Designing light harvesting proteins and photoactive enzymes for artificial photosynthesis

Supervisory team:
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Project description:
Electron and captured energy flow within proteins is essential to life; these phenomena underpin cellular respiration and photosynthesis, both of which are dependent on complex protein machinery supporting chains of redox active cofactors or chromophores. Despite the apparent complexity of the natural multiprotein assemblies responsible for these processes, there are simple engineering rules that govern photosynthetic and respiratory protein assembly and function. For instance, by minimising intermolecular distances between cofactors or chromophores, highly efficient and rapid energy and electron transfer can be achieved in soluble or membrane-bound designer proteins. Such artificial or 'de novo' proteins present a particularly attractive platform to understand and exploit desirable properties of their natural counterparts as they contain little, or no sequence information derived from natural proteins; this eliminates natural protein features that are unnecessary for probing or harnessing the function of interest. They are also incredibly robust, thermostable and amenable to change, characteristics that render them appealing for probing fundamental principles and implementing them in real world devices and applications. The goal of our laboratory is to construct such de novo proteins equipped with chains of redox-active cofactors and chromophores to gain both a deeper understanding of photosynthesis and cellular respiration, while providing a framework for exploiting – on our own terms - such exceptional properties as efficient photon capture and energy transduction, long range and directional electron transfer, and transmembrane proton translocation.

The aims of this project are to use powerful computational and iterative approaches to the de novo design of multi-chromophore, light harvesting proteins. We will employ a combination of state-of-the-art machine learning protein design algorithms (e.g. protein MPNN), well-established Rosetta protein design protocols, biomolecular simulation and calculations (e.g. molecular dynamics), thereby facilitating an unparalleled control and precision over the protein sequence, structure and biophysical characteristics. Once expressed and purified from E. coli, these designs will be subjected to an array of biophysical and structural techniques to assess protein structure, thermal stability, chromophore binding and their subsequent spectroscopic properties. We will then use ultrafast single and multidimensional spectroscopy to probe and map energy capture and transfer, uniquely providing insight into the behaviour of individual and paired chlorophyll-like molecules within a protein environment. Finally, we will explore the utility of these light harvesting proteins when incorporated into multiprotein, artificial photosynthetic systems and/or biophotovoltaic devices.

Our aim as the SWBio DTP is to support students from a range of backgrounds and circumstances. Where needed, we will work with you to take into consideration reasonable project adaptations (for example to support caring responsibilities, disabilities, other significant personal circumstances) as well as flexible working and part-time study requests, to enable greater access to a PhD. All our supervisors support us with this aim, so please feel comfortable in discussing further with the listed PhD project supervisor to see what is feasible.