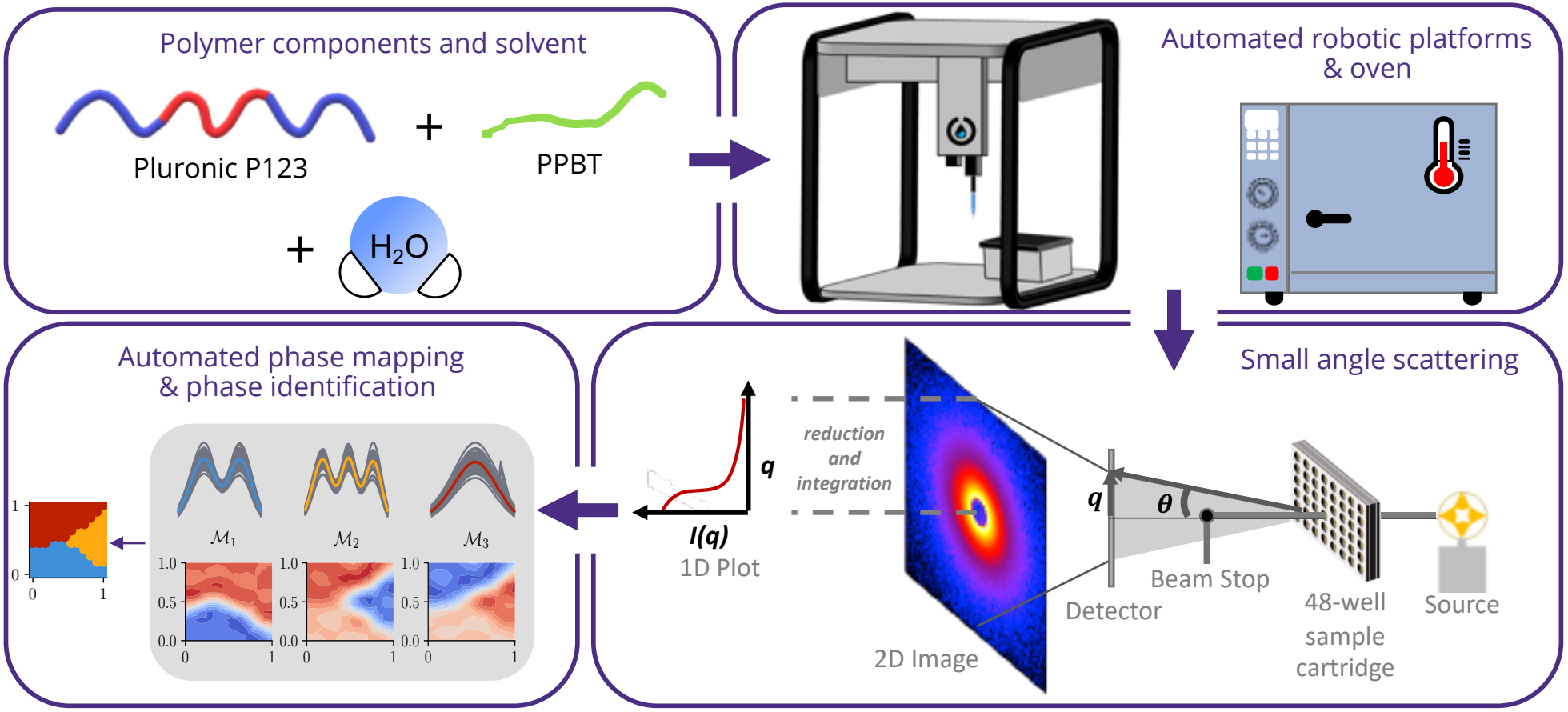


https://github.com/pozzo-research-group/Automation-Hardware

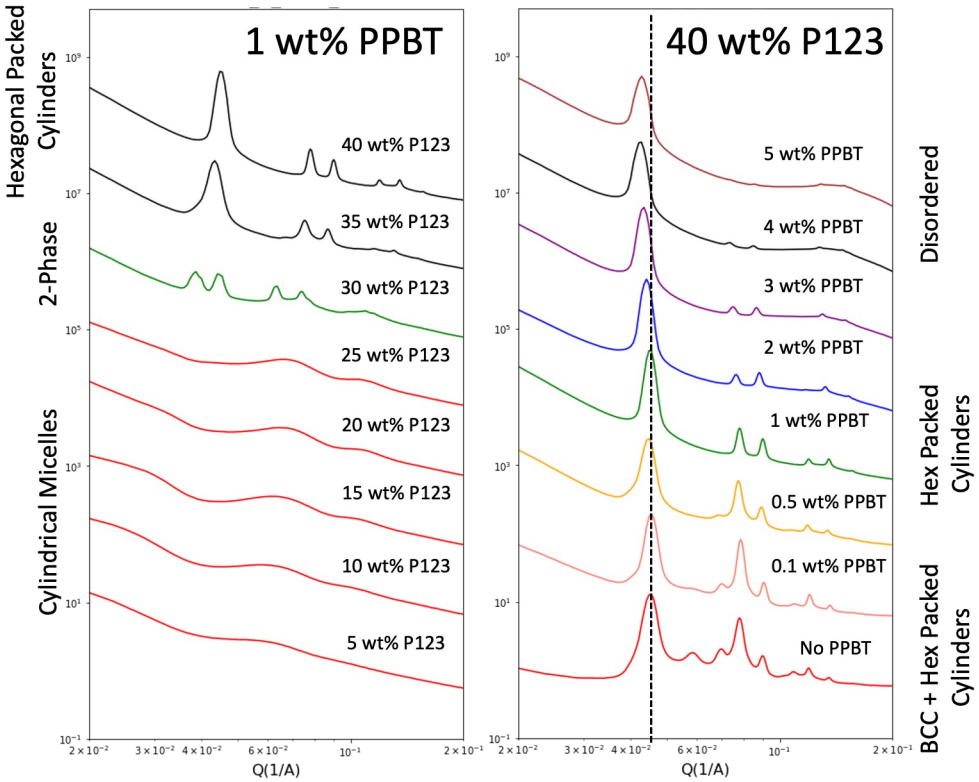
Phase-Mapping: Conjugated Polymer + Copolymer

