

The Department of Chemical Engineering Presents:



*“Investigating crystal structure formation and stability in self-assembly simulations”*

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3:30PM via Zoom:

<https://rochester.zoom.us/j/98875611576?pwd=RHY3bmhrRFZEMGhiUW5wZ0VlaDNuUT09>

**Abstract:** Self-assembly processes in soft condensed matter have been leading to the discovery of increasingly complex ordered structures. Many of these mesoscale structures have geometric equivalents on the atomic scale. We investigate the variety of crystal structures stabilized by minimalistic particle models via numerical simulations and examine the robustness of their structure formation. Isotropic particles that interact with multi-well pair potentials can form structures that correspond to atomistic systems with various types of chemical bonding, as well as those that have no known equivalents at all. We study the process of crystal growth, as well as the structural behavior of such particle systems when additional parameters like polydispersity and confinement are introduced. Our goal is to provide design targets for soft materials with new properties, with enhanced assembly robustness, and with tunable characteristics. By investigating these behaviors and features in abstract systems, we aim to deduce overarching rules of structure formation in order to identify fundamental principles of the emergence of order in condensed matter.

**BIO:** Dr. 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 earned the Max-von-Laue award from the German Crystallographic Society in 2015 and an Outstanding Postdoctoral Fellow Award of the University of Michigan in 2016. She co-authored a book entitled “Intermetallics – Structures, Properties, and Statistics”, published in 2016 by Oxford University Press