Computational Design and Modeling of Semiconductor Biohybrids via DNA Voxel Guided Self-Assembly

Emily Yao[1], Thi Vo[2]

[1]Department of Materials Science & Engineering, Johns Hopkins University, [2]Department of Chemical Engineering, Johns Hopkins University
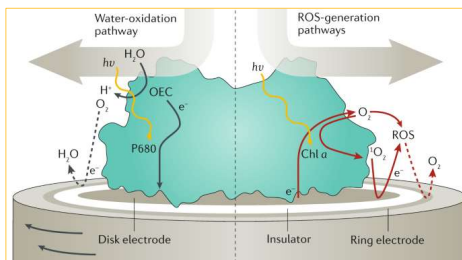
Abstract

Through a novel approach involving **DNA voxel guided self-assembly** and crystallization, this project aims to **decouple the interactions between organic and inorganic components** to design a system that is not only structurally efficient but also leverages the efficiency of natural photosynthesis.

This project aims to engineer complex materials systems with precision by drawing inspiration from photosynthesis to enhance systems' performance and innovating sustainable energy solutions that boast a minimized ecological footprint.
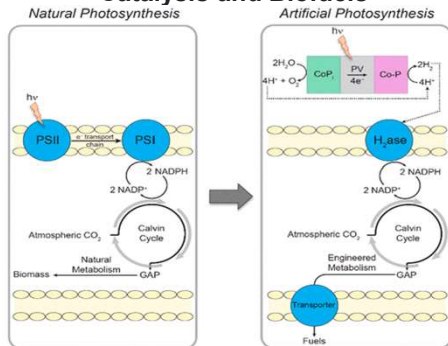
Self-Assembling a Biohybrid System

Aim 1: Design and Assembly of DNA Building Blocks

Nano-Objects   Directional (tip-to-tip) Interactions   2D Kagome Lattice

Properties Analysis

Aim 3: Analysis of Diffusive Properties

Understanding how particles diffuse and interact is crucial for predicting and controlling the self-assembly process.

Stokes-Einstein Equation

$$D = \frac{kT}{\xi}$$
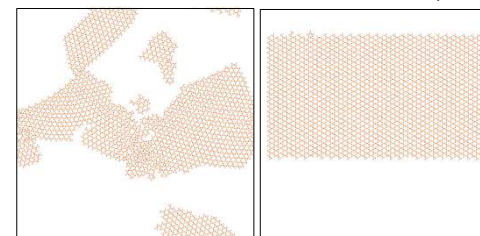
Field Strength ≥3   Field Strength <3
t = 14000 steps   t = 14000 steps

|Force Field|	Stability
1	✓
2	✓
3	✗

Future Development

1. **Experimental Validation**: Conduct laboratory experiments to correlate simulated predictions with real data.
2. **Stability and Long-term Behavior**: Investigate the longevity and resilience of organic materials within biohybrid systems, focusing on their stability and degradation behaviors.

Applications

Electrode-Enhancing Interfaces

Zhang et. al Nature Review Chem (2020)

Catalysis and Biofuels
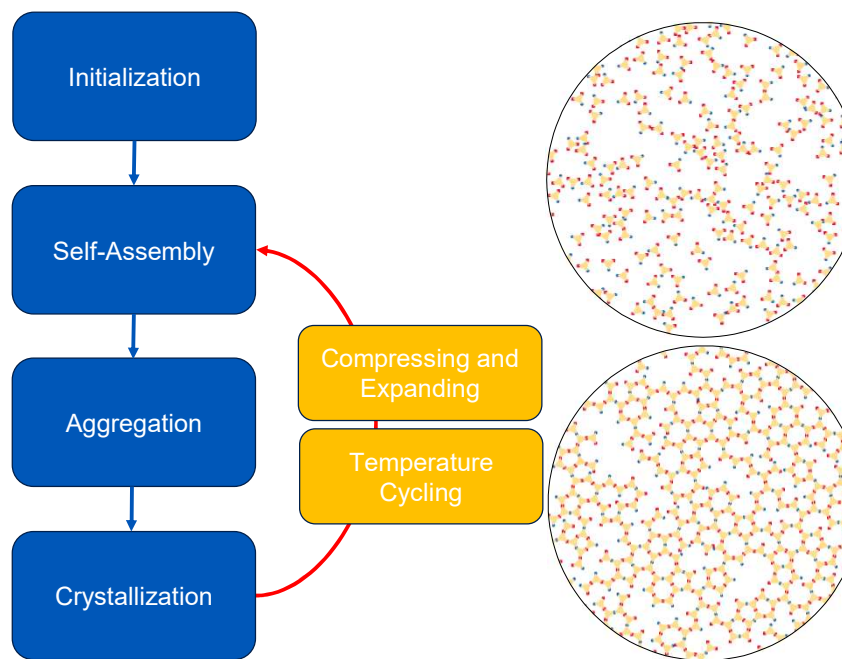

Dogutan et. al ACS (2019)

Molecular Dynamics Simulations

Aim 2: Protocol Development for Self-Assembly

Initialization

Self-Assembly

Aggregation

Crystallization

Compressing and Expanding

Temperature Cycling

References

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[3] V. Ramasubramani, B. D. Dice, E. S. Harper, M. P. Spellings, J. A. Anderson, and S. C. Glotzer. freud: A Software Suite for High Throughput Analysis of Particle Simulation Data. Computer Physics Communications Volume 254, September 2020, 107275. doi:10.1016/j.cpc.2020.107275.

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