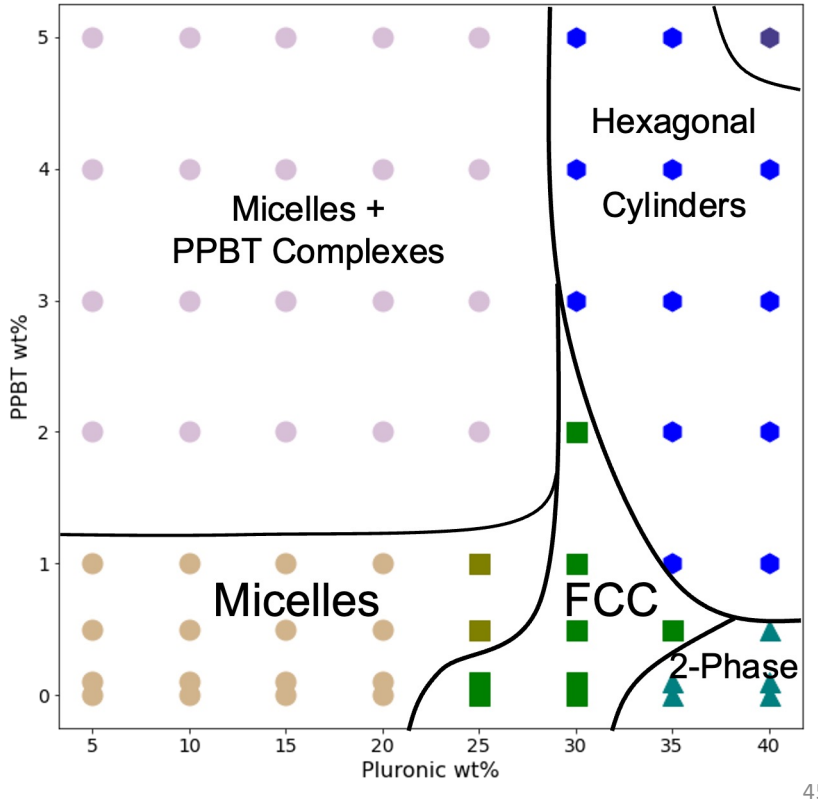


Automated High-Throughput OMIEC Formulation and Analysis



HT SAXS Mapping of Structured Blend Phase-Diagram



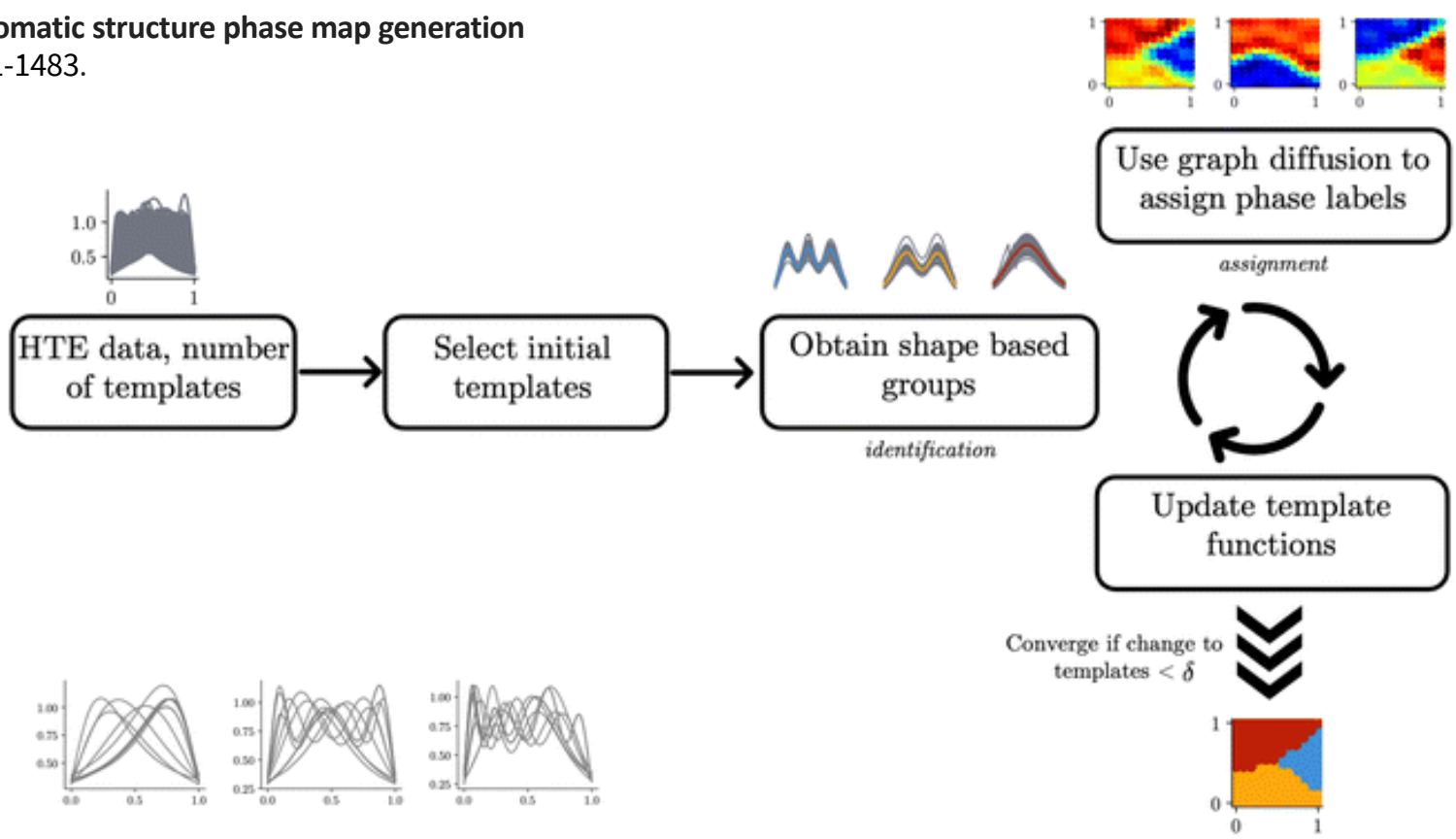


