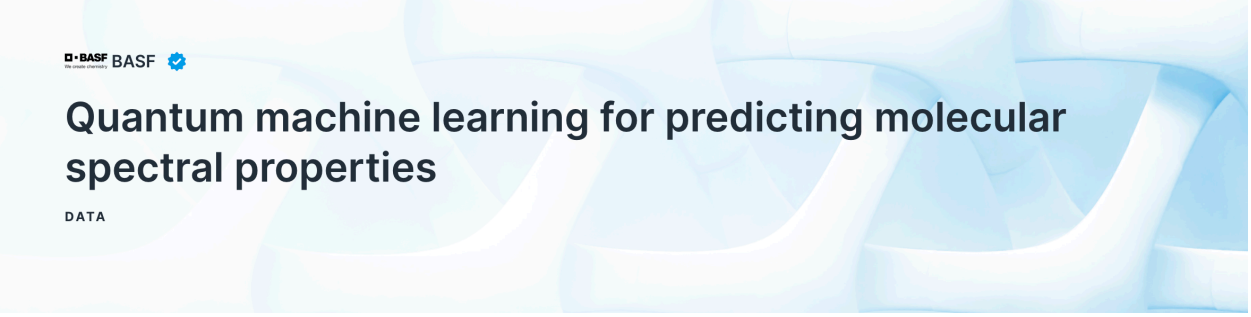

Background

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
- Provide relevant references that support your QML approach

What's out of scope:

- Solutions that require external proprietary datasets.
- Black-box approaches - we would like to understand the QML method for joint research.
- Purely classical approaches – we are interested in quantum computing solutions.

Acceptable technology readiness levels (TRL): Levels 1-4
1. Basic principles observed
2. Concept development
3. Experimental proof of concept
4. Validated in lab conditions
5. Validated in relevant environment
6. Demonstrated in relevant environment
7. Regulatory approval
8. Product in production
9. Product in market

What we can offer you

Eligible partnership models:

Sponsored research

Benefits:

Sponsored Research

Funding will be proposal dependent, mutually agreed upon and milestone dependent.

Expertise

Partners will have access to internal experts.

Reviewers

Lauren Junker
Technology Scout

Tom Holcombe
Collaboration & Scouting NA

Kavita Bitra
Technology scout

Sophia Steffens
Innovation & Scouting

Ricarda Schulte
Senior Associate Venture Portfolio Management

Nicole Klein Stocke
Community Manager

Please contact the University of South Florida Technology Transfer office representative for submission – Karla Schramm at kschramm@usf.edu