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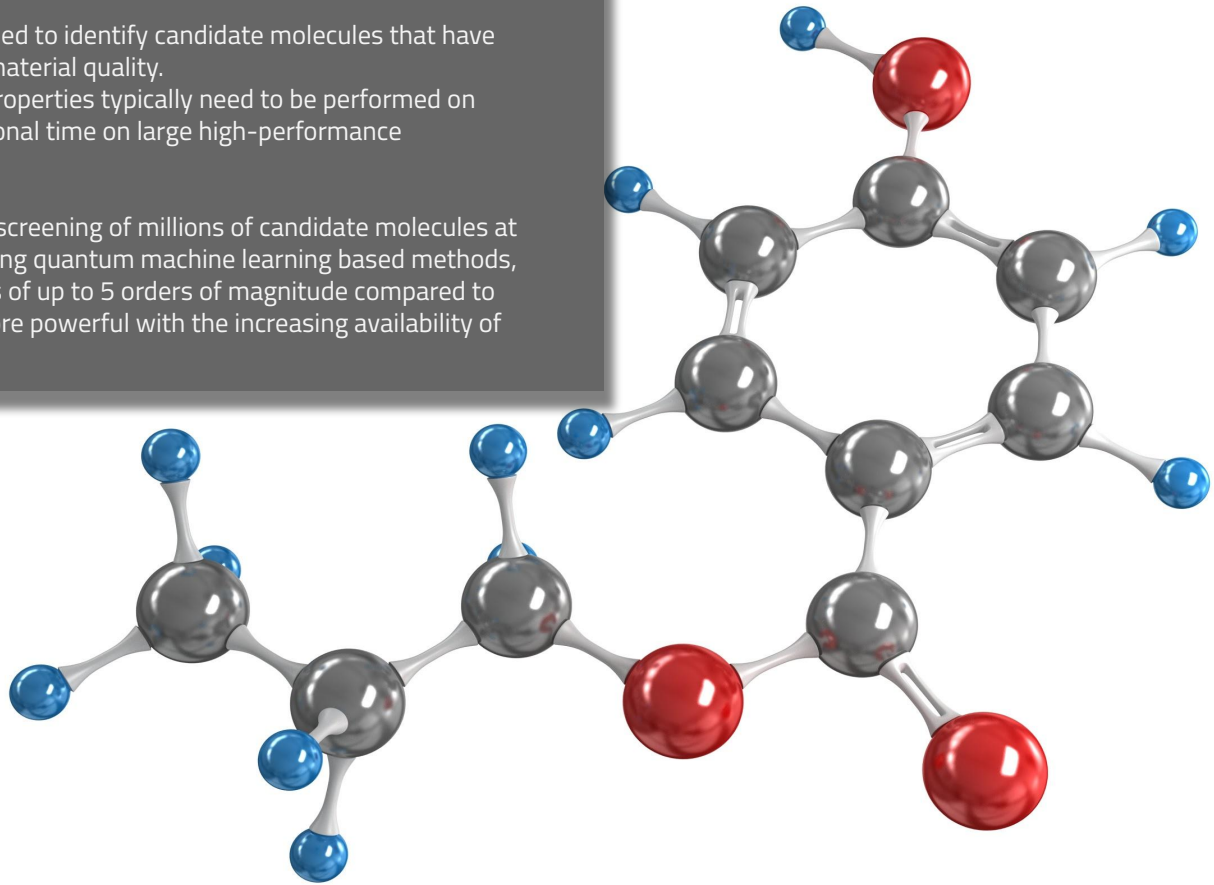
Quantum Machine Learning

Improving the discovery process with machine learning

Quantum Machine Learning based High Throughput Screening

Virtual high throughput screening of molecules is widely used to identify candidate molecules that have specific target properties, such as drug toxicity or battery material quality.
Computational experiments to evaluate and predict such properties typically need to be performed on millions of candidates, which can take weeks of computational time on large high-performance computers.

Rahko enables customers to generate and perform virtual screening of millions of candidate molecules at drastically reduced computational costs and timescales using quantum machine learning based methods, accelerated by the cloud. These methods provide speedups of up to 5 orders of magnitude compared to traditional approaches today and will gradually become more powerful with the increasing availability of quantum computers.



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ML Accelerates Drug Discovery

Computational drug discovery investigates the ability of drug chemical compounds to inhibit protein molecules (targets). To identify a drug which has the right properties to inhibit the protein, many steps are required starting from an informed proposal of a drug candidates to molecular dynamics simulations which explore the potential energy landscape. This is a time consuming and expensive process, typically involving millions of core hours for larger molecules.

Rahko's machine learning based approaches dramatically accelerate the speed of molecular generation and simulation, by using specialised machine-learned interatomic potentials. This additionally increases the overall accuracy, and also allows the evaluation of more complex materials.

Our machine learning based approaches can reduce the overall cost for by up more than 90%.

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Crystal Structure Prediction (CSP)

Most drugs such as paracetamol (acetaminophen) are in crystalline form. Drug patents and regulatory approval only apply to a single polymorph - meaning that patents with the wrong polymorph can become useless. *In silico* CSP offers the promise of predicting the experimentally likely polymorph structures.