Autonomous Phase-Mapping with Shape-Similarity Distance Metrics

Kiran Vaddi, Karen Li, and Lilo D. Pozzo.

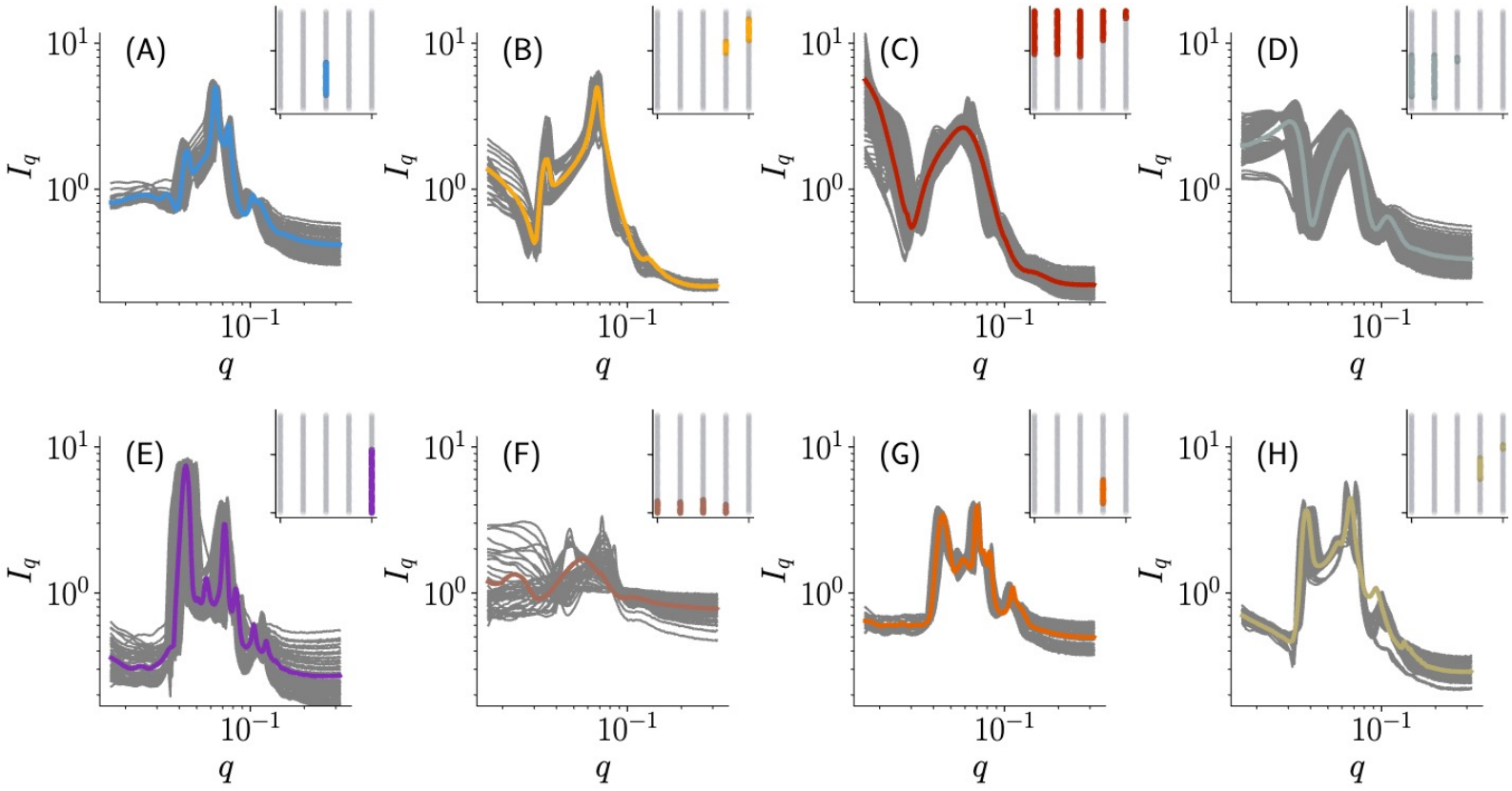
Metric geometry tools for automatic structure phase map generation

Digital Discovery, 2023,2, 1471-1483.



