

# Machine Learning Based Computational Methods For Analyzing Small Angle Scattering Data From Soft Materials

A. Jayaraman<sup>a,b</sup>, Z. Wu<sup>a</sup>, C. Heil<sup>a</sup>, N. Gupta<sup>a,\*</sup> and S.V.R. Akepati<sup>c,\*</sup>

<sup>a</sup>Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE 19716, USA

<sup>b</sup>Department of Materials Science and Engineering, University of Delaware, Newark, DE 19716 USA

<sup>c</sup>Master of Science in Data Science Program, University of Delaware, Newark, DE 19716 USA

My research group's expertise lies in the development of physics-based molecular models and simulation methods as well as data-driven machine learning models for designing and characterizing soft macromolecular materials. In this talk, I will highlight examples from my group's recent work to showcase how we develop and use computational tools (e.g., CREASE [1-2], CREASE-2D [3], and PairVAE [4]) to interpret experimental characterization data from small angle scattering and electron microscopy. I will also show how we use these methods with experimental data that are either in the literature or shared by our collaborators in order to establish structure-property relationships (e.g., [5, 6]) for soft materials.

For interested researchers, we direct them to the *readme* documents for CREASE: <https://crease-ga.readthedocs.io/en/latest/> and codes shared openly in <https://github.com/arthijayaraman-lab>

## References

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- [5] C. M. Heil *et al.*, *Science Advances* **9**, 21, 10.1126/sciadv.adf2859 (2023).
- [6] A. Patil *et al.*, *ACS Materials Letters* **4**, 9, 1848–1854 (2022).

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Submitting Author: arthij@udel.edu