

Chemistry Departmental Colloquium

Spectrum, Form, Function: Exploring structure-spectrum relationships in photosynthesis and beyond

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Abstract: Biological photosynthesis offers a tantalizing glimpse of the clean-energy opportunities at the interface of synthetic biology, chemical catalysis, molecular excitonics, and soft-matter physics. However, this sophisticated system is optimized in nature for biological objectives (competitive fitness) that are often at odds with human concerns such as overall energy-storage efficiency. While some progress has been made in reconfiguring native photosystems for biofuel production, advances are limited by gaps in our understanding of the "structure-spectrum-function" relationship, i.e., of the mechanisms by which protein structures tune pigment optical properties and, in turn, how these optical properties translate into biological function. In this talk, I will describe our recent efforts to bridge these gaps by building a robust toolset – from pen-and-paper theory to high-throughput experiments – for “translating” between structural and spectroscopic data. On the experimental side, we are working to build high-throughput, low-cost methods for the recombinant expression and spectroscopic characterization of isotope-tagged proteins and chlorophyll-protein mutants. On the theoretical front, we develop excitonic lineshape descriptions (both vibrational and electronic) that incorporate realistic interactions with the environment. At the intersection between these efforts is our development of “point-and-click” online spectroscopy simulation tools, which both guide our design of modified proteins with “interesting” spectroscopic features and are themselves refined against experimental data. Together, these efforts pave the way for the rational (re)design of photosynthetic light harvesting systems tailored for efficient biofuel production.



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