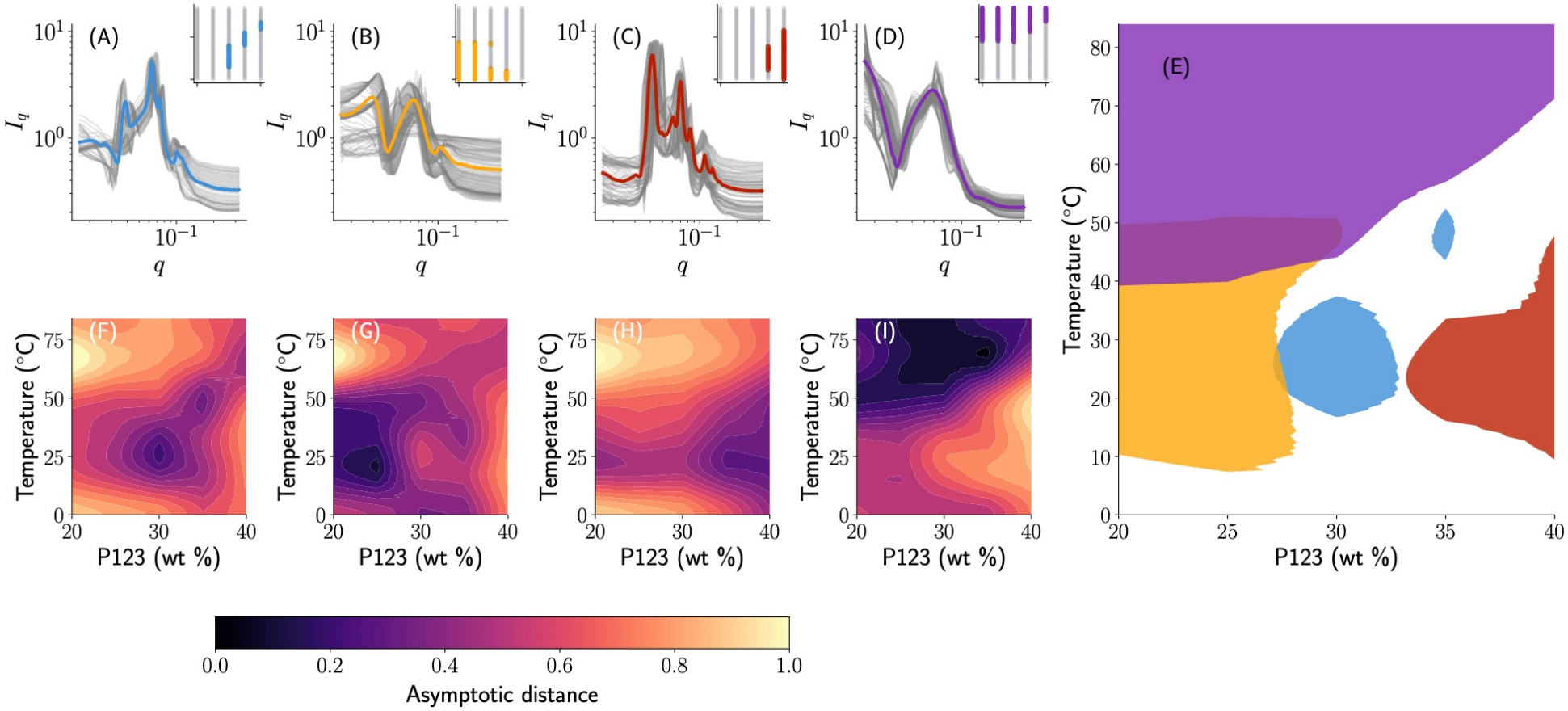
Code GitHub Repo

Distance Metrics in Autonomous Phase Mapping

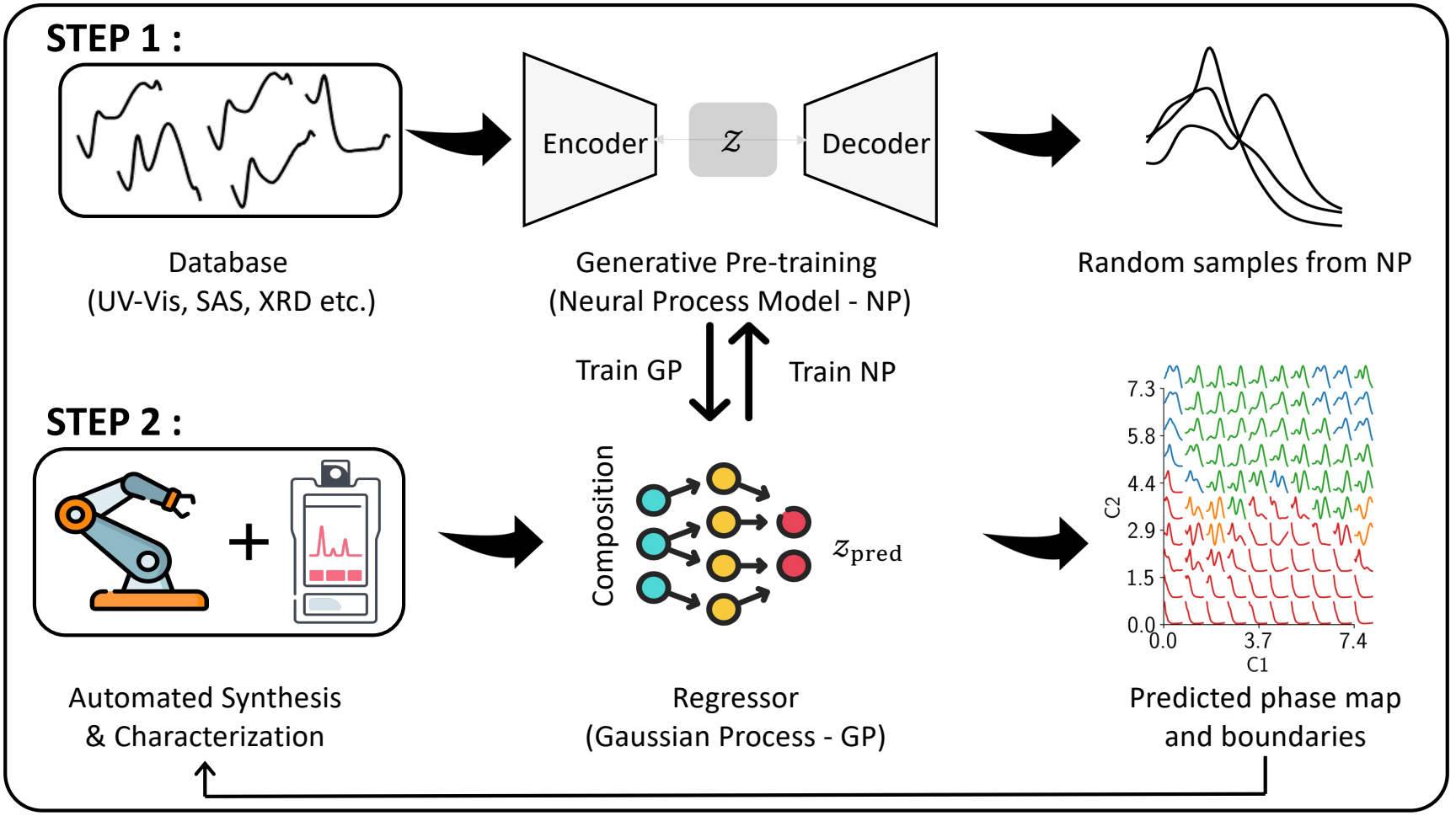


"Metric geometry tools for automatic structure phase map generation", K. Vaddi[2], K. Li[2], L. Pozzo, Digital