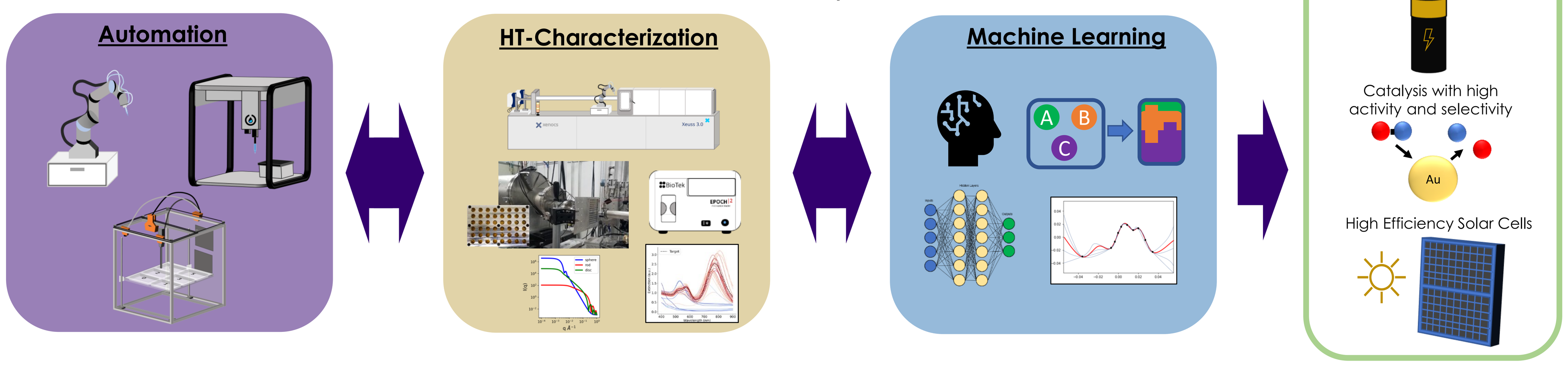
High-Throughput Scattering Characterization Combined with AI/ML to Accelerate Material Discovery

Huat Thart Chiang[1], Kiran Vaddi[1], Zhiyin Zhang[2], Akif Tezcan[2], Lilo Pozzo[1]

[1]Department of Chemical Engineering, University of Washington, Seattle WA USA
[2]UCSD Department of Chemistry and Biochemistry, University of California San Diego, CA USA

UNIVERSITY of WASHINGTON

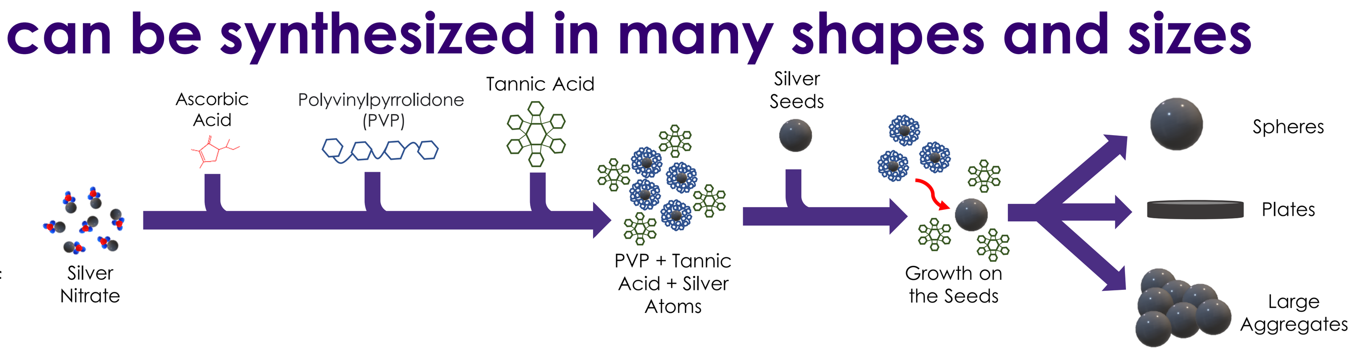
High-throughput characterization can be combined with sample automation and AI/ML to accelerate the discovery of new materials



