

SPRING 2023

MSE 690 SEMINAR SERIES

FRIDAY, APRIL 21ST, 2023 | 3:30 REFRESHMENTS | 3:45PM SEMINAR | ARMS 1010

“Free Energy Contributions to Template-Assisted Self-Assembly of Nanoparticles”

Abstract: Directed self-assembly of nanoparticles (DSA-n) over a templated surface has attracted a lot of interests for a wide variety of applications in semi-conducting, plasmonic, and photovoltaic devices, and molecular-specific imaging and sensing. It is commonly thought that the wedge-mechanism of DSA of micrometer sized particles onto templated surfaces would apply to DSA of sub-10 nm particles. Using particle simulations, we present a model to understand the mechanisms of DSA of sub-10 nm particles onto array of nanocavities as a template. The simulation results suggest that random hopping mechanism ahead of the receding meniscus plays the major role in DSA of sub-10 nm particles. We present a phase diagram of DSA yield as a function of liquid film thickness (confinement) and nanoparticle density, and discuss the impact of template geometry, nanocavity size and spacing, and nanoparticle ordering in the bulk on the DSA yield. We also predict the free energy contribution to DSA-n over a templated surface for both stagnant and receding liquid film. Our simulation results suggest that the impact of the receding liquid film on the free energy associated with DSA of a nanoparticle is similar to that of stagnant liquid film. Taken together, the results provide new insights into the potential mechanisms of DSA of nanoparticles onto templated substrates and the relevant driving factors, which help future experimental design of DSA onto templated surfaces to increase the yield and decrease the defect density.

Biography: Shafigh Mehraeen is an Assistant Professor of Chemical Engineering at the University of Illinois at Chicago (UIC). He received his Ph.D. from Stanford University in 2011. After a post-doctoral appointment at Georgia Institute of Technology, and later at MIT, he joined the faculty at the University of Illinois at Chicago. His group’s research focuses on understanding nanoparticle self-assembly, and enabling materials design using atomistic and molecular simulations and machine learning. His research has been funded by several funding agencies including NIH, SERDP, Argonne National Laboratory, Microsoft, and Nvidia. He was the 2018 and 2019 recipient of outstanding teaching awards from the College of Engineering at UIC.



SHAFIGH MEHRAEEN

Assistant Professor
Department of Chemical
Engineering
University of Illinois at
Chicago (UIC)



PURDUE
UNIVERSITY®

School of Materials Engineering