Discovery, 2, 1471-1483, (2023)

Distance Metrics in Autonomous Phase Mapping

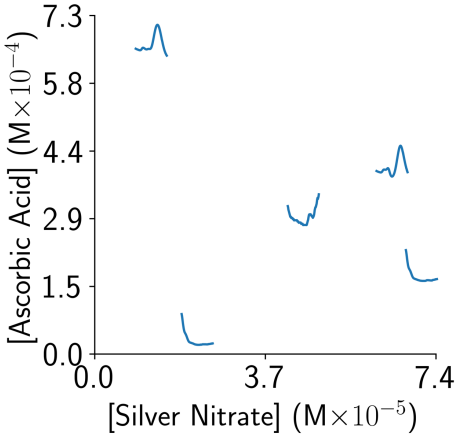


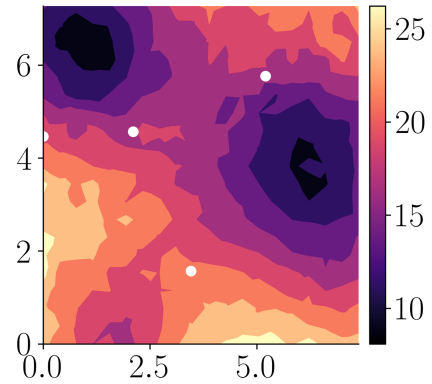
Two-step workflow for "differentiable" phase mapping