Structural Control of Silver Nanoparticles

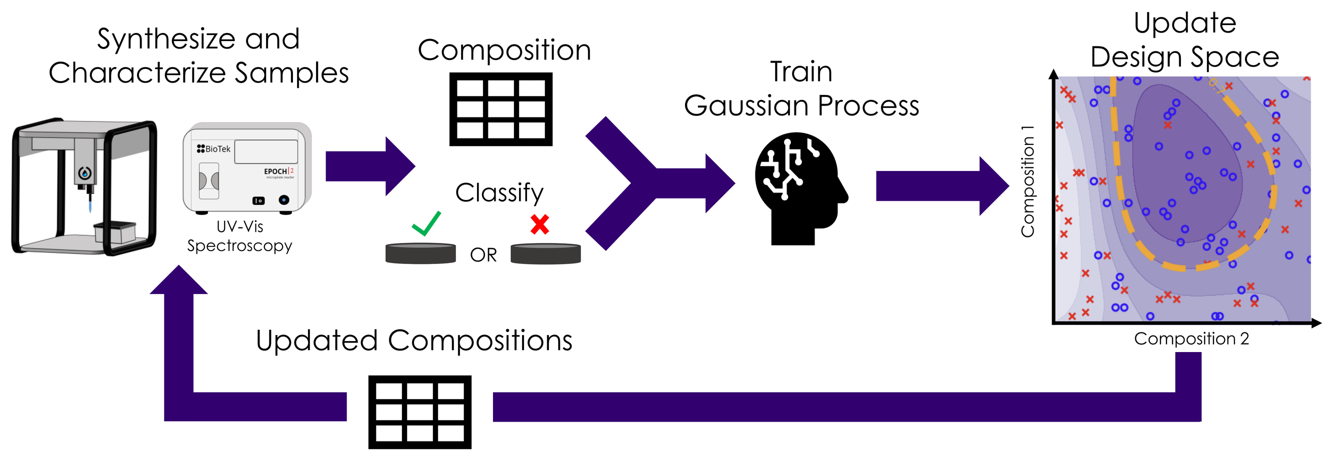
1. Silver nanoparticles can be synthesized in many shapes and sizes

- The experimental design space consists of Silver Nitrate, Ascorbic Acid, Polyvinylpyrrolidone, Tannic Acid, and Silver Seeds
- How can we synthesize nanoparticles of a desired shape and size?

