# BIOENGINEERING SEMINAR

FALL 2022

## DNA at the Multi-Scale: Theory and Applications


### Abstract

The Holliday junction motif in nucleic acids is utilized as a building block to create strand crossovers between duplexes of DNA, and repeated use of this motif allows the creation of large-scale wireframe structures in arbitrary 2D and 3D shapes, called DNA origami. In this talk, we investigate the properties of DNA at various scales, including electronic-level properties, sequence effects at the junction level, and overall dynamics of large-scale DNA origami assemblies. Accurate electronic structure calculations of DNA sequences are difficult-to-impossible due to extremely inefficient scaling of quantum chemical calculations as the system size increases. It is shown that a machine learning algorithm based on Euclidean neural networks, where the training data includes accurate electronic structure calculations of smaller fragments of DNA, namely, the relevant base-pair steps, can be utilized to reproduce the electron density of arbitrary DNA sequences to an error of less than 1%. DNA junctions are utilized as the basic building block of DNA origami, but the base sequence effects on these junctions are not well understood. By utilizing molecular dynamics simulations at the junction-level, it is shown that changing the core sequence at the junction has a dramatic effect on the isomerization energies and dynamics of the Holliday junction motif. The system-level effect of motif design on large-scale DNA origami structures is difficult to quantify, but global system dynamics of these DNA origami structures can be simulated as well using molecular dynamics. Different strategies for creating these large-scale DNA origami structures are presented, with an emphasis on the level of control available with regards to the structural fidelity. Finally, we will consider why it is important to understand the properties of DNA at these various levels of scale with an energy transfer application. DNA origami can be utilized as a scaffold for photoactive molecules, with the goal of creating an efficient energy transfer network. It is seen that both the local and global properties of the DNA scaffold itself influence the energy transfer between scaffolded photoactive molecules, hence it is important to fully understand DNA at the multi-scale.


### Biography

Prof. William Bricker is an Assistant Professor in the Department of Chemical and Biological Engineering at the University of New Mexico, starting in the Fall of 2019. He received his PhD in Energy, Environmental, and Chemical Engineering at Washington University in St. Louis, where he studied the theory of energy transfer in natural biological light-harvesting complexes from photosynthesis. As a postdoctoral associate in the Biological Engineering department at MIT, he utilized computational chemistry tools to research novel synthetic excitonic devices using DNA as a scaffolding material. His current research focuses on attempting to understand structure-to-function relationships in biology by utilizing tools from computational chemistry.


## William P. Bricker, PhD

Assistant Professor,
Chemical and Biological Engineering
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**Thursday, September 8th**
**12:00-1:00 pm**

Fairfax Campus:
**Horizon Hall, Rm 1012**

Live streaming to SciTech Campus: KJH 258

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