Manipulating the light absorbing properties of artificial protein – chromophore assemblies

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The initial step of photosynthesis, namely charge separation, occurs with outstanding efficiencies.[1] Photosynthetic organisms achieve this *via* protein – pigment complexes that implement a number of strategies termed "design principles of charge separation",[1] which involve a delicate landscape of (vibrational and electronic) energy levels. To implement these "design principles" in an artificial system, the energy position of the lowest excited state is a fundamental property that must be known and precisely tailored.

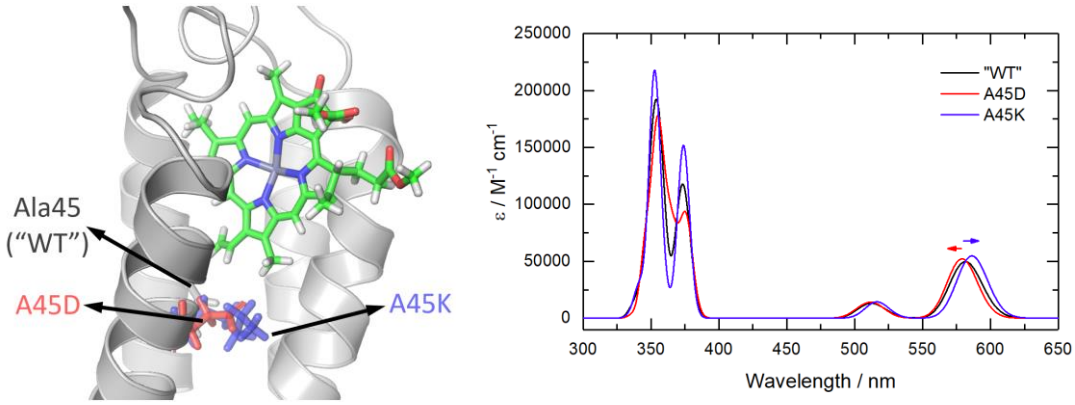

Figure 1. *Left: Structure of a protein – chromophore assembly, highlighting one of the bound chromophores and an Ala amino acid (grey) in the "wild type" structure that is changed to Asp (red) or Lys (blue) in the mutated ones. Right: Calculated absorption spectra of the "wild type" and the mutated structures.*

In this contribution, we present computational results on a series of artificial protein – chromophore assemblies based on the four alpha-helix bundle motif (**Figure 1**, left) and porphyrin-like chromophores. By systematically mutating the protein in positions close to the binding site of the chromophores, we are able to study and manipulate the light absorbing and spectroscopic properties of the assemblies (**Figure 1**, right). The latter include circular dichroism spectra, which we compare to experimental data to validate the computational models. This work is part of a larger study to provide rules for the rational design of artificial systems with good charge-separation properties, to be employed as light-driven catalysts.

References

[1] E. Romero, V. Novoderezhkin, R. van Grondele *Nature* **2017**, *543*, 355-365.