Women in Science – 3rd Erlangen Symposium

# Excited-State Odyssey: Charting Maps with Data-Driven Strategies

*Carolin Müller*[1]

[1]Computer-Chemistry-Center, Nägelsbachstraße 25, 91052 Erlangen, Germany
carolin.cpc.mueller@fau.de

Photochemistry offers a promising route to sustainable chemical processes. However, to exploit its full potential, it is necessary to explore the potential energy landscapes of different excited states. This exploration resembles an odyssey, because in the absence of design principles and detailed structural information for excited states, detailed maps for these surfaces are lacking.
Quantum chemical simulations provide glimpses on these landscapes, yet their accuracy is hampered by computational costs associated with quantum chemical methods, restricting their use to small systems (*e.g.*, ≤100 atoms) and short timeframes (ranging from femto- to picoseconds). Here, data- and science-driven strategies emerge as a guiding force. For example, by leveraging existing quantum chemical data across various molecular configurations and excited states, machine learning approaches can accelerate photodynamics simulations to navigate the excited state manifold or drive static approaches to localize critical points on various excited-state surfaces.
This presentation provides an overview of how machine learning can streamline the charting of maps for the landscape of photochemical reactions involving various excited states. Introducing the machine learning method, **SPaiNN** [1], and its companion database, **SHNITSEL** [2,3], we delve into a promising duo driving the exploration and prediction of excited-state landscapes. **SHNITSEL** serves as a comprehensive repository housing computational data for various photochemical reactions, meticulously crafted as the **S**urface **H**opping **N**ewly **I**nvented **T**raining **S**et for **E**xcited-state **L**earning. Specialized in training and predicting excited state properties, **SPaiNN** will be showcased using examples from the **SHNITSEL** database, marking the commencement of an Excited-State Odyssey, charting maps with data-driven strategies.

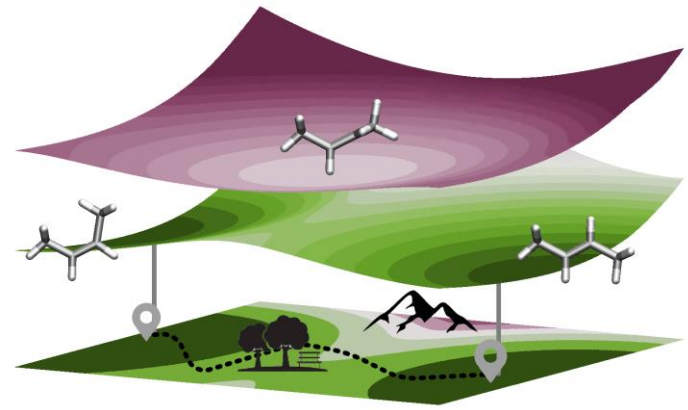

**Figure 1.** Schematic illustration of the excited state map of buten.

## References

[1] S. Mausenberger, C. Müller, A. Tkatchenko, P. Marquetand, L. Gonzalez, and J. Westermayr, *in preparation* **2024**
[2] T. Röhrkasten, R. Curth, J. Westermayr, and C. Müller, *in preparation* **2024**
[3] C. Müller, *https://shnitsel.github.io* **2023**