Quantum Computing: Fundamentals, Trends and Perspectives for Chemical and Biochemical Engineers

Preprint

Amirhossein Nourbakhsh
Geomatics Engineering
Lassonde School of Engineering
York University
Toronto, ON M3J 1P3
Canada

Mark Nicholas Jones
Molecular Quantum Solutions
Maskinvej 5
2860 Søborg
Denmark

Kaur Kristjuhan
Molecular Quantum Solutions
Maskinvej 5
2860 Søborg
Denmark

Deborah Carberry
Department of Chemical and Biochemical Engineering
Technical University of Denmark
Søltofts Plads
2800 Kongens Lyngby
Denmark

Jay Karon
Intelligent Data Analytics
Toronto, ON M3J 1P3
Canada

Christian Beenfeldt
Knowledge Hub Zealand
Biotech City Kalundborg
4400 Kalundborg
Denmark

Kyarash Shahriari
Intelligent Data Analytics
Toronto ON M3J 1P3
Canada

Martin P Andersson
Department of Chemical and Biochemical Engineering
Technical University of Denmark
Søltofts Plads
2800 Kongens Lyngby
Denmark

Mojgan A. Jadidi
Geomatics Engineering
Lassonde School of Engineering
York University
Toronto, ON M3J 1P3
Canada

Seyed Soheil Mansouri
Department of Chemical and Biochemical Engineering
Technical University of Denmark
Søltofts Plads
2800 Kongens Lyngby
Denmark

January 11, 2022

*mark@mqs.dk
†mjadidi@yorku.ca
‡seso@kt.dtu.dk
ABSTRACT

We use the benefits and components of classical computers every day. However, there are many types of problems which, as they grow in size, their computational complexity grows larger than classical computers will ever be able to solve. Quantum computing (QC) is a computation model that uses quantum physical properties to solve such problems. QC is at the early stage of large-scale adoption in various industry domains to take advantage of the algorithmic speed-ups it has to offer. It can be applied in a variety of areas, such as computer science, mathematics, chemical and biochemical engineering, and the financial industry. The main goal of this paper is to give an overview to chemical and biochemical researchers and engineers who may not be familiar with quantum computation. Thus, the paper begins by explaining the fundamental concepts of QC. The second contribution this publication tries to tackle is the fact that the chemical engineering literature still lacks a comprehensive review of the recent advances of QC. Therefore, this article reviews and summarizes the state of the art to gain insight into how quantum computation can benefit and optimize chemical engineering issues.

A bibliography analysis covers the comprehensive literature in QC and analyzes quantum computing research in chemical engineering on various publication topics, using Clarivate analytics covering the years 1990 to 2020. After the bibliographic analysis, relevant applications of QC in chemical and biochemical engineering are highlighted and a conclusion offers an outlook of future directions within the field.

Keywords Quantum · Computing · Chemical · Engineering · Review

1 Introduction

The term quantum computer was first coined by Paul Benioff in 1979 when he constructed a microscopic quantum mechanical model to perform computation. [Benioff, 1980] In the early 70’s, Stephen Wiesner proposed his idea of “Conjugate Coding,” which is a cryptographic tool, and submitted an article to the IEEE Transactions on Information Theory. His paper was rejected because it seemed incomprehensible to the referees. [Brassard, 2005] In October 1979, Benioff and Wiesner found a way to use Wiesner’s coding scheme with the concept of public-key cryptography. [Diffie and Hellman, 1976] Finally, the result of their collaboration led to the generation of new topics in the field, such as teleporting an unknown quantum state by using dual classical and Einstein-Podolsky-Rosen channels [Bennett et al., 1993], entanglement distillation [Bennett et al., 1996], strengths and weaknesses of quantum computing [Bennett et al., 1997], and quantum cryptography [Bennett et al., 1992].

Richard Feynman’s description of how to accurately calculate quantum physical system on a quantum computer architecture can be seen as the first description of a quantum computer architecture. He submitted the description on the 7th of May 1981 to International Journal of Theoretical Physics. The article was then published in volume 21, June, 1982.