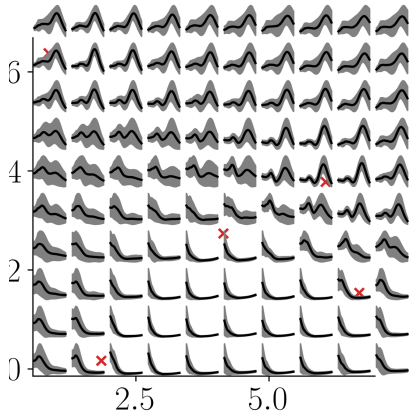


Learning to predict spectra from experiments

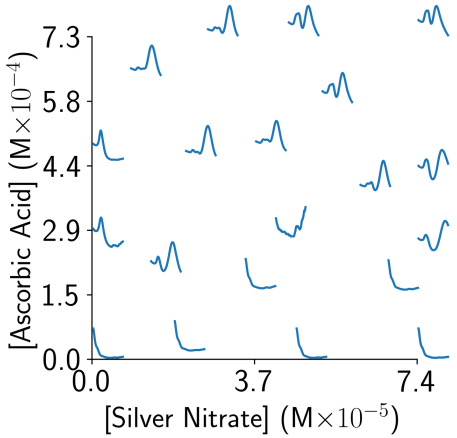
Iteration 1

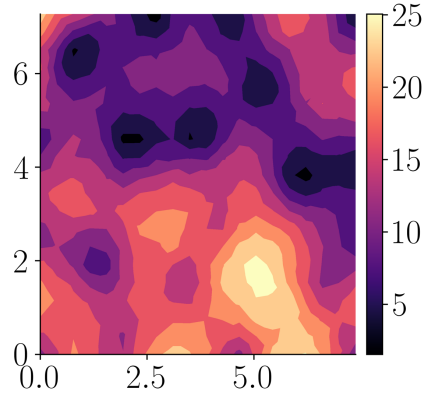


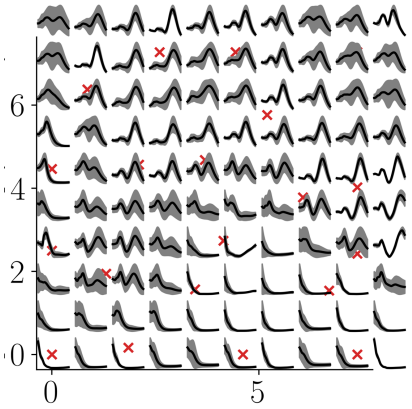




Iteration 5



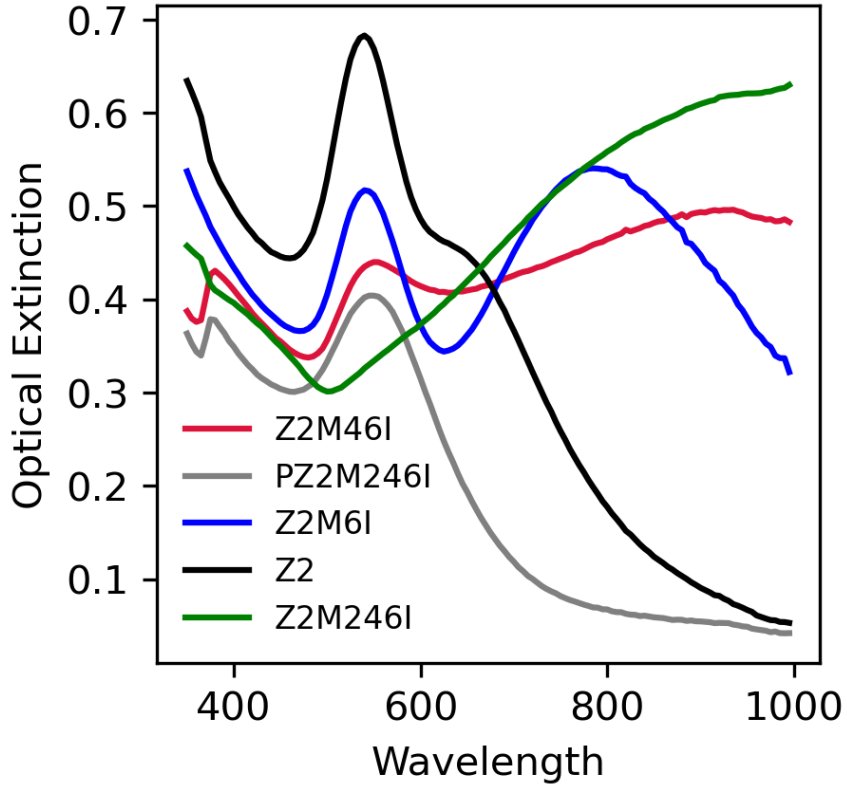


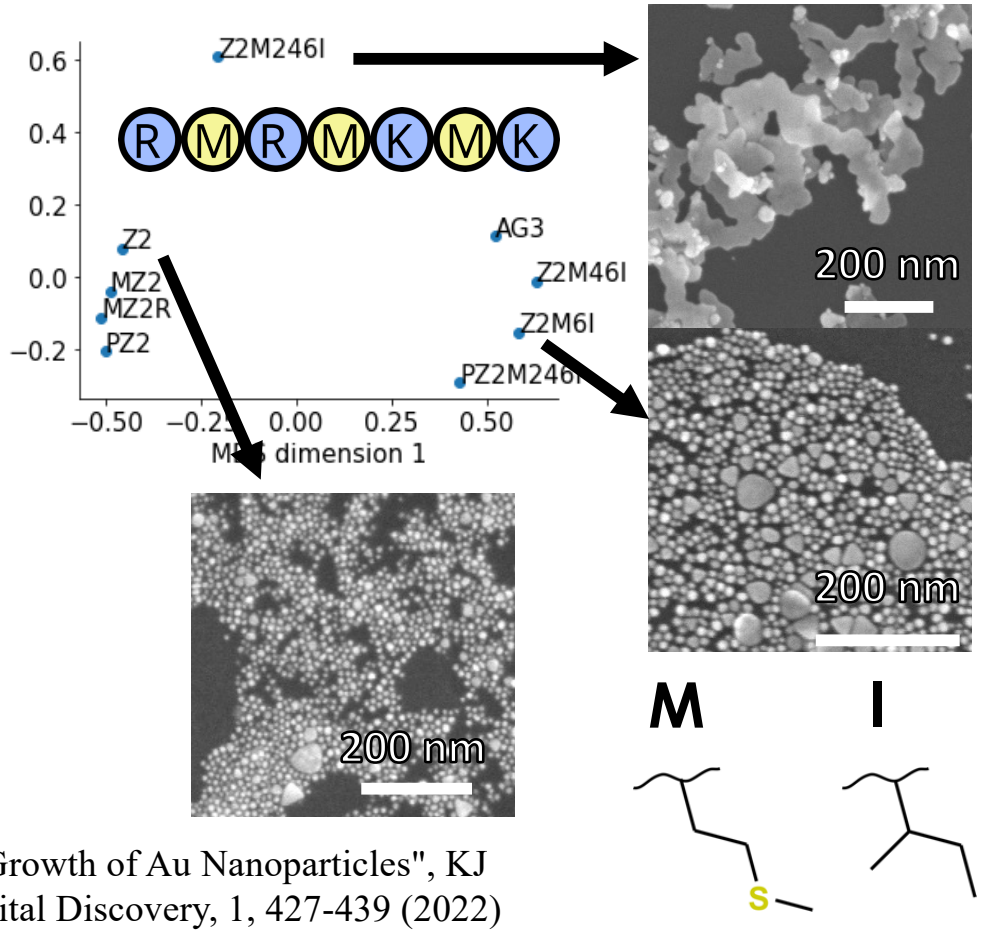


Timed Intervention

