UNIVERSITY of HAWAIʻI at MĀNOA™
MECHANICAL ENGINEERING

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Holmes Hall 287
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Discovering Self-Assembly Properties of Patchy Particles using Inverse Design

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Abstract
Soft materials, including colloids, polymers, and biological assemblies, exhibit complex self-organization driven by weak, highly tunable interactions. Their ability to form structures across length scales makes them central to the study of self-assembly and materials design. Within this class, patchy particles provide a coarse-grained, minimal, and highly tunable model for directional interactions, retaining only essential features, such as building-block geometry and binding specificity. These particles can be engineered to assemble into targets ranging from finite clusters to bulk crystals, spanning synthetic colloids and biological analogs such as viral capsids. Despite this flexibility, the design space is effectively unbounded, yielding a high-dimensional landscape that can be systematically explored using inverse design techniques. Although prior work has developed frameworks for targeted assembly, the interplay between key design parameters remains poorly understood. Here, we address this gap using differentiable molecular dynamics with JAX-MD. We show that the design landscape is governed by structural floppiness, and that stiff and sloppy parameter directions can be identified through Hessian analysis of the full optimization space.

About the Speaker
Gregory Snyder is a PhD student in Mechanical Engineering working under the supervision of Dr. Chrisy Xiyu Du. Gregory received his MS in Mechanical Engineering from the University of Hawai`i and his BS in Aerospace engineering from the Pennsylvania State University. His current research focuses on the implementation of inverse design techniques in the development of self-assembling patchy particles. His previous research covered applications of Koopman operator theory with autonomous mobile platforms.