David Deutsch described in 1985 his idea of an universal quantum computer. He mentioned that a computing machine with quantum theory characteristics can be built and that it can have many remarkable properties which cannot be found in Turing machines. [Deutsch, 1985]

Quantum computing has been studied for decades and ranges from information theory to details of hardware technologies, computational models implemented on the specific hardware and problem formulations which can be solved on a certain hardware type. It has applications in nearly every field that contains or utilizes computations with high complexity. Quantum computers have the potential to impact many aspects of current domains of science, including computer science, mathematics, and chemical engineering. Generally, to compare classical computing and quantum computing, computational problems can be divided into three categories. The first category contains problems that cannot be solved by classical computers in any feasible amount of time, but which are possible to solve with quantum computers. This is one of the main goals of quantum computing, which is termed “quantum supremacy” or ”quantum advantage”. John Preskill published a paper in November 2012 about quantum supremacy and the consequences it will have to several critical applications in society such as: cryptography and optimization. [Preskill, 2012]

In October 2019, Google claimed to have achieved quantum supremacy using a programmable superconducting processor. [Arute et al., 2019] Google scientists used a quantum processor called “Sycamore” to sample the output of a pseudo-random quantum circuit. They used 53 qubits representing a state space of $2^{53}$ dimensions. The process took about 200 seconds to solve a complex computation, while that process would have taken about 10,000 years with a classical computer. [Arute et al., 2019] However, IBM stated that the computation of the Google experiment could be performed on a classical computer in 2.5 days rather than 10,000 years. [Edwin Pednault, 2019] The second category of
computational problems is related to the issues that can be solved with both classical computers and quantum computers, though with less computational complexity when using a quantum computer. The third category is comprised of problems that cannot be solved more efficiently with quantum computers. Thus, a careful analysis of the mathematical complexity of a mathematical problem formulation must be made to assess which computational system/architecture should be applied.

Figure 1 represents which Qubit technologies enable which kind of quantum computing model. Each provider has its model of QC technology. The details of the different QC technologies are described in Section 2 and 3.

2 Fundamentals of Quantum Computing

There are four computation models in quantum computers:

1. gate model (circuit)
2. adiabatic
3. measurement based
4. topological.

In the following sections, these models are described.

2.1 Gate-based Quantum Computing

Superposition and entanglement are one of the features of quantum physics that quantum computing makes use of and are being introduced in the following. In classical computers a bit can only be in one of two states, usually represented as 1 and 0. However, a qubit, the basic building block of QC, can be in a superposition state of 1 and 0. Another difference between a bit and a qubit is that measuring a bit has no effect on its state. However, the measurement of a qubit changes its state, except if already being in the computational basis state of 0 and 1. Moreover, a classic system, given the same inputs, will always yield the same results. However, QCs with the same system and inputs will give different results with a certain probability. 

There exist different theoretical approaches to depict a state of a qubit, many times related to the technological implementation of a qubit. One of the well-known ways to depict a qubit state is by utilizing the Bloch sphere diagram. As Figure 2 shows, every qubit state can be described in polar coordinates by two angle parameters, \( \theta \) and \( \phi \), which give us a point on the sphere; the zero state \( |0\rangle \) is located on the north pole of the Bloch sphere and the one state \( |1\rangle \) is located on the south pole.

This allows to visualize 2-dimensional states in the 3-dimensional space. In other words, instead of considering a qubit
as a 2-dimensional complex vector space on the unit sphere, we can equivalently consider the state of the qubit as sitting on the surface of a 3-dimensional unit sphere by introducing the two parameters $\alpha$ and $\beta$:

$$|\Psi\rangle = \alpha |0\rangle + \beta |1\rangle$$

(1)

where $|\Psi\rangle$ represents the state of the qubit and $\alpha$ and $\beta$ are complex numbers and $|\alpha|^2 + |\beta|^2 = 1$. Based on the definition of complex vectors in polar coordinate systems the qubit state can be expressed as:

$$|\Psi\rangle = r_0 e^{i\phi_0} |0\rangle + r_1 e^{i\phi_1} |1\rangle, \quad r_0^2 + r_1^2 = 1$$

(2)

which leads to:

$$|\Psi\rangle = e^{i\phi_0} [r_0 |0\rangle + r_1 e^{i(\phi_1 - \phi_0)} |1\rangle]$$

(3)

The term $e^{i\phi_0}$ does not change the result after each measurement of the system and can therefore be neglected. Moreover, $r_0$ and $r_1$ can be replaced by $\cos \frac{\theta}{2}$ and $\sin \frac{\theta}{2}$. Thus, the following equation describes the general state of the qubit on the Bloch sphere by using two parameters in 3-dimensions.

$$|\Psi\rangle = \cos \frac{\theta}{2} |0\rangle + e^{i\phi} \sin \frac{\theta}{2} |1\rangle$$

(4)

The variables $\theta$ and $\phi$ parametrize the entire Bloch sphere, and every possible quantum state of a single qubit can be expressed by formula (4). A selection of quantum states is illustrate in Figure 3.

