OPTIMAL

Organic **P**hotovoltaics and **T**riplet states via **I**nnovative **M**achine learning and **A**dvanced **L**ogic

Katharina Boguslawski

May 2025

We propose interdisciplinary and innovative approaches to design and optimize modern organic materials that are important for developing photovoltaics and organic light emitting diodes (OLEDs) with improved physicochemical properties. Our unique strategy will combine physicists, chemists, and computer scientists to enhance the predictive power of state-of-the-art theoretical and experimental techniques. These include

- the development of novel quantum-mechanical methods
- improved code efficiency via machine learning (ML) and ML-assisted GPU and multi-GPU computing (exploring the GH200 or newer hybrid computer architectures)
- ML-assisted prescreening of new materials with desired properties
- theoretically-driven materials design
- experimental ML-assisted probing of promising materials candidates and their experimental realizations
- extensions of our methodologies to quantum computers

The project's culmination will be the theoretical and experimental prediction of organic polymers, important for organic electronics (photovoltaics and OLEDs), using our quantum algorithms and ML techniques.