

SPECIAL SEMINAR

Building the Future, One Interaction at a Time: Emergent Architectures & Functions from Self-Assembly of Nanoparticles & DNA



... **Prof. Gaurav Arya**

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This talk will discuss the role of molecular simulations in designing new material architectures and functions based on the assembly of polymer-grafted nanoparticles and DNA origami nanostructures. First, I will show how molecular simulations have played an instrumental role in developing a new strategy for assembling nanoparticles into unique higher-order structures. This approach harnesses the competition between interparticle and interfacial interactions at a fluid-fluid interface to assemble nanoparticles into tunable clusters, strings, networks, superlattices, and perforated structures. These architectures have potential applications in plasmonics, optics, membranes, and catalysis, where precise control over particle orientation and spatial arrangement is critical for function. Second, I will highlight how simulations can reveal the behavior of DNA origami nanostructures from their folding to their collective dynamics. I will discuss how simulations elucidate the folding mechanisms of individual origami structures, provide insight into their higher-order assembly into superlattices, and reveal the emergent collective behavior of dynamic DNA nanostructure assemblies, including mechanically mediated communication and order-disorder transitions. Such programmable systems, capable of exhibiting complex architectures or collective phenomena, could enable new approaches to sensing, soft robotics, photonics, and energy harvesting. Finally, I will highlight how AI and machine learning are increasingly enhancing molecular simulations by helping capture complex many-body interactions, accelerating the development of coarse-grained models, and enable the inverse design of hierarchical architectures with targeted properties.

Tuesday, September 22, 2026 at 3:30pm

Mani L. Bhaumik Collaboratory

Dongwon Yoo Seminar & Conference Hall (Young Hall 4222C)

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