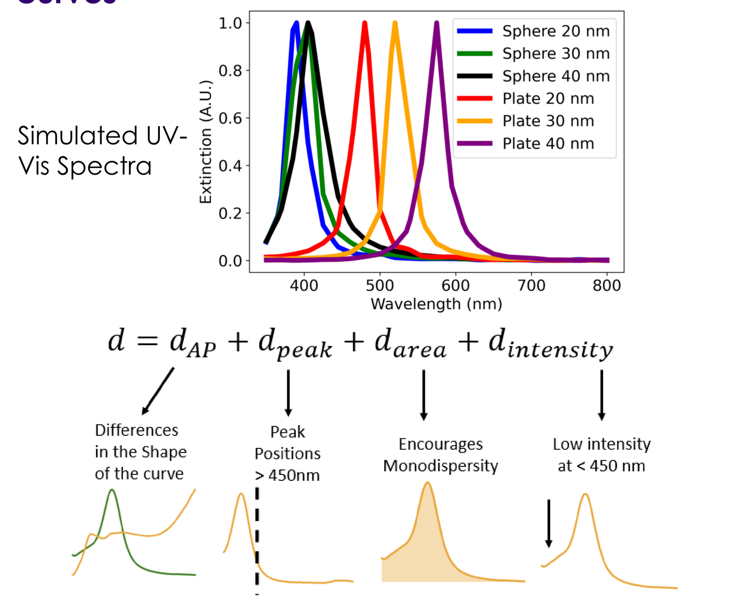


2. Fast Spectroscopic Exploration

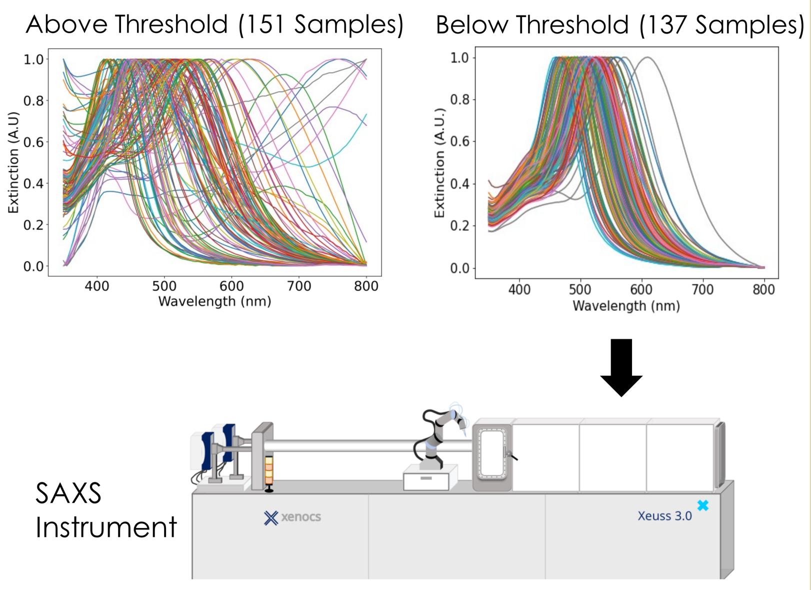
- Our method can be used to iteratively narrow down the design space until we form the targeted nanoparticles
- Our target will be small, colloidally stable, monodisperse, plate-like particles
- The use of UV-Vis spectroscopy allows for a fast and inexpensive characterization method



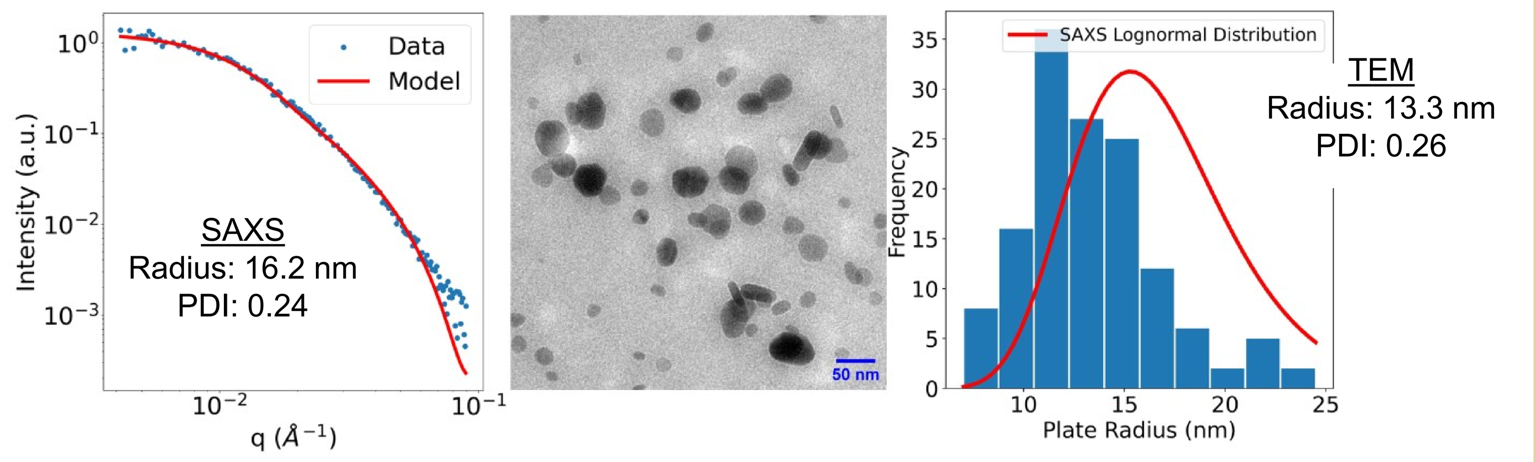
Distance Metric to Classify spectroscopy curves