States Out-of-Equilibrium

Dynamic Intervention: Peptide-Mediated Growth





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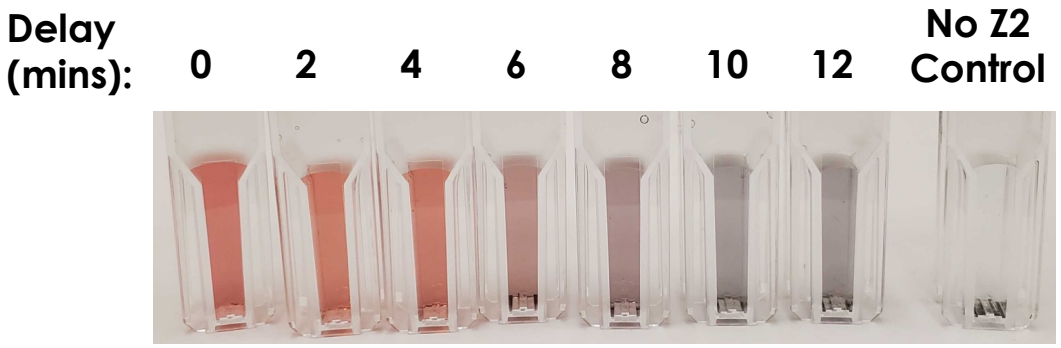
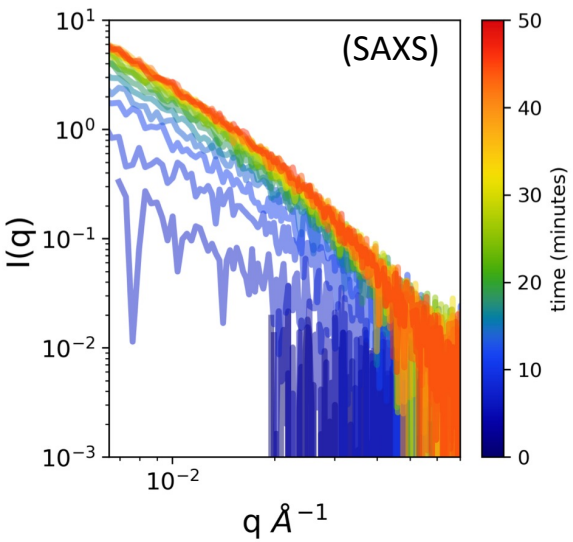
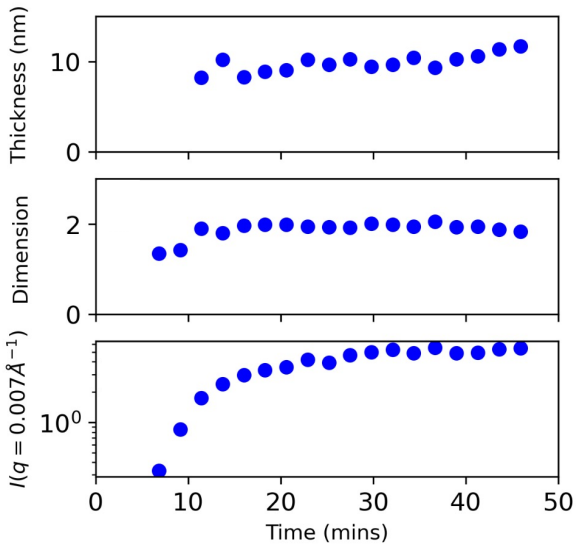
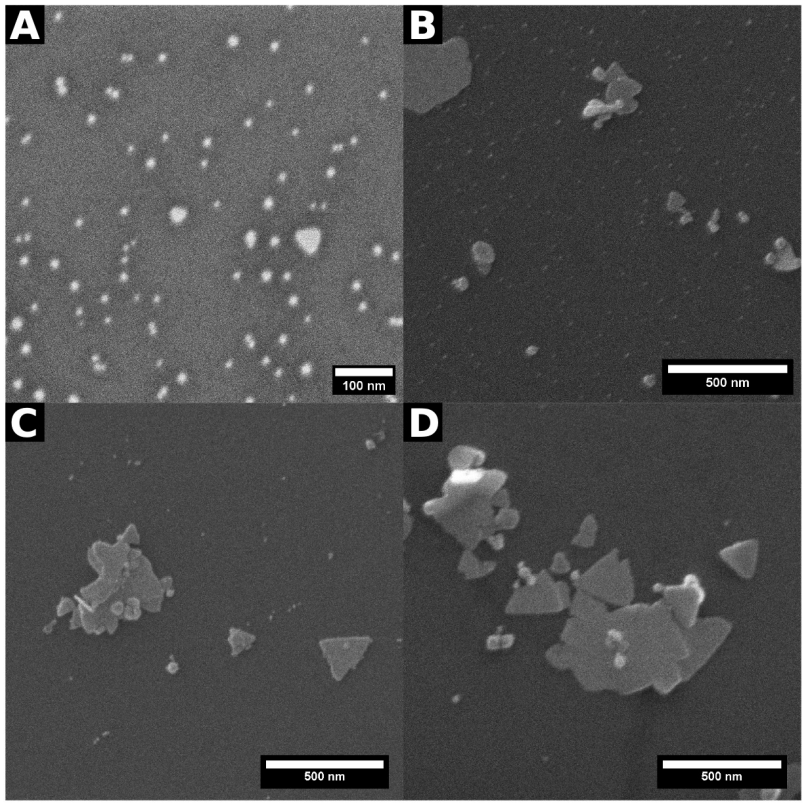
Dynamic Intervention: Accessing Out of Equilibrium States

