

VISTA Seminar

Seminar 61

December 6, 2023

**10:00 am – 11:30 am EST / 3:00 – 4:30 pm GMT London / 4:00 pm –
5:30 pm CET Paris / 11 pm CST Beijing**

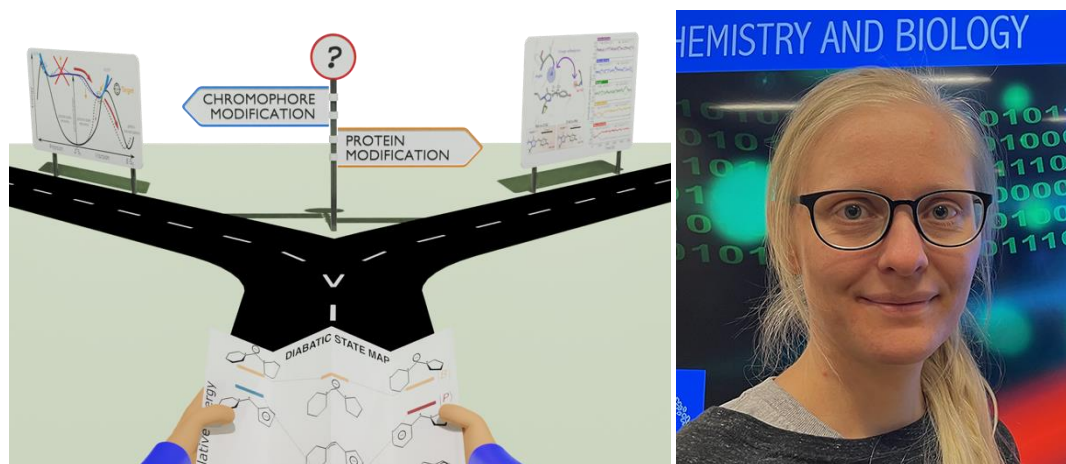
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Dimming the lights and switching the twist. Chemical and environment control of the GFP chromophore

Nanna Holmgaard List

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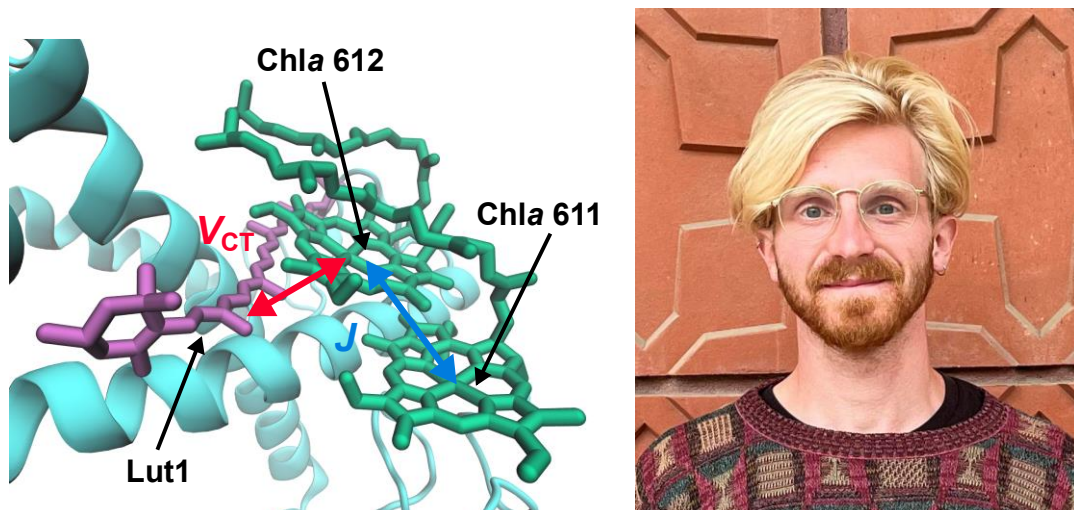


Fascinating and diverse biological functions have emerged by the combination of light-absorbing chromophores and protein scaffolds in photoactive proteins. The initial electronic excitation induces ultrafast dynamics localized at the chromophore that is captured and amplified by the surrounding protein environment ultimately leading to a larger-scale photofunctional response. Importantly, the photoinduced behavior of the chromophore often change substantially when embedded in a protein matrix. This tunability is explored in biotechnology to engineer tools that exploit light to activate, drive or report on (bio)chemical processes. For instance, directed evolution using random mutagenesis and high-throughput library screening are successfully being employed to expand the palette of photoactive proteins, such as GFP-like proteins. However, our understanding of the fitness landscapes remains opaque. Multiscale quantum-classical approaches offer a possible strategy to help chart out purposeful design factoring in photofunction, but it comes with many challenges. In this talk, I will discuss some of these challenges through presenting our recent efforts to understand how the chromophore in GFP-like proteins may be modulated photochemically.

Coupled electron and energy transfer dynamics in light harvesting complexes: a hybrid hierarchical equations of motion approach

Thomas P. Fay, David T. Limmer

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In this talk I will describe a method for simulating exciton dynamics in protein–pigment complexes, including effects from charge transfer as well as fluorescence. The method combines the hierarchical equations of motion, which are used to describe quantum dynamics of excitons, and the Nakajima–Zwanzig quantum master equation, which is used to describe slower charge transfer processes. We have studied the charge transfer quenching in light harvesting complex II, a protein postulated to control non-photochemical quenching in many plant species. Our calculations reveal that the exciton energy funnel plays an important role in determining quenching efficiency, a conclusion we expect to extend to other proteins that perform protective excitation quenching.

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 61

Time: Dec 6, 2023 10:00 AM Eastern Time (US and Canada)

Join Zoom Meeting

<https://buffalo.zoom.us/j/96465847706?pwd=TG14ZHpjTHlaQzZmNDluTkRyck5GQT09>

Meeting ID: 964 6584 7706

Passcode: 084488