QUANDELA

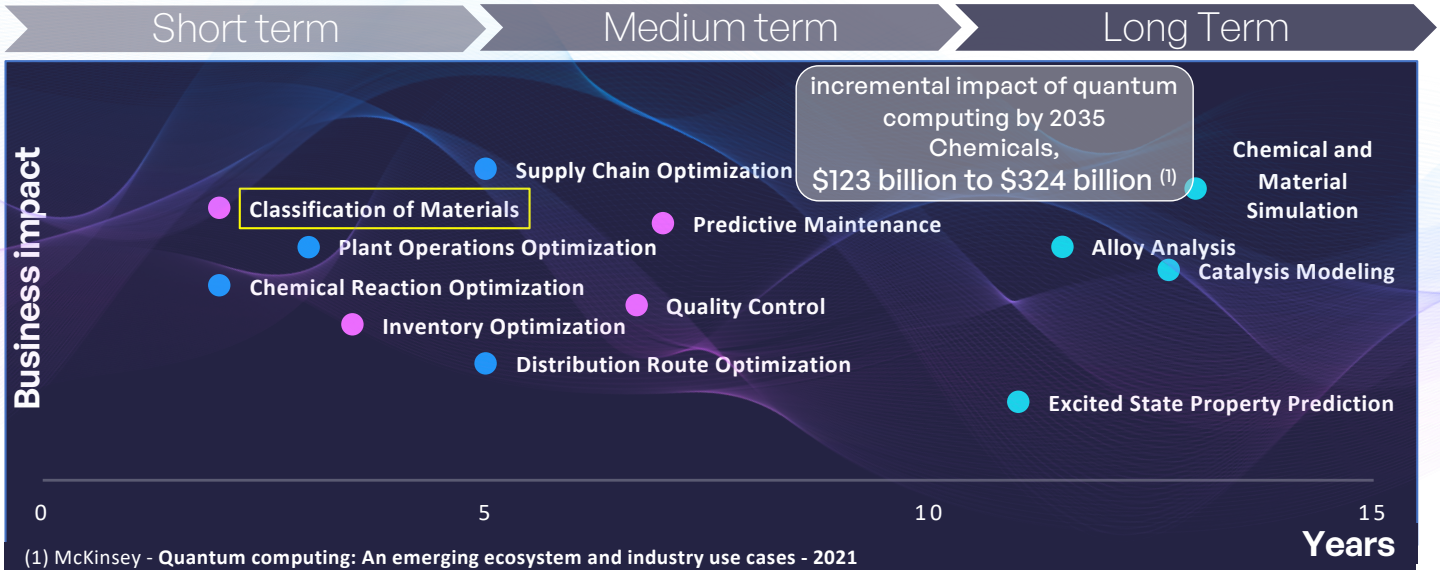
2023- Case story

Chemicals & Materials

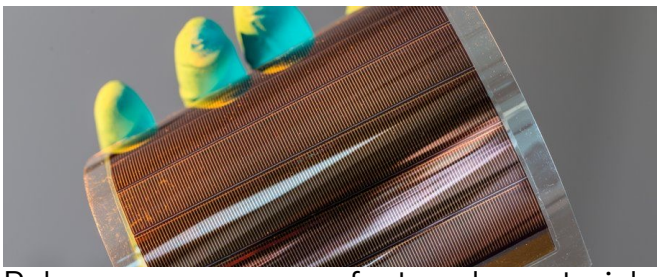
Alysophil accelerates the discovery of new polymers with Quantum Machine Leaning

Use-cases for Chemicals & Materials

Quantum Machine Learning	Classification of materials, Predictive Maintenance, Quality Control, Inventory Optimization,
Quantum Simulation	Chemical and Materials Simulation, Catalysis Modeling, Chemical Dynamics Simulation
Quantum Optimization	Chemical Reaction Optimization, Plant Operations Optimization, Distribution Route Optimization, Supply Chain Optimization, Alloy Analysis, Excited State Property Prediction



Challenge for manufacturers : designing new polymer materials with specific properties



Polymers are manufactured materials **ubiquitous in the industry**= electronics, cosmetics, drug design, carbon capture, aerospace, automotives, clothing, communication, 3D printing, organic photovoltaic, etc. To target specific needs, industrial manufacturers try to synthesis polymers with given properties, mostly from a process of trial and error, but this is costly and time-consuming.

A designing process has emerged with high-performance computation, using Deep Learning. But this sophisticated models are hard to develop and to run on classical computers due to the **gigantic chemical space of polymers** and to the complexity to search for an optimum.

A new approach should be explored. Quandela and Alysophil focused on the opto-electronic properties of polymers. To be more specific, the goal is to classify whether a polymer belongs to the near-infrared or the visual class. This **work paves the way towards designing new organics photovoltaic materials,** useful for recycling solar panels, a big challenge in the solar panel industry.

contact@quandela.com www.quandela.com

QUANDELA

2023- Case story

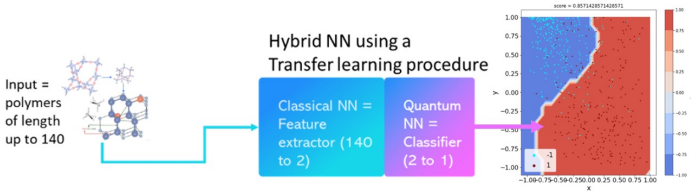
Chemicals & Materials

"With Quandela we implemented state of the art methods that outperform today's standard in production.

By joining forces, Quandela and Alysophil developed today and tomorrow best solutions."

Philippe Robin, Founder & President Alysophil, leader in AI methods for continuous-flow chemistry

Solution : develop a hybrid algorithm mixing Machine Learning with Quantum



The chosen solution is a **hybrid algorithm**. The **classical part** takes as an input a numerical representation of polymers and provides a representation in lower dimension of this dataset. The output dimension must be sufficiently small such that the **Quantum Computer** can then classify those data. In scheme above, the method is described = an embedding step, a training step and the classification in the visual (blue) or near-infrared class (red).

The results are already conclusive. This algorithm is converging, and the accuracy for the classification is comparable to what the state-of-the-art classical method obtains. This is a demonstration of a treatment of **real chemical data using a hybrid approach for classification.**

Targeted extensions to other polymers properties

In the coming years, as the size of the Quantum Computer will increase, the classical pre-processing part can be reduced, until the capability is reached to run fully the algorithm on a Quantum computer. For this reason, this hybrid approach yields best of both world and paves the way for even more success.

It must be underlined that this hybrid approach is generic. Thus, many variations might be explored to classify and to predict other polymers properties but also different chemicals and materials.

To go further, read Stoyanova et al., Photonic Quantum Computing For Polymer Classification, https://arxiv.org/abs/2211.12207

Get onboard the Quantum Journey with Quandela

It is time to make your industry start with Quantum computing, our teams are dedicated to help corporates in their first steps in the quantum world, from the target of problems to their implementation on real QPUs

QUANDELA

Identification of computational problems where Quantum will bring you the most value

Consultation with Quantum scientists to explore the best approaches

Test and benchmark these approaches on state-of-the-art Quantum Processors (QPU)

contact@quandela.com

www.quandela.com