To change the state of a qubit, quantum gates are applied. There are many kinds of quantum gates as well as many different physical implementations of them. Some of them are basic gates and can transform one or two qubits at the moment. Others are constructed from specific arrangements of several basic quantum gates, called compound gates. Any movement on the Bloch sphere is spanned by the 3-dimensional rotation group $SO(3)$, which is isomorphic to the special unitary group $SU(2)$. All elements of this group can be represented as 2-dimensional unitary matrices with unit determinant. In this representation, the qubit basis states are represented as vectors:

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

(5)

A selection of commonly used single qubit gates are represented in Table 1.
Figure 3: Visualization of 3 different qubit states. Figure (a) is described with $\theta = 30^o$ and $\phi = 60^o$. In Figure (b), the state $|\psi\rangle$ is described by $\phi = \theta = 90^o$ and is in an equal superposition of $|0\rangle$ and $|1\rangle$. In Figure (c), the state $|\psi\rangle = |1\rangle$ has no defined value of $\phi$, because the first term in equation (4) is zero for $\theta = 180^o$, making $\phi$ part of the global phase variable $\phi_0$, which was neglected after equation (3).

Table 1: Single qubit gates with their matrices, their effect on the $|0\rangle$ state and a general description.

| Gate   | Matrix          | Input | Output | Description                                               |
|--------|-----------------|-------|--------|-----------------------------------------------------------|
| Pauli-X| $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ | $|0\rangle$ | $|1\rangle$ | Performs a rotation of $\pi$ around the $X$ axis. Also called the NOT gate. |
| Pauli-Y| $\begin{bmatrix} 0 & -1 \\ i & 0 \end{bmatrix}$ | $|0\rangle$ | $i|1\rangle$ | Performs a rotation of $\pi$ around the $Y$ axis. |
| Pauli-Z| $\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ | $|0\rangle$ | $|0\rangle$ | Performs a rotation of $\pi$ around the $Z$ axis. |
| Hadamard| $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$ | $|0\rangle$ | $\frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$ | Performs a rotation of $\pi$ around the $Z$ axis, followed by a rotation of $\pi/2$ around the $Y$ axis. |
| $R_\phi$| $\begin{bmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{bmatrix}$ | $|0\rangle$ | $|0\rangle$ | Movement along the latitudinal direction, by an angle of $\phi$. Also called shift gate, where the $\phi$ is the phase shift. |
| I-gate | $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ | $|0\rangle$ | $|0\rangle$ | Does not change the state. Also called the identity or no-op gate. |
| S-gate | $\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$ | $|0\rangle$ | $|0\rangle$ | Performs a phase shift of $\pi/2$ |
| T-gate | $\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$ | $|0\rangle$ | $|0\rangle$ | Performs a phase shift of $\pi/4$. |

was representable as a 2-dimensional unitary matrix, then an $n$ qubit gate is representable as a $2^n$-dimensional unitary matrix. The simplest and most commonly occurring example is a two qubit gate called the CNOT gate, given by the matrix

$$\text{CNOT} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

(6)

It is useful for creating entanglement between two qubits, meaning that it can create a two qubit state which cannot be expressed as a direct product of two single qubit states. An example is the two qubit Bell state

$$|\Psi\rangle = \frac{1}{\sqrt{2}} |00\rangle + \frac{1}{\sqrt{2}} |11\rangle$$

(7)

which can be prepared from the $|00\rangle$ state by applying a Hadamard gate on the first qubit, followed by a CNOT gate controlled by the first qubit and targeted on the second qubit. Both of the qubits are in an equal superposition of $|0\rangle$ and $|1\rangle$, but they are correlated with each other - no matter the measurement outcome, we know that the two qubits will be in the same state.

The physical implementation of quantum gates is specific to each qubit technology. However, there is a universal trade-off that has to be considered by all of them. Namely, to apply gates to qubits, they must be susceptible to
interactions, or else we cannot address them. Unfortunately, this also produces susceptibility to noise. This is especially problematic for entangled states, where each additional degree of entanglement will increase the amount of interference from noise.

2.2 Adiabatic Model

In this section, the adiabatic quantum computation model is described. The Hamiltonian is an operator that can be used to determine the total energy of a system and consists of kinetic and potential energy. Let \( N \) be the number of qubits available on the quantum hardware system. \( N \) qubits are set up in the ground state of \( H_0 \). \( H_0 \) is gradually transformed into a new Hamiltonian \( (H_f) \). In other words, \( H_0 \) is the initial Hamiltonian, and \( H_f \) is the final Hamiltonian. A gradual transformation can be described with the following equation:

\[
H(t) = (1 - t)H_0 + tH_f
\]

