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SÉRIE DE SÉMINAIRES

SEMINAR SERIES

Arthi Jayaraman

Dept. of Chemical and Biomolecular Eng. & Materials Science and Eng., University of Delaware, Newark, DE

Title | **Computational methods for analyses of small angle scattering and microscopy measurement results from macromolecular soft materials**

Abstract | My research group's expertise lies in the development of molecular models and simulation methods as well as machine learning workflows towards designing and characterizing new and improved soft macromolecular materials. In this talk, I will present our recent work developing machine learning workflows (e.g., CREASE [1,2] and PairVAE [3]) to interpret soft materials' structural characterization data from small angle scattering and microscopy. These methods provide an objective understanding of the distributions of length scales and patterns found within hierarchical structures in polymer materials. These workflows also help automate and/or accelerate structural characterization tasks towards establishing design-structure-property relationships in synthetic- & bio- polymers and formulations.

1. Christian M. Heil, et al. ACS Central Science (2022), 8, 7, 996-1007
2. Christian. M. Heil et al. JACS Au (2023) 3, 3, 889–904
3. S. Lu and A. Jayaraman, JACS Au (2023) 3, 9, 2510–2521

Bio | 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).

Contact | Audrey Laventure < audrey.laventure@umontreal.ca>

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