

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

Prof. Arthi Jayaraman

*Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE 19716, USA*  
*Department of Materials Science and Engineering, University of Delaware, Newark, DE 19716 USA*  
*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

- [1] C. M. Heil *et al.*, *ACS Central Science* **8**, 7, 996-1007 (2022).
- [2] C. M. Heil *et al.*, *JACS Au* **3**, 3, 889-904 (2023).
- [3] S.V.R. Akepati *et al.*, *JACS Au* **4**, 4, 1570-1582 (2024).
- [4] S. Lu and A. Jayaraman, *JACS Au* **3**, 9, 2510-2521 (2023).
- [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).

## Biography

Arthi Jayaraman is currently a full professor in the Departments of Chemical and Biomolecular Engineering and Materials Science and Engineering at the University of Delaware (UD), Newark. She is also the director for an NSF-funded NRT graduate traineeship program on 'Computing and Data Science Training for Materials Innovation, Discovery, and Analytics'.

She received her Ph.D. in Chemical Engineering from North Carolina State University and conducted her postdoctoral research in Materials Science and Engineering at the University of Illinois-Urbana Champaign.

Jayaraman's research has been recognized with honors/awards including AIChE COMSEF IMPACT Award (2021), Fellow of the APS (2020), ACS PMSE Young Investigator (2014), and AIChE COMSEF Young Investigator Award (2013), and Department of Energy (DOE) Early Career Research Award (2010)

Honors recognizing Jayaraman's excellence in teaching include Univ. of Delaware College of Engineering faculty award for excellence in teaching (2023), Univ. of Colorado chemical and biological engineering's outstanding graduate teaching award (2014), and Univ. of Colorado chemical and biological engineering's outstanding undergraduate teaching award (2011).

