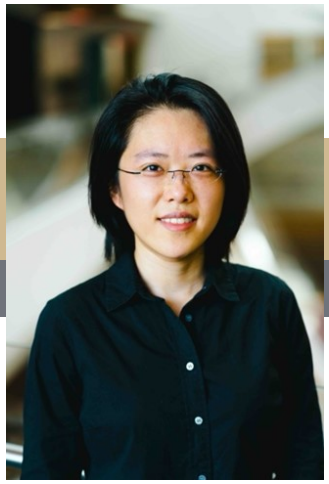
Physical Chemistry Seminar

Computational Strategies for Designing Macromolecular Photocatalysts: Physics-Based Simulations, Data-Driven Approaches, and Quantum Computing

Dr. Sijia Dong

Assistant Professor, Department of Chemistry and Chemical Biology
Affiliated Faculty, Department of Physics and Department of Chemical Engineering
Northeastern University



The understanding and design of photophysical and photochemical processes in macromolecules is critical in developing molecular systems for solar to chemical energy conversion, new chemical synthesis strategies, and light-responsive materials. For example, photoenzymes are emerging protein-based photocatalysts that are repurposed from natural enzymes for non-natural reactions difficult for small-molecule catalysts. They exhibit extraordinary selectivity, scalability, and tunability, and offer a promising new toolbox for solar energy conversion and chemical synthesis. However, the understanding and design of photoenzymes and other macromolecular photocatalysts pose several challenges. First, accurate first-principles simulations of the electronic structure of macromolecules are usually computationally expensive, especially those that involve strong electron correlation. In this talk, I will discuss our computational strategies, including data-driven methods and quantum computing, particularly quantum annealing, to tackle this challenge. Second, existing enzyme design strategies do not consider electronic excited states, and photoenzyme engineering has mainly relied on directed evolution. I will discuss our work on physics-informed computational photoenzyme design, where we combine physics-based simulations and data-driven methods to demonstrate that microenvironment tuning is a promising design strategy for photoenzymes and other macromolecular photocatalysts.

Wednesday, September 10, 2025 **10:30am** **BRWN 4102**

PURDUE UNIVERSITY | James Tarpo Jr. and Margaret Tarpo Department of Chemistry

Dong Bio

Dr. Sijia Dong is an assistant professor in the Department of Chemistry and Chemical Biology at Northeastern University, with affiliations in the Department of Physics and the Department of Chemical Engineering. Sijia is passionate about accelerating science using computation and automation. She received her PhD in Chemistry from California Institute of Technology in 2017, advised by Prof. William A. Goddard III. She carried out her postdoctoral research at the University of Minnesota with Prof. Donald G. Truhlar and Prof. Laura Gagliardi, and then at Argonne National Laboratory with Prof. Giulia Galli. Research in the Dong Lab focuses on developing and applying physics-based and data-driven computational methods on both classical and quantum computers to accelerate chemical discoveries, especially on leveraging microenvironment tuning to design new chemistry and physics. Sijia has been selected a Scialog Fellow for Automating Chemical Laboratories by Research Corporation for Science Advancement, has won the Northeastern University College of Science Excellence in Mentorship Award, has a Maximizing Investigators' Research Award for Early Stage Investigators from the National Institutes of Health, and is recognized as an Emerging Investigator by the Journal of Chemical Physics, American Institute of Physics. Sijia also co-chairs the Early Career Board of the Journal of Chemical Theory and Computation.