MASTER THESIS PROJECT Physical chemistry

Photocontrol of electron transfer pathways

One of the key challenges for society today is to find **sustainable ways to produce fuels and high value chemicals**, like transforming CO_2 to CH_4 . This requires energy input, for example by light in photoreactions, and importantly it also requires the transfer of several electrons in a single reaction to form the desired product. It is well known that molecules typically are very unstable in highly oxidized or reduced states and thus susceptible to degradation. On the other hand, molecules are excellent at providing selectivity for a reaction, which is also a necessity for success.

In this project we will look at the selectivity problem in detail and address whether it is possible to control the rates, yields and mechanisms of multielectron transfer in photoactive hybrid materials by using light both as an energy input to start the reaction and to control the pathway.

This idea builds on results presented in Science^[3] by Julia Weinstein and coworkers a few years ago, demonstrating that through selective light excitation into certain vibrational modes, they could activate and deactivate specific electron transfer routes. In this proposal, we hypothesize that it is possible to design a photoactive hybrid material in which we can control the mechanism of a photocatalytic process using dual light excitation using both the visible and the IR region of the electromagnetic spectrum. Specifically, we will address the following questions:

- Can we control electron transfer mechanisms by using an additional light source subsequent to photoexcitation with visible light?
- Can we control formation of a specific desired product in cleverly designed hybrid materials?
- Can it be applied to catalytically active systems to gain control over product selectivity?

The project covers everything from synthesis of model compounds and characterization of properties with spectroscopic methods to complex laser spectroscopy experiments to study the influence of a second light pulse. Projects can be designed based on the students interest.



Contact:

Postdoc Andrew Maurer (maurer@chalmers.se) PhD student Hassan Mourad (<u>hassanmo@chalmers.se</u>) Professor Maria Abrahamsson (abmaria@chalmers.se)