where \( t \) is a given time that gradually increased from 0 to 1 until \( H_f \) is reached. The ground state of \( H_f \) is \( |\Psi_f\rangle \), which is unknown. Finding \( |\Psi_f\rangle \) is the problem that adiabatic quantum computing is trying to solve. The quantum adiabatic theorem states that if one starts from the ground state of the initial Hamiltonian and the transformation is done slowly enough, then the final state of the system is the ground state of the final Hamiltonian. [Kato, 1950] One limitation is that the minimal required time needed to perform the transformation scales as follows:

\[
T = \frac{1}{(\text{Min}(g(t)))^2}
\]

where \( g(t) \) is the difference between the two smallest eigenvalues of \( H(t) \) (the difference between the ground energy and the first excited energy). Adiabatic quantum computing has been shown to be capable of achieving a speedup over classical algorithms [Roland and Cerf, 2002], where similar to Grover’s algorithm [Grover, 1996], finding any given element in an unstructured list could be done in \( O(\sqrt{N}) \) steps (as opposed to the requisite \( O(N) \) for classical computers.

2.2.1 Quantum Annealing

Quantum annealing belongs to the category of adiabatic quantum computing and is a meta-heuristic algorithm, which is able to find the minimum of a discrete cost (energy) function. Not all optimization problems can be solved with this approach, but there exist physical implementations that are able to find the ground state of a specific spin-lattice model called the transverse Ising model [Kadowaki and Nishimori, 1998], where each of the spins on the lattice is represented by a qubit. Quantum annealing is performed by preparing the ground state of a certain configuration of the spin-lattice model, described by some parameters, and subsequently changing those parameters to adiabatically transform the model such that it has a Hamiltonian that corresponds to the energy function of interest. Classically, finding the minimum of a discrete energy function can be considered as a combinatorial optimization problem.

The Hamiltonian of a transverse Ising model is:

\[
\hat{H} = \sum_i h_i \hat{\sigma}_z^i - \sum_{i,j} J_{ij} \hat{\sigma}_z^i \hat{\sigma}_z^j
\]

where \( i \) and \( j \) enumerate the different qubits, \( \hat{\sigma}_z \) are Pauli Z operators, \( h_i \) are called qubit biases and \( J_{ij} \) are called coupling strengths. By configuring a network of radio frequency superconducting quantum interference devices (RF-SQUIDs), the values of \( h \) and \( J \) can be configured and smoothly adjusted during operation. [Harris et al., 2010] To solve a problem with a discrete energy function \( E(s) \), where \( s \in \{-1, 1\} \), a corresponding Hamiltonian \( \hat{H}(\hat{\sigma}) \) with the same functional form needs to be prepared on the quantum computer. This is done by defining a time-dependent hamiltonian, which adiabatically transforms an easily preparable Hamiltonian \( \hat{H}_X(\hat{\sigma}) \) into the problem Hamiltonian \( \hat{H}(\hat{\sigma}) \):

\[
\hat{H}(t, \hat{\sigma}) = A(t)\hat{H}_X(\sigma) + B(t)\hat{H}(\hat{\sigma})
\]

where \( A(t) \) and \( B(t) \) are functions that make up the so-called annealing schedule and \( A(t) \gg B(t) \) at the start of annealing \( t = t_{\text{start}} \) whereas \( A(t) \ll B(t) \) at the end of annealing \( t = t_{\text{end}} \). In the RF-SQUID based approach, the starting Hamiltonian has a form of

\[
\hat{H}_X(\sigma) = \sum_i \hat{\sigma}_z^i
\]
If the system is prepared in a ground state of $\hat{H}_X(\sigma)$ at $t = t_{\text{start}}$, then it will be in a ground state of $\hat{H}(\sigma)$ at $t = t_{\text{end}}$ if $t$ changes sufficiently slowly in accordance with the adiabatic theorem provided before. Therefore measuring the states of the qubits will yield the ground state of the problem Hamiltonian, which represents the lowest-energy configuration of the original energy function, with high probability.

2.2.2 Quadratic unconstrained binary optimization (QUBO)

To make use of current quantum annealing hardware (e.g. from D-Wave or Atos), one has to formulate the problem at hand as either an Ising problem

$$E_{\text{Ising}} = \sum h_i s_i - \sum_{ij} J_{ij} s_i s_j$$

or a quadratic unconstrained binary optimization (QUBO) problem:

$$E_{\text{QUBO}} = x^T Q x = \sum_{ij} Q_{ij} x_i x_j$$

where $x$ is a binary vector and $Q$ is a matrix. The energy function of a QUBO resembles the Ising formulation except that the binary variables are either 0 and 1 in comparison to the spin values of the Ising model being -1 and 1. The two models are easily convertible to each other, and the QUBO form is often simpler to handle mathematically. Although this format of problem input may seem restrictive, many important NP complexity class problems can be expressed in this manner [Lucas 2014a].

