



**CHEMISTRY &
BIOCHEMISTRY**

DATE 11/15/2024 | **TIME** 01:30pm | **LOCATION** COB1 267

CHEMISTRY & BIOCHEMISTRY SEMINAR SERIES: Folding, surface-placement, and higher-order assembly of DNA nanostructures

Abstract:

DNA nanotechnology is a rapidly growing field that holds great promise for creating nanodevices capable of complex functions, including drug delivery, molecular sensing, nanomanufacturing, and molecular computing. However, for many of these applications to become a reality, the devices need to be assembled into macroscopic arrays to achieve higher throughput and more complex functions. As the PI of a molecular modeling lab, I will discuss how our lab is addressing this challenge using statistical mechanics, molecular simulations, and machine learning, often in close collaboration with experimentalists. Specifically, I will describe our ongoing efforts in: (i) understanding the dynamical process by which DNA origami (a design approach for efficiently fabricating DNA nanostructures) fold; (ii) creating brush-functionalized DNA origami and assembling them into superlattices with guidance from machine learning algorithms; (iii) developing assemblies of dynamic origami devices capable of exhibiting emergent functions like signal communication and macroscopic order-disorder transitions; and (iv) controlling the energy landscape of origami-surface binding to achieve orthogonal placement of multiple DNA structures on surfaces.



Gaurav Arya

Professor
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About the Speaker:

Gaurav Arya is a Professor of Mechanical Engineering and Material Science, Biomedical Engineering, and Chemistry at Duke University. Prior to joining Duke in Fall 2017, he was an Assistant Professor and then Associate Professor in the Department of NanoEngineering at UC San Diego. He obtained his B.Tech. degree in Chemical Engineering from IIT Bombay in 1998, and Ph.D. degree, also in Chemical Engineering, from the University of Notre Dame in 2003. He carried out postdoctoral research at Princeton University and New York University. Professor Arya's research focuses on molecular-scale modeling of biological and soft materials. Specifically, he uses simulations, often combined with theory or machine learning, to predict material properties and gain molecular-level understanding of material behavior, with the overarching aim of discovering new phenomena and developing new materials. His current research falls within the themes of nanoparticle-polymer composites, DNA nanotechnology, and DNA translocation motors, and is well-supported by grants from NSF, DOE, and NIH. His group has published over 100 peer-reviewed articles and 2 book chapters.

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