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~~Abstract~~ Book

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Design of new proteins for enhanced photosynthesis using deep learning

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ABSTRACT

Proteins mediate the critical processes of life, including the light-driven reactions of photosynthesis that power the biosphere. Despite the evolutionary success of photosynthesis, its overall efficiency is low. Oxygenic photosynthesis fails to capture the abundant energy in the near-infrared region of the solar spectrum, and it loses energy to thermalization and the thermodynamically downhill electron-transfer steps of charge separation. Our long-term goal is to design new photosystem proteins that address these limitations to enhance photosynthetic efficiency. In contrast to traditional protein engineering efforts, which have focused on modifying naturally occurring proteins, we design new proteins from scratch. Increasingly, we develop and use deep learning methods to design amino acid sequences that are predicted to fold to desired structures and functions. We produce synthetic genes and express the designed proteins in *E. coli*, photosynthetic bacteria, and plants. We characterize the protein structures and functions experimentally using spectroscopy, electrochemistry, cryo-electron microscopy, and X-ray crystallography. In this talk, we will highlight recent designs that assemble multi-pigment light-harvesting arrays, redox centers for light-responsive electron transport chains, and new metal-oxo clusters for catalysis. We are working to combine these cofactor-binding modules to assemble functional photosystems. This work may lead to photosystems with higher overall solar-to-chemical energy conversion efficiency for enhanced yields of food crops, renewable solar fuels, and sustainable ammonia for fertilizer.