2.3 Measurement based model

Measurement-based quantum computing (MBQC) is an approach to quantum computing, where the computation is implemented by performing a sequence of measurements on a quantum computer. This is possible because measurements change the state of the quantum computer, and can thus be used to emulate the action of quantum gates, enabling the processing of quantum information. In fact, universal quantum computation is possible within this framework, first shown by Raussendorf and Briegel in 2001, where they devised a so-called one-way quantum computer, which could implement the universal gate set using single-qubit measurements. [Raussendorf and Briegel 2001]

Although measurements can be used to create entanglement [Pfaff et al. 2013], it is more often the case that measurements destroy entanglement instead. For example, when performing any single-qubit measurement, the state of the measured qubit must necessarily collapse to a pure state, thus removing any entanglement it had in relation to other qubits. Because of this feature, MBQC most often relies on preparing a highly entangled state, called a resource state, on the quantum computer beforehand, where entanglement can be thought of as a resource, which is successively used up by the measurements needed to perform the computation. The specific design of a resource state has to be carefully considered, because it was discovered by Gross et al., that if the resource state is chosen randomly (from the Haar measure), then MBQC offers no speedup for computation. [Gross et al. 2009] Unfortunately, finding a suitable resource state for a given computation is in general more difficult than the computation itself [Morimae 2017]. Moreover, physical hardware and design constraints limit the possible resource states that can be efficiently prepared, as it is very challenging to develop the capability to prepare arbitrarily entangled states. Perhaps the one of the most simple examples of a resource state is a cluster state, which consists of a regular lattice of entangled qubits, such as the square lattice used in the original one-way quantum computer. [Raussendorf and Briegel 2001]

Another crucial aspect to keep in mind with the MBQC scheme, is that results of measurements are inherently random. As a consequence, the unitary transformations induced by those measurements are concatenated with a random Pauli operator called a byproduct operator. [Morimae 2014] To avoid an indeterministic calculation, this randomness can be mitigated by selecting the basis of each measurement based on the results of the measurements preceding it. This extra classical processing of information can be harmful insofar as it may cause a time-delay, which can lead to increased decoherence in the quantum computer.

MBQC is particularly appealing for quantum computing with photons, where creating highly entangled cluster states is possible and performing single-qubit measurements is immensely simpler than performing multi-qubit operations required for the gate-based model. [Larsen et al. 2019] Additionally, Broadbent, Fitzsimons and Kashefi discovered that MBQC can be used for blind quantum computation, where a client can outsource their computations to a server in a way where the server cannot decipher what computation is being performed [Broadbent et al. 2009], which is especially useful for future applications that have a high demand for security and privacy, [Fitzsimons 2017] For a more in-depth review of MBQC, see [Wei 2021], [Briegel et al. 2009], [Browne and Briegel 2016].
2.4 Topological model

A common feature of all the previously described computational models is that information is encoded into qubits locally. Through decoherence, information is lost when qubits interact with their local environment. The time that this process takes is called the decoherence time and it limits the accuracy and length of calculations that can be performed on quantum computers.

The topological model of quantum computation proposes to circumvent decoherence by encoding information non-locally, into global characteristics known as topological invariants. A classical example of this, shown in Figure 4, is encoding information by braiding ropes into knots that differ by their knot invariant. The two knots shown in the figure are topologically inequivalent, which means that one cannot be deformed into the the other without cutting the rope. This is a global property, since no particular part of either rope carries this information.

![Figure 4: The trivial knot (left) and the left-handed trefoil knot(right). These knots are topologically inequivalent. If this difference is used as a basis for encoding information, then the information is protected from all rope deformations besides cutting.](image)

Certain quantum states could also be braided along space and time dimensions, visualized in Figure 5. Superpositions of the occupation number of those states enable the storage of quantum information. Many interactions with the environment occur over small length scales, and are exponentially suppressed as the braiding is performed over larger distances. Only specific kinds of processes may still destroy the information. One such example is quasiparticle poisoning, where the environment introduces additional particles into the system. These particles might braid and fuse with the existing particles in the system, but the rate of this process is still estimated to allow for decoherence times on the order of seconds. [Karzig et al., 2021]

![Figure 5: Real-space trajectories of three particles (a), and the braiding of their worldlines (b). If the particles are non-Abelian anyons, then the final many-body quantum state is different than the initial one and information can be encoded as states that are related by different, topologically inequivalent braids. Deformation of the trajectories by noise or inaccurate control do not alter the stored information, as long as the particles do not come into contact. This robustness provides resilience to errors.](image)
The quantum states that possess the necessary properties describe particles called non-Abelian anyons. [Stern, 2010] Elementary particles of this type have not been discovered in nature, but it could be possible to create quasiparticle excitations within low-dimensional solid-state systems, which fit into this specific class of particle. [Wilczek, 2009] Recent experimental research shows evidence for the existence of anyons [Bartolomei et al., 2020; Nakamura et al., 2020], but so far there has been no conclusive observation of any non-Abelian anyons. Consequently, no topological computers or qubits have been built to date.

