Séminaire

Mardi 16 septembre 2025 à 10h30

Amphithéâtre Henri Benoît

Arthi Jayaraman

Dep. of Chem. and Biomol. Engineering, Dep. of Materials Science and Engineering, Data Science Institute,
University of Delaware, Newark, DE

Machine learning based analyses and interpretation of structural characterization data from soft materials

My research group specializes in developing physics-based molecular models and simulation methods, as well as data-driven machine learning models, for designing and characterizing soft macromolecular materials. In recent years, we have dedicated significant efforts to creating machine learning–based computational methods that accelerate and automate the interpretation of structural characterization data from scattering and microscopy techniques. In this talk, I will highlight several examples to showcase our recent work (e.g., CREASE [1-4], PairVAE [5], microscopy analyses [6,7]). I will explain the key features of these methods and how we apply them to experimental data shared by our collaborators to establish structure-property relationships across a broad range of soft materials.

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] R. Adhikari *et al., J. Appl. Cryst*, 58, 1384–1398 (2025)
[5] S. Lu and A. Jayaraman, *JACS Au* 3, 9, 2510–2521 (2023)
[6] A. Paruchuri *et al., Digital Discovery,* 3, 2533-2550 (2024)
[7] S. Lu and A. Jayaraman, *Progr. in Polymer Sci.* 153, 101828 (2024)

Users interested in the open-source codes can access them here: https://github.com/arthijayaraman-lab

CV on back.

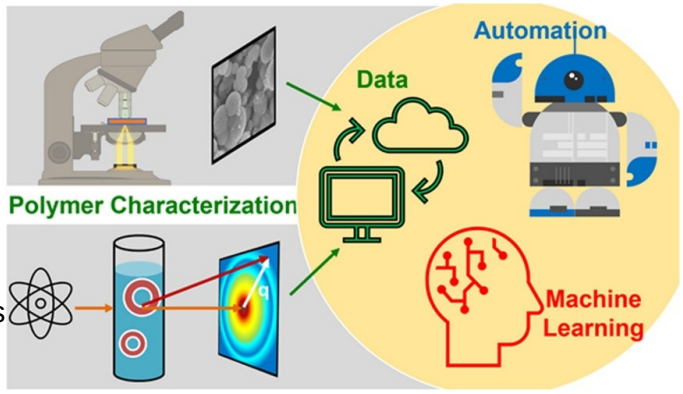

Figure 1: Image from Lu & Jayaraman [7]

Les personnes souhaitant rencontrer A. Jayaraman sont priées de prendre contact avec J. Baschnagel.

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 also directs an NSF-funded NRT graduate traineeship program on 'Computing and Data Science Training for Materials Innovation, Discovery, and Analytics'. She serves as an associate editor for Macromolecules and was the inaugural deputy editor for the first three years of ACS Polymers Au.

Jayaraman earned her Ph.D. in Chemical Engineering from North Carolina State University and completed her postdoctoral research in Materials Science and Engineering at the University of Illinois at Urbana-Champaign. After serving as the Patten Assistant Professor in the Department of Chemical and Biological Engineering at the University of Colorado (CU) Boulder, she joined UD faculty in 2014. Her research focuses on developing and applying computational techniques to study polymer nanocomposites, blends, solutions, and biomaterials.

Her honors include the American Chemical Society (ACS) PMSE Fellowship (2024), UD College of Engineering Faculty Award for Excellence in Teaching (2023), AIChE COMSEF Impact Award (2021), American Physical Society (APS) Fellowship (2020), Dudley Saville Lectureship at Princeton University (2016), ACS PMSE Young Investigator (2014), AIChE COMSEF division Young Investigator Award (2013), CU Provost Faculty Achievement Award (2013), Department of Energy (DOE) Early Career Research Award (2010), and CU Department of Chemical and Biological Engineering's outstanding undergraduate teaching award (2011) and graduate teaching award (2014).

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