Background

Spectral properties of molecules are crucial for understanding and analyzing chemical reactions. These properties result from interactions between molecules and electromagnetic radiation, such as ultraviolet (UV), visible (Vis), and infrared (IR) light. By studying these interactions, scientists can gain valuable insights into the molecular structures, dynamics, reaction environments, and material properties.

Currently, we utilize classical simulation methods, such as density functional theory (DFT), to predict molecular spectral properties. While such classical simulation methods provide reliable results, they have limitations in computational efficiency and accuracy, especially for larger, more complex molecules or reactions. To overcome these challenges and enhance predictive power, BASF is interested in exploring Quantum Machine Learning (QML) techniques, which have the potential to significantly improve both the speed and precision of spectral property predictions.

What we're looking for

We are looking for promising QML methods with the potential to exceed classical methods in terms of speed and accuracy. In a joint research project, we would like to evaluate the proposed QML method.
The developed method should ultimately be applicable to different molecules, perform well on provided datasets, and be demonstrated on similar use cases.
Solutions of interest include:

- Quantum computing algorithms that can be adapted to predict specific spectral properties of molecules

Our must-have requirements are:

- Clear, high-level description of the quantum architecture
- Strong rationale for potential quantum advantage

What's out of scope:

- Solutions that require external proprietary datasets.
- Black-box approaches -