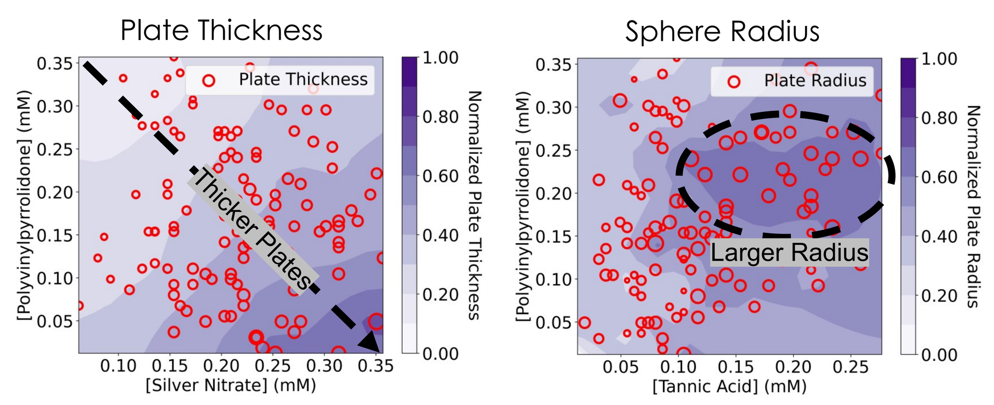


3. SAXS Structural Exploration



TEM and SAXS Have Good Agreement





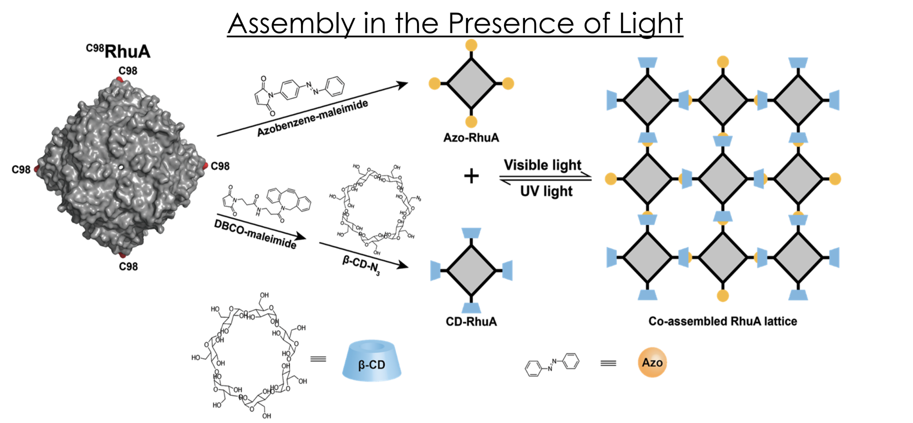
Size of markers are proportional to plate thickness (left) sphere radius (right)