Current proposals involve fabricating semiconductor-superconductor hybrid nanostructures to engineer topological superconductors, which are theoretically predicted to host non-Abelian quasiparticles at their boundaries. [Lutchyn et al., 2018; 2010; Oreg et al., 2010] This approach has the potential to offer a path towards a scalable, fault-tolerant topological quantum computer. Similarly to superconducting qubits, extremely low temperatures are required for operation. [Karzig et al., 2017; Kitaev, 2003]

3 Quantum technology

There are many different types of quantum technologies, with each type having its specific characteristics with different advantages and disadvantages. This section will focus on three of those technologies: superconducting circuits, trapped ions and photonic qubits.

3.1 Superconducting circuits

Superconducting qubits use energy levels of superconducting circuits as computational basis states. Based on the degree of freedom, three main categories have been proposed for this type of qubit [Kjaergaard et al., 2020]: a) charge qubits, b) phase qubits and c) flux qubits.

Two factors can be influential in determining these three categories: Josephson energy (JE), which describes the energy stored in a Josephson junction, and charging energy (CE), which describes the energy described in a capacitor. The ratio JE/CE can distinguish the classes. In Figure 6, a) represents the charge qubit, which is also called the cooper pair box. In this case, the CE is larger than the JE (JE/CE << 1). The basis states in the charge qubits are the charge states, which means the presence or absence of cooper pairs on the island. The state of the qubit can be changed by changing the number of cooper pairs that cross the junction.

In Figure 6, b) depicts the flux qubit circuit diagram. In this case, the JE is larger than CE (1 < JE/CE < 100). The state of the qubit can be changed by changing the bias flux \( \Phi \).

In Figure 6, c) depicts the phase qubit, which is a current-biased circuit where JE is much larger than CE. Accordingly, the JE/CE ratio is considerably larger than the ratio for the charge qubit.

Additionally, different types of superconducting qubits can be derived by combining features of the three mentioned main types. For example, C-shunt flux [Yan et al., 2016], Transmon [Koch et al., 2007], and Hybrid qubits [Steffen et al., 2010].

![Figure 6: (a) Charge, (b) flux and (c) phase qubit](image-url)

| Advantage | Disadvantage |
|-----------|--------------|
| Faster gate speed | Poor connectivity to other qubits |
| The most mature of all the types | Requires near absolute zero temperature to operate |
| Can be built using existing semiconductor approaches | Susceptible to noise |
| Easy to reproduce qubits | Keeps qubit states for short period |
3.2 Trapped Ions

The first quantum gate for the trapped-ion systems was proposed by Ignacio Cirac and Peter Zoller. [Cirac and Zoller, 1995] This was the first step to turn quantum computing from theory into an experimental issue. Today it is one of the leading candidates in quantum computing [Bruzewicz et al., 2019], with Honeywell’s H1 system achieving the highest recorded quantum volume, which is a measure of performance capability for quantum computers [Cross et al., 2019]. In 2021, Katz [2021] This qubit technology uses ions, such as Yb$^{3+}$ [Kindem et al., 2020], suspended in vacuum, where certain internal electronic states of the ions are used as the computational basis states. Based on which states are chosen for this, four types of qubits are distinguished: hyperfine qubits [Blinov et al., 2004], zeeman qubits [Brown and Brown, 2018], fine structure qubits [Bruzewicz et al., 2019], and optical qubits [Bruzewicz et al., 2019]. The most important difference of these types is the amount of energy by which the internal states differ, enabling (and requiring) different photon energies for control and readout, which in turn provides unique benefits and drawback to each sub-approach.

The general advantages and disadvantages of trapped ion qubits are shown in Table 3.

Table 3: Advantage and disadvantage of trapped ion qubits

| Advantage                                      | Disadvantage                                             |
|-----------------------------------------------|----------------------------------------------------------|
| Stability (long coherence time)               | Slow gate speed                                          |
| Optimal connectivity (all to all)             | Many lasers are needed                                    |
| Entanglement of qubits is easy                | Vacuum needed for operation                              |
| Near absolute zero temperature is not needed  |                                                          |

3.3 Photons

Quantum theory describes light as consisting of individual particles called photons, which can be used to carry quantum information. The aim of photonic quantum computing (PQC) is to embed the processing of quantum information on photons into electronics so that it can be used for quantum computation. To perform PQC, photons need to be generated and quantum information needs to be encoded onto them. Subsequently, the photons must be manipulated to perform the computation and then detected to retrieve the result. Each of these steps have unique requirements and challenges associated with them. [Slussarenko and Pryde, 2019, Flamini et al., 2018] The general advantages and disadvantages of PQC are displayed in Table 4.

