Leveraging Quantum Machine Learning for the synthesis of polymers

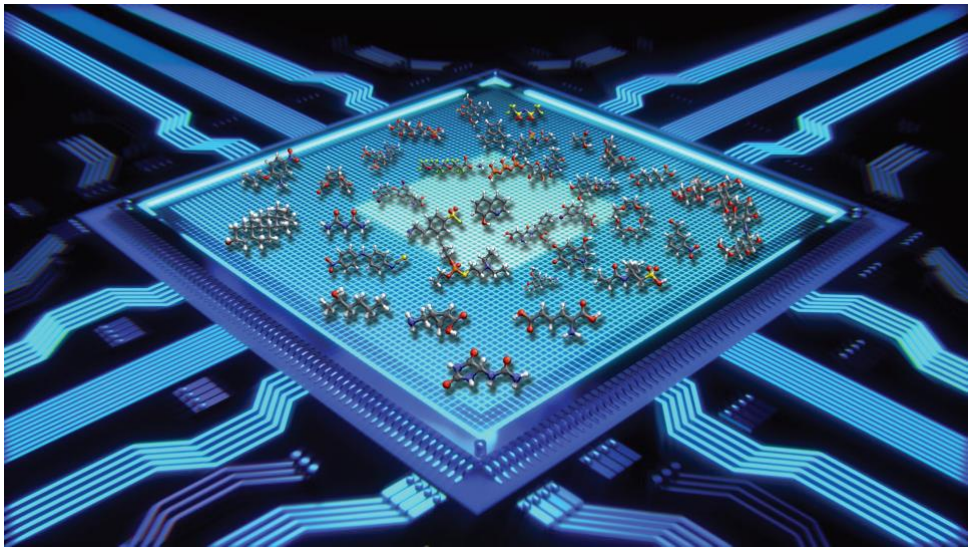
Can single-photons help industry discover new polymer architectures in the coming ten years? A feasibility study performed recently by Alysophil and Quandela, in partnership with MBDA, has shown how this could be achieved.

Enabled by the rapid growth in computing power and algorithmic developments, deep-learning technologies are widely used today in a variety of domains: image, speech, and automatic language processing, product recommendations, online fraud detection, cybersecurity, stock market trading, and medical diagnosis. Channeling the ever-growing amount of data through sophisticated algorithms that can detect intricate patterns and correlations has revealed the huge potential of those technologies to extract valuable knowledge. Natural sciences like chemistry, physics, and biology have also joined the race in leveraging machine-learning models to gain insights into complex (bio-)molecular structures, chemical reactions, and materials properties.

The ubiquity of machine learning today is reminiscent of the rise of Minitel, an electronic terminal that boomed in the 1980s before eventually declining with the arrival of personal computers. While it is hard to compare the hardware revolution to the evolution in machine learning, some trends can be observed. For example, recent boosts in the development of quantum hardware are accompanied by developments of quantum analogues to traditional machine learning algorithms. Will these Quantum Machine Learning approaches be the next revolution to eclipse classical machine learning models?

While quantum phenomena have been studied in-depth by chemists and physicists for over a hundred years, they are only recently getting the attention they deserve from broader fields. This interest came after realizing that quantum computers can solve problems involving complex correlation patterns in input data like images and language structures. Such correlations are harder to detect by classical machines, even when the latter are enabled by powerful computing units such as the Graphics Processing Units. Quantum computing on quantum hardware, however, allows calculations in higher dimensional spaces that enable the use of more complex learning models. Faster computations and more general models are thus expected.

Naturally, the question of “quantum advantage” in machine learning arises: for which tasks and data executing a machine learning algorithm on a quantum computer would we expect a real computational advantage in terms of precision and time? Invoking the concept of a “quantum advantage”, we should also mention the areas of quantum physics and quantum chemistry. These sciences are expected to gain overwhelming advantages since both involve quantum simulations on atomic and molecular systems. Benefits in terms of computation time, and hence in optimization efficiency, could be of several orders of magnitude compared to current and future classical computers. As the famous physicist Richard Feynman said, “Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.”



In silico design of new macromolecules with the help of deep learning.

Embarking on the quantum adventure, Quandela, Alysophil, and MBDA conducted a feasibility study on what would be the impact of Quantum Machine Learning on the discovery of new polymers and polymer composites. The first findings were compelling, and two strategies scheduled for a 2-year project were designed to take aim at the prediction of polymer structures and properties. This project will also enroll MBDA and Alysophil in the race of the second quantum revolution. The two strategies are based on state-of-the-art machine learning methods and their quantum analogues combined with simulations then run on Optical Quantum Computers. As they are highly versatile, we expect them to be applicable to a wide range of applications and domains, where the use of polymers is important: cosmetics, drug discovery, tyres and sealings, structural materials, propulsion, carbon capture.

If you would like to know more about the project, feel free to contact us at philippe.robin@alysophil.com and arno.ricou@quandela.com.

About Alysophil

Alysophil is a company that develops new concepts of industrial chemistry to produce high-added-value molecules by combining flow chemistry and artificial intelligence. These technologies enable the development process to be accelerated, by identifying molecules more quickly to meet complex needs and then defining and implementing high-performance syntheses. The combination of artificial intelligence and flow processes will enable Alysophil to have frugal, compact, mobile production units made autonomous by neural chips, considerably improving manufacturing performance (safety, environmental footprint, costs, independence, etc.). The company is based in Strasbourg and currently employs 10 people.

For more information, visit our website and social channels which are listed below. Website – LinkedIn – Twitter

About Quandela

Founded in 2017 by three scientists, Quandela is an innovative company with high technological content. Quandela works currently on several research projects from the Centre for Nanosciences and Nanotechnologies (C2N - CNRS/University of Paris-Saclay) in Palaiseau. Quandela's main activity is to develop and market a range of modular technologies for the quantum tech industry. Today, starting from an international leadership position in the R&D market, Quandela is developing an optical quantum computer. This computer will be accessible via an online service and will enable industry to optimize several problems that are known to be difficult to solve with classical computers.

For more information, visit our website and social channels which are listed below. Website – LinkedIn – Twitter – YouTube – Medium

About MBDA

MBDA is the only European defence group capable of designing and producing missiles and missile systems that correspond to the full range of current and future operational needs of the three armed forces (land, sea and air). MBDA is at the core of our home nations and their allies' sovereignty by providing decisive military capabilities to protect the freedom of our nations.

MBDA's mission is to enable its customers' armed forces to maintain their operational superiority and sovereignty across all military domains. We provide fast, efficient and precision effects complex weapon systems, which are decisive force multipliers in military operations. The group offers a range of 45 missile systems and countermeasures products already in operational service and more than 15 others currently in development. MBDA is jointly owned by Airbus (37.5%), BAE Systems (37.5%), and Leonardo (25%).

For more information, visit our website and social channels which are listed below.

Website – LinkedIn – Twitter – YouTube

The continuation of a collaborative project between Alysophil, Quandela, and MBDA is under discussion after a successful first phase.

For more information, please visit:

quandela.com
alysophil.com
mbda-systems.com