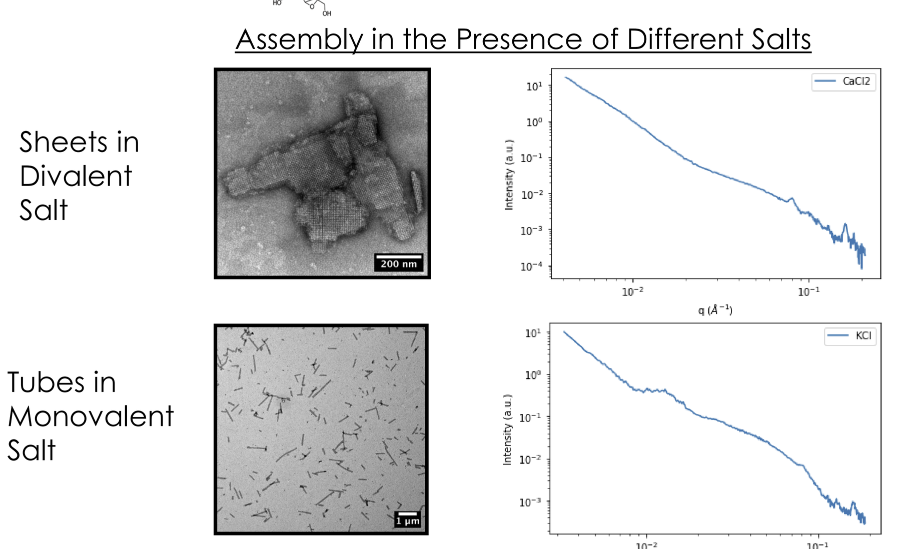
Conclusion

- A gaussian process was trained with UV-Vis spectroscopy data to find the experimental design space where small, monodisperse, plate-like particles are most likely to be formed
- SAXS was used to obtain information on the structure of the plates

Controlling the Self-Assembly of Photoresponsive Proteins

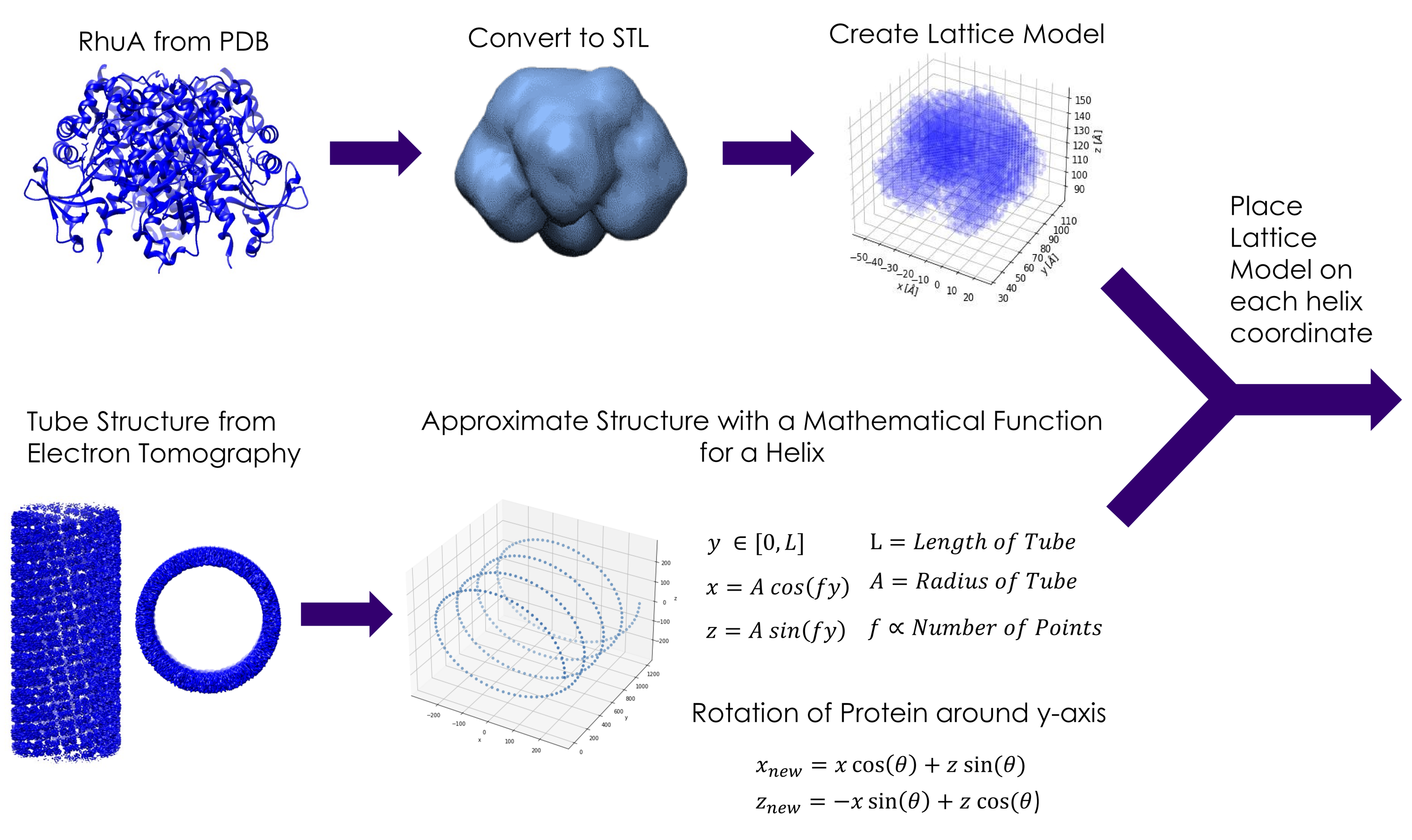
1. The RhuA protein can assemble in many structures

