

VISTA Seminar

Seminar 64

March 6, 2024

**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**

TOC:

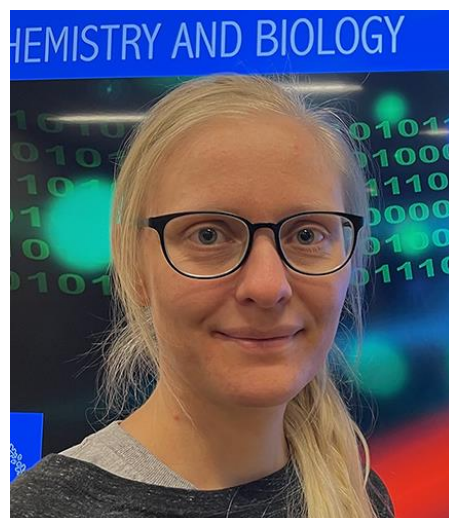
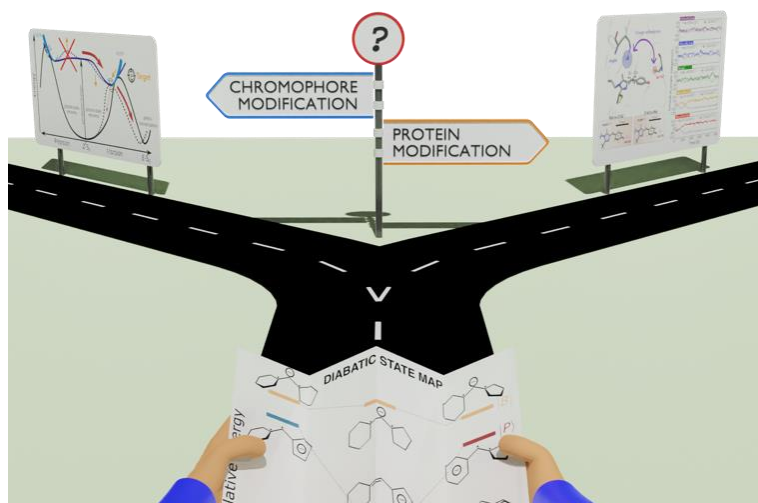
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Dimming the lights and switching the twist. Chemical and environment control of the GFP chromophore

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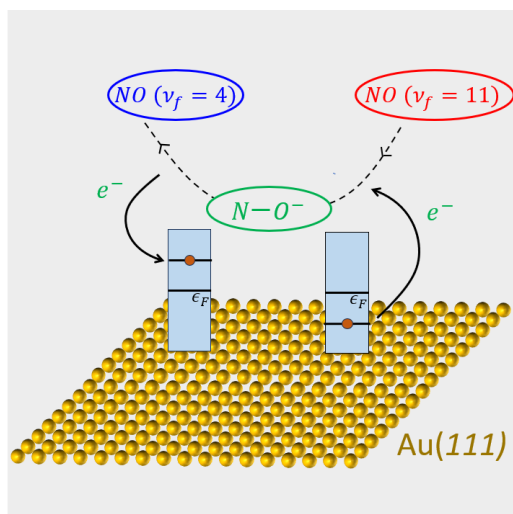


Fascinating and diverse biological functions have emerged by the combination of light-absorbing chromophores and protein scaffolds in photoactive proteins. The initial electronic excitation induces ultrafast dynamics localized at the chromophore that is captured and amplified by the surrounding protein environment ultimately leading to a larger-scale photofunctional response. Importantly, the photoinduced behaviour 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.

Simulating the Non-Adiabatic Vibrational Relaxation of *NO* Scattering from Au(111) using Linearized Semiclassical Dynamics.

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We study the vibrational relaxation of *NO* scattering from a Au(111) surface, which has been the focus of many experimental and theoretical investigations. Transient electron transfer from the metal is suspected to play a crucial role in the vibrational relaxation by facilitating energy transfer into electron hole pair excitations. Our approach employs Linearized Semiclassical dynamics and can capture the role of transient electron transfer to predict accurate vibrational relaxation for the initial vibrational state $\nu_i = 3$. For the more challenging case of $\nu_i = 16$, our simulations capture significant multi-quantum relaxation but fall short of predicting the experimental vibrational distributions. Investigations into the mechanism of electron transfer provide some insights into this shortcoming.

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 64

Time: Mar 6, 2024 10:00 AM Eastern Time (US and Canada)

Join Zoom Meeting

<https://buffalo.zoom.us/j/99896357887?pwd=bUpuM1FUWm5JSHR4WHVBaXF4cnJkZz09>

Meeting ID: 998 9635 7887

Passcode: 322950