Table 4: Advantages and disadvantages of photonic quantum computing

| Advantage                                               | Disadvantage                                                |
|---------------------------------------------------------|-------------------------------------------------------------|
| Extremely long coherence time                          | Multi-qubit gates hard to implement                          |
| Possible room temperature operation                     | Deterministic photon generation and detection difficult     |
| Easy to generate entanglement                           | Qubits are destroyed by measurement                          |
| Easy to perform reliable single-qubit gates             |                                                             |
| Scalable architectures possible                          |                                                             |
| Supports quantum communication and distributed QC       |                                                             |

3.3.1 Photon Generation

Photons can be generated easily and in high numbers. For example, a common light bulb emits $\sim 10^{20}$ photons each second. The difficult task is to build a mechanism for deterministic single photon generation, which would be capable of emitting precisely one photon on demand, such that it is directed into an optical fiber or other specific element of the photonic circuit. Moreover, when using many photons within a computation, they need to be indistinguishable from each other in order for two-photon interference effects to give predictable and usable results.

Improving the reliability of deterministic single photon sources is an active area of research and many advancements have been made in recent years using trapped ions [Higginbottom et al., 2016], colour centers [Benedikter et al., 2017] and quantum dots [Lodahl, 2017] [Uppu et al., 2020], [Dusanowski et al., 2019]. A near-deterministic source could also be constructed by combining logical control operations on probabilistic processes. For example, spontaneous parametric downconversion (SPDC) probabilistically converts one higher energy photon into two lower energy photons. Detecting one of the photons heralds the other, which can then be routed into the circuit for computation. [Caspani et al., 2017]
3.3.2 Encoding information onto photons

Information can be mapped onto photon states in numerous ways. A qubit can be constructed from photons by choosing two orthogonal photon states that represent the logical states $|0\rangle$ and $|1\rangle$ of the qubit. This is sometimes referred to as dual-rail encoding. For example, a photon with horizontal polarization could represent $|0\rangle$ and a photon with vertical polarization could represent $|1\rangle$. A single photon has the ability to be in an arbitrary superposition of these two states and could as such be used as a qubit. A different example would be to send photons through two possible paths and a photon going through one path would represent $|0\rangle$ while a photon going through the other path would represent $|1\rangle$. Again, photons can travel through a superposition of many paths, experimentally easily achievable with a beam splitter. Many other encoding schemes exist as well and multiple encodings can be used simultaneously, meaning a single photon could encode multiple qubits in different ways at the same time. [Kagalwala et al., 2017] Moreover, some degrees of freedom are not just restricted to two possible states, but rather a plethora or even continuum of states, which could be used to encode *qudits*, the higher-dimensional version of qubits. As an example, a single optical mode can be in a superposition of Fock states $|n\rangle$, each of which represent a state with a certain number of photons $n$. There is, in principle, no limit to the amount of photons in a Fock state, allowing for an arbitrary amount of information to be encoded into one such optical mode, provided we have the capability to accurately prepare such states and distinguish between them.

3.3.3 Computation on photons

Perhaps the most difficult aspect of PQC is performing the actual computation itself. More specifically, the ability to perform multi-qubit operations is a necessary requirement for a universal quantum computer and for most quantum algorithms. The issue is that in normal circumstances, photons do not exhibit non-linear interactions with each other, which is good for avoiding unwanted cross-talk between qubits but detrimental to engineering multi-qubit gates. Early attempts to perform multi-qubit gates on photons involved using non-linear optical elements such as a Kerr media [Chuang and Yamamoto, 1995], but the viability of this approach is severely limited because this effect is extremely weak in all known materials. [Kok et al., 2002]

Consequently, most of the effort in the field focusses on linear optical quantum computing (LOQC), which uses only linear optical elements and measurements. [Kok et al., 2007] An important advancement came with the discovery of the KLM scheme, which probabilistically performs a two-qubit gate using just these components. [Knill et al., 2001] This scheme was quickly improved upon by others to perform almost deterministic two-qubit gates. [Kok et al., 2007] This shows that universal photonic quantum computing is in principle possible, even in the framework of LOQC.