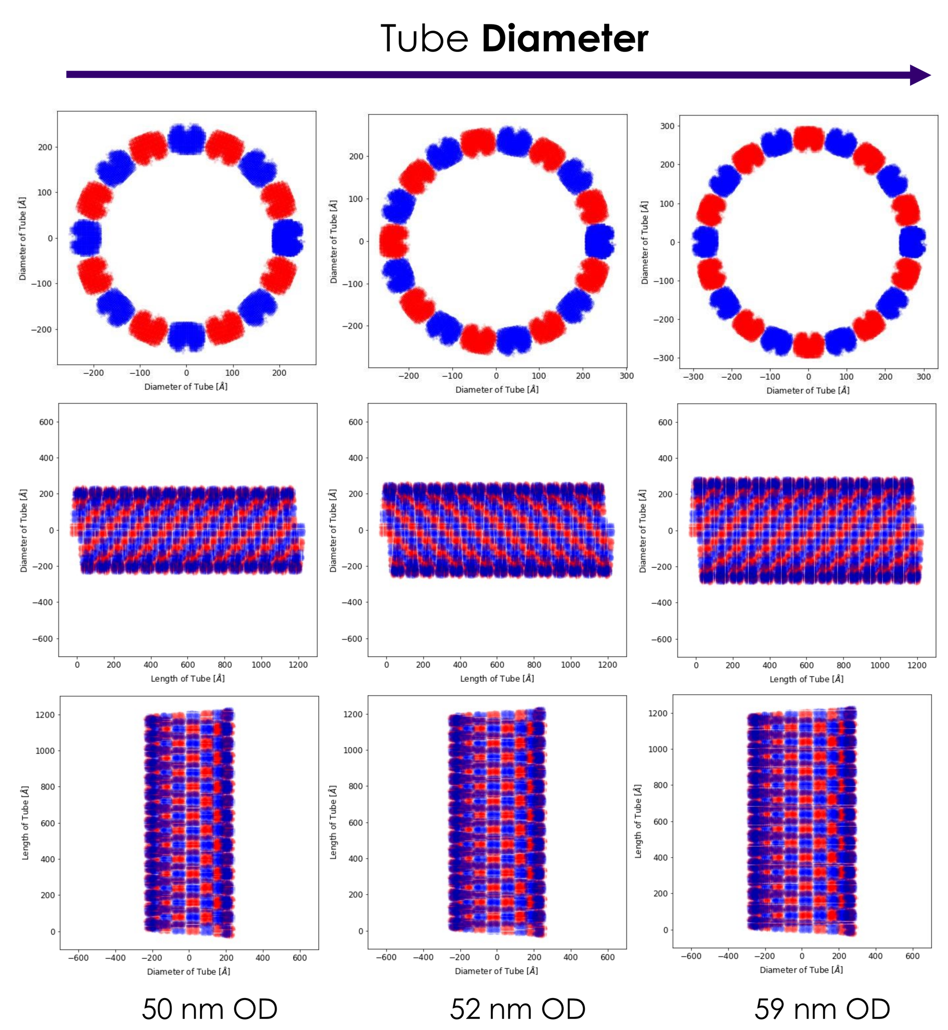




How do we interpret the SAXS curves?

