

THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT
FALL COLLOQUIUM SERIES PRESENTS:

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Emerging crystalline order in self-assembly simulations of complex structures

In both hard and soft condensed materials, spanning length scales from atomic to mesoscopic, have crystal structures of increasing diversity and complexity been discovered over decades of structural research. On all scales, the complexity spectrum spans from the simplest sphere packings to structure types with large unit cells or even aperiodic crystals. Moreover, the same intricate crystal structures can be observed in disparate materials systems, implying that general principles of structure formation underlie the processes of crystal growth and stabilization. We study the assembly and structural features of complex crystals via numerical simulations, in order to investigate the emergence of long-range order from short-range interactions. By employing simple coarse-grained models, we gain systematic insights into the phenomena that lead to the crystallization of complex types of order, with the ultimate aim to generate a deeper knowledge of structure formation that will allow for the design of tailored, functional materials in the future.

Dr. Julia Dshemuchadse received her Diploma degree in Physics from TU Dresden, Germany, and her PhD in Materials Science from ETH Zurich, Switzerland. In her doctoral work she investigated structural principles of complex intermetallic compounds with crystallographic methods and data mining. As a postdoctoral researcher, Dr. Dshemuchadse joined the University of Michigan, Ann Arbor on a fellowship from the Swiss National Science Foundation and performed computational research of the self-assembly behavior of soft matter. Dr. Dshemuchadse joined the Department of Materials Science and Engineering at Cornell University as an Assistant Professor in 2019. Her group studies abstract model systems to discover fundamental principles of crystal structure formation and stability.

Dr. Dshemuchadse co-authored a book entitled “Intermetallics – Structures, Properties, and Statistics”, published in 2016 by Oxford University Press. She was awarded an NSF CAREER Award in 2021, as well as a Machine Learning in the Chemical Sciences and Engineering Award by the Camille and Henry Dreyfus Foundation in 2022.

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In person only; no Zoom

Questions? Contact allison.macknick@northwestern.edu and megan.ray@northwestern.edu