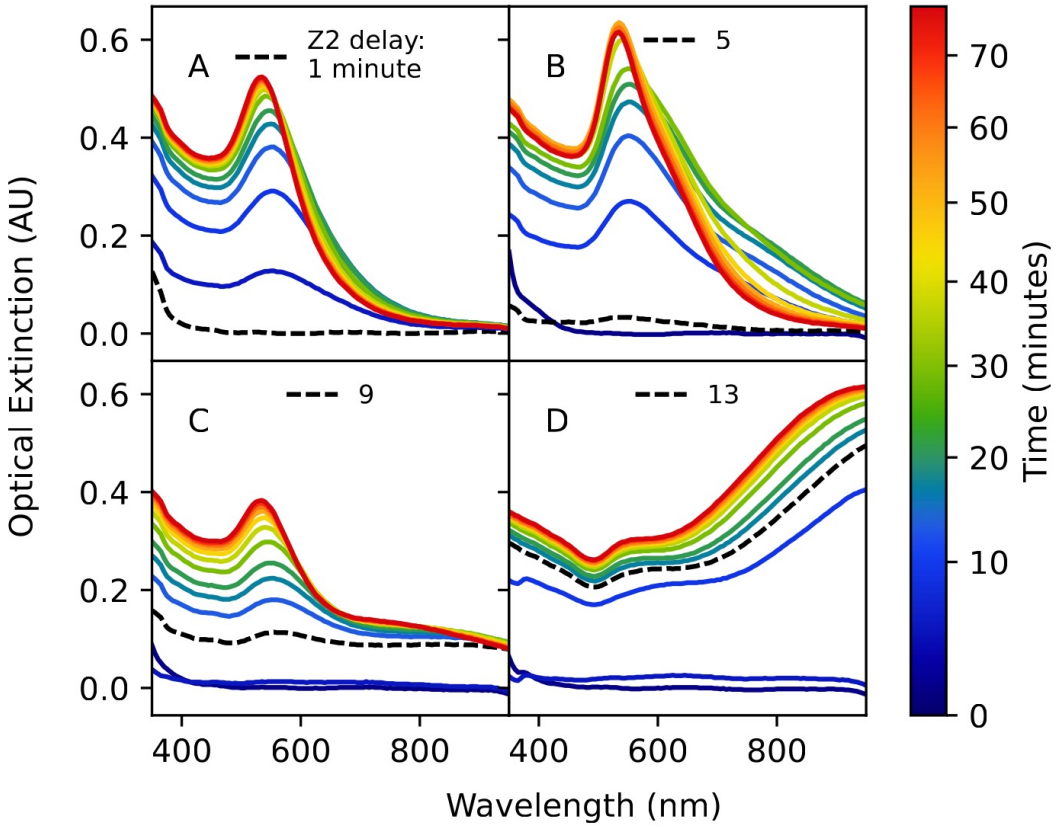


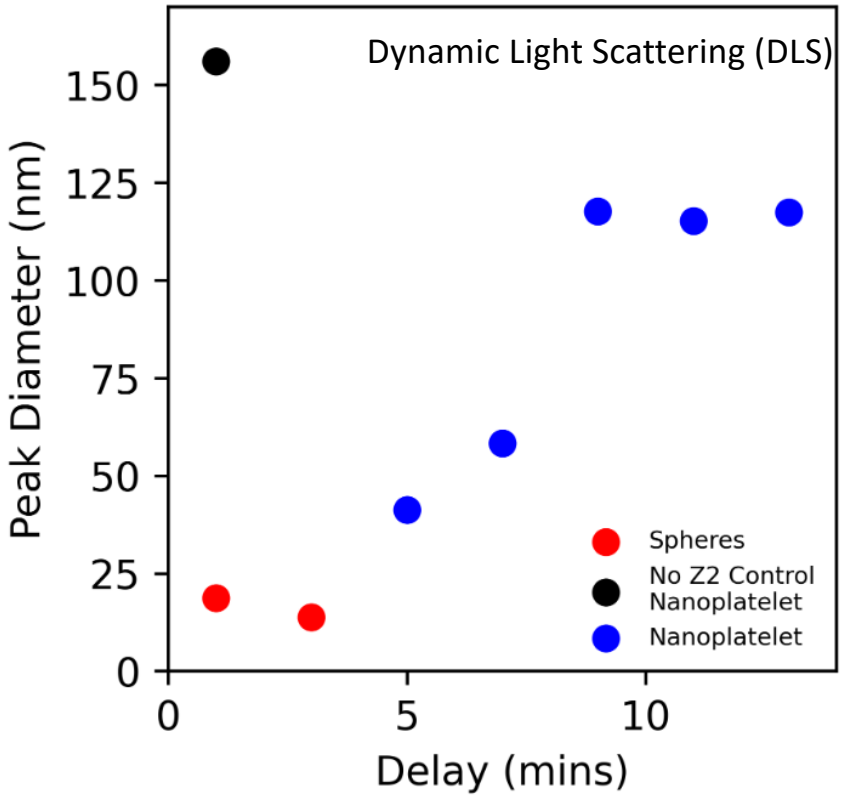






Dynamic Intervention with Z2 Stabilizes Small Plates





"Anisotropic Gold Nanomaterial Synthesis Using Peptide Facet Specificity and Timed Intervention" K. J. Lachowski, H. T. Chiang, K. Torkelson, W. Zhou, S. Zhang, J. Pfaendtner, L. D. Pozzo, Langmuir 39 (45), 15878-15888, (2023)

Conclusions

- Presented Tools for Broad Adoption of SDLs
- Distance metrics play an important role for AI agents working on functional data
- 'Shape Matching' distance (Amplitude-Phase) outperforms standard Euclidean and expert defined metrics
- Next Steps:
  - Multi-fidelity optimization with automated SAXS data
  - Pathway manipulation in non-equilibrium systems

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