2. Simulating the SAXS Curve of RhuA in a Tube Assembly





3. Fitting the Model

Using the Spherical Harmonics Method to solve the Fourier Transform

$$I(q) \propto \langle |A(q)|^2 \rangle_\Omega = \int_V \Delta\rho(r) e^{-iq\cdot r} dv$$

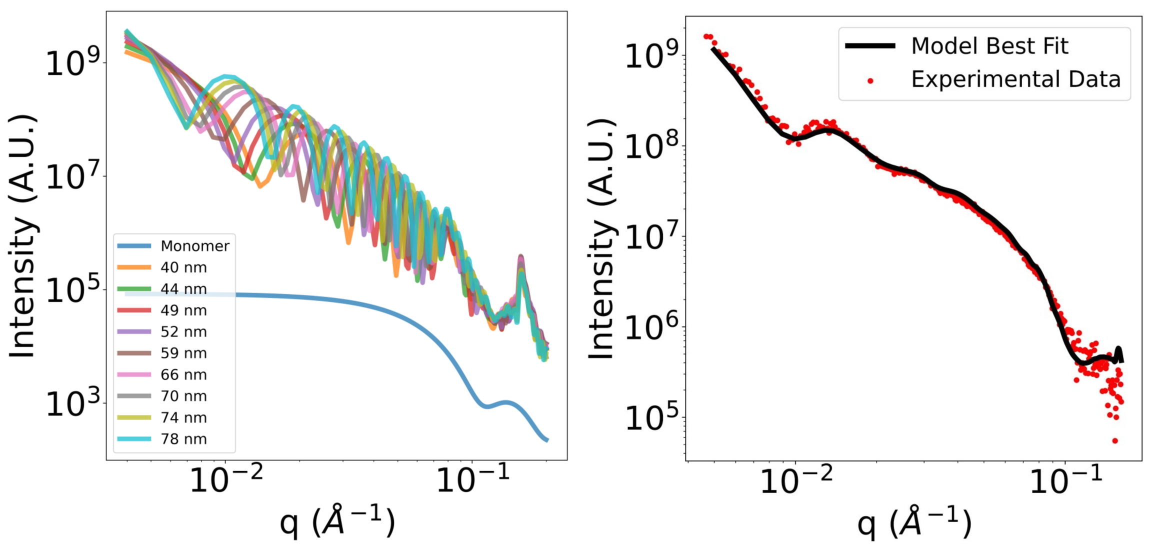
$$I(q) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \left| 4\pi i^l \sum_{j=1}^{N} \Delta\rho(r) j_l(q r_j) Y_{lm}^*(\theta_j, \varphi_j) \right|^2$$

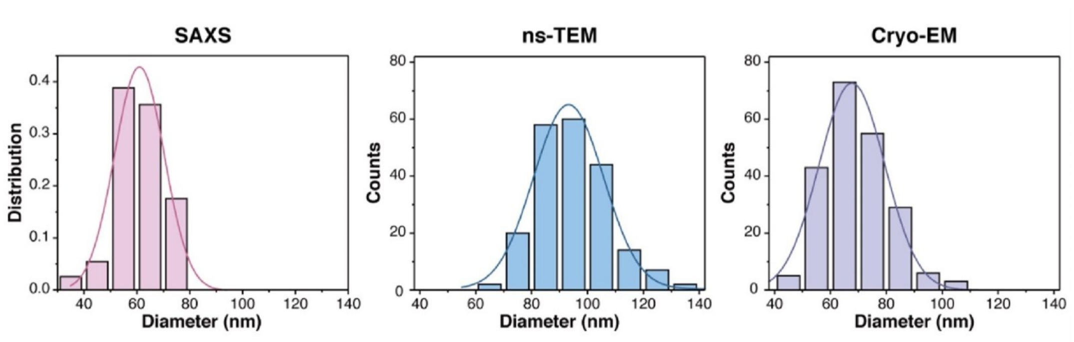
Fit the model to the Data

$$I(q)_{model} = w_{monomer}(I_{monomer}(q)) + w_1(I_1(q)) + \ldots + w_n(I_n(q))$$

$$Score = \sum_{q=0}^{\infty} \left| \log(I(q)_{model}) - \log(I(q)_{Exp\_data}) \right|$$