In collaboration with several multinational pharmaceutical companies Rahko has achieved a reduction in customer DFT costs for CSP of up to 98%, while also detecting important structures which were incorrectly filtered out during the traditional CSP process.

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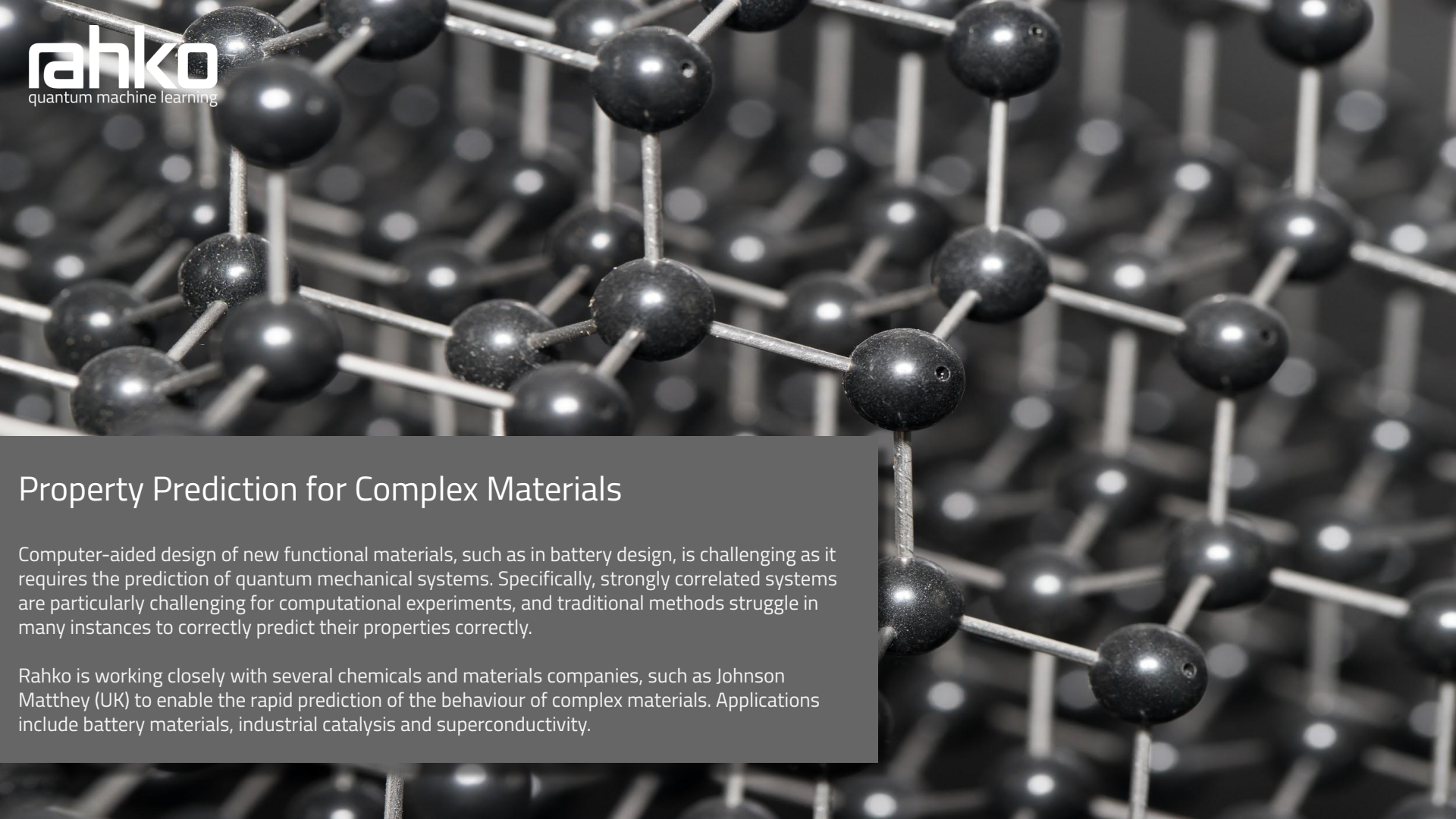

Property Prediction for Complex Materials

Computer-aided design of new functional materials, such as in battery design, is challenging as it requires the prediction of quantum mechanical systems. Specifically, strongly correlated systems are particularly challenging for computational experiments, and traditional methods struggle in many instances to correctly predict their properties correctly.

Rahko is working closely with several chemicals and materials companies, such as Johnson Matthey (UK) to enable the rapid prediction of the behaviour of complex materials. Applications include battery materials, industrial catalysis and superconductivity.

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Computer Aided Fertilizer Design

Efficient use of fertilizers, such as nitrogen, is essential and strategically highly important for agricultural production. The efficiency of fertilizers depends highly on slow- or controlled-release products. Computational methods, such as molecular dynamics can be used to probe the structure and dynamics of chemical systems, and characterize these in terms of their physicochemical properties, such as dielectric properties or hydrogen bonding. For example, these computational methods can be used to investigate the release of nutrients from coated fertilizer granules across a multitude of candidates through computational experiments.

Rahko's machine learning driven approaches enable extremely fast computational experiments for the computer-aided R&D process.

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Get in touch!

Email: info@rahko.ai