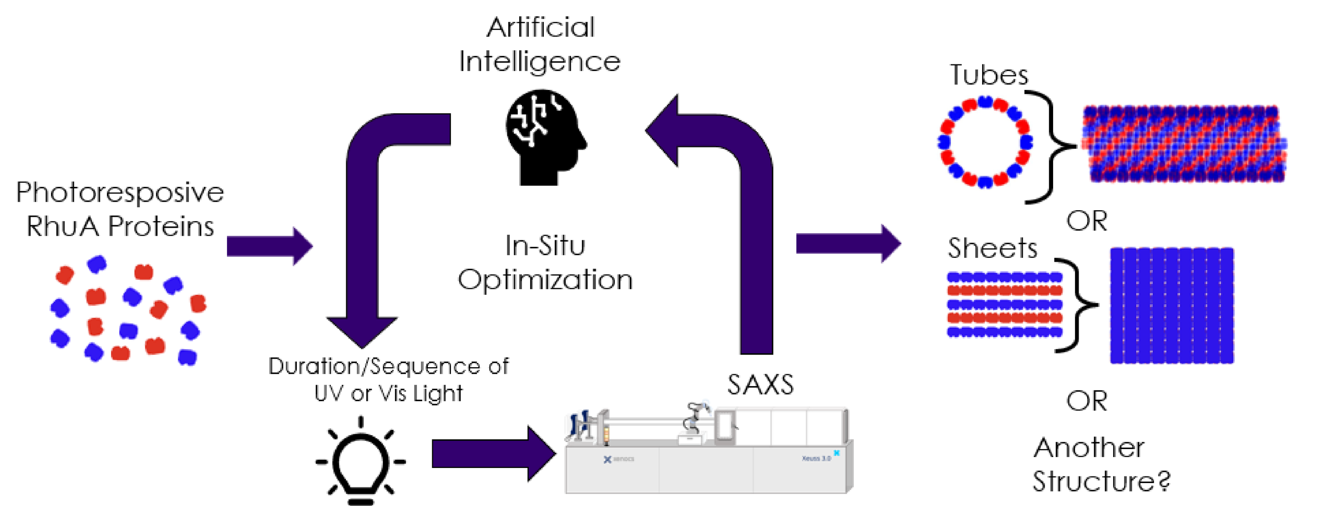
Find the optimal weights ($w_{monomer}, w_1, \ldots, w_n$) to minimize *Score*





Histogram of the Tube Sizes in the Sample

4. Future Work: Can we control the assembly?

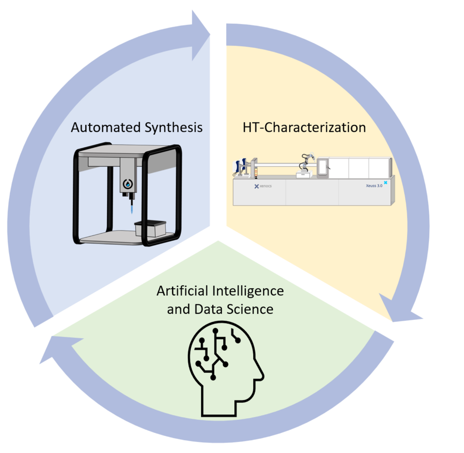


Conclusion

- SAXS is a fast (~3 minutes) *in situ* characterization method for the structures that the RhuA protein assembles in
- We can model different structures and fit them to our SAXS curves to find out the size of the structures that are formed and their polydispersity
- Our next objective is to control the structures that are formed using artificial intelligence, automation, and SAXS in a closed loop design

Conclusion

- High-throughput scattering characterization can be combined with AI/ML and automation to explore large experimental design spaces
- SAXS is a fast and information rich characterization technique for a diverse set of materials



Acknowledgements

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References

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