A related, but conceptually different approach is to perform measurement based quantum computing on optical cluster states [Nielsen, 2003], where the goal is to generate a pre-determined highly entangled network of qubits as the input and perform quantum computation by only using single-qubit gates conditioned on projective measurements. Recent experiments have demonstrated that it is possible to create optical cluster states with thousands of qubits [Larsen et al., 2019] [Asavanant et al., 2019] and perform deterministic multi-qubit operations on them. [Larsen et al., 2021]

Finally, a non-universal quantum computational scheme called boson sampling has been pursued actively in recent years. The basic task of boson sampling is to send a number of input modes through a linear interferometer and sample the distributions of the photons at the output. [Aaronson and Arkhipov, 2011] One variant called gaussian boson sampling uses gaussian states of light as input rather than single photons, thereby circumventing the difficulties of developing reliable single-photon sources. [Hamilton et al., 2017] The task of simulating the sampled photon distribution with a classical computer has no known efficient algorithm, which is why researchers have been able to claim a demonstration of quantum supremacy based on this problem. [Zhong et al., 2020] Numerous near-term applications for this computational scheme have been found and compact, scalable and programmable devices are being developed for broader commercial use. [Bromley et al., 2020] [Arrazola et al., 2021]

3.3.4 Photon detection

Due to the bosonic nature of photons, many photons may occupy the same quantum state at once. Broadly, photon detectors can be classified into two groups: photon number resolving (PNR) detectors, which can discriminate between different photon occupation numbers, and threshold detectors, which can only signal whether or not at least one photon occupies the state. PNR capabilities are obviously preferred, but may not be necessary for some algorithms and experiments. Current state-of-the-art for experiments are silicon avalanche photodiodes (APDs), operating in Geiger mode, which are threshold detectors with limited wavelength coverage. [Eisaman et al., 2011] Improving the capabilities of photon detection is an active area of research, with perhaps the most notable direction being superconducting nanowire single-photon detectors (SNSPDs). [You, 2020] These detectors require cryogenic cooling to a few kelvin to enable superconductivity, which is still much more readily achievable than the millikelvin temperatures...
involved in superconducting qubits. Current state-of-the-art with PNR technology resides with transition-edge sensors
(TESs), which are capable of resolving photon numbers but suffer from slow operation [Burenkov et al., 2017; Calkins
et al., 2011], roughly two orders of magnitude slower than what is considered practical for PQC. [Slussarenko and
Pryde, 2019].

3.4 Other quantum technologies

There exist a range of other quantum technologies which we decided not to cover in this publication. These technologies
are based on silicon quantum dots [Chatterjee et al., 2021; Ferraro and Prati, 2020], diamond vacancies or neutral
atoms and the interested reader is referred to the referenced literature [Pezzagna and Meijer, 2021; Henriet et al., 2020;
Saffman, 2019].

4 Bibliography Analysis

In the past 30 years, quantum computing has experienced continuous expansion and diversification. This section
describes trends and perspectives for quantum models, qubit technology, and the use of quantum computing in chemical
and biochemical engineering. Publications are a suitable source of data that can be used as a factor to analyze the
growth rates of scientific fields and for this bibliography analysis data is collected from Web of Science (WOS). Figure
shows a quantitative analysis of published articles from 1993 to 2020. In this section, “search in topics” means search
through the input fields for title, abstract, author keywords, and keywords. The figure is based on a list of composite
keywords:

- (“quantum computing” OR “quantum computation”) AND “adiabatic quantum”
- (“quantum computing” OR “quantum computation”) AND (“gate based” OR “logic gate” OR ”circuit based”
  OR “digital quantum”)
- (“quantum computing” OR “quantum computation”) AND (“measurement based” OR “measurement-based”
  OR “one-way”)
- (“quantum computing” OR “quantum computation”) AND “topological quantum”

In total, 2,346 articles were found, from which 680 articles belong to the topological quantum model, 857 articles to the
measurement-based models, 418 articles to the adiabatic quantum models, and 391 articles to the gate-based models.
The first published paper on quantum models is related to the gate-based model. [Mizutani, 1993] From 1998 to 2001,
11 articles have been found and classified as relating to measurement-based quantum computing models. [Castagnoli
and Finkelstein, 2001; Castagnoli and Rasetti, 1993; Fortnow and Rogers, 1999; Castagnoli, 1998; Fortnow and Rogers,
1999; Csurgay and Porod, 2000; Yamasaki et al., 2000; Ambainis et al., 2000; Handel, 2001; Servedio, 2001] However,
based on citations, paper [Raussendorf and Briegel, 2001], with 3,918 citations, is the most significant paper on this
model. This paper discusses one-qubit measurements of cluster states. The first publication on the topological quantum
model was in 1998. [Freedman, 1998].

During the 90s, the gate-based models were at the top of the chart (from 1993 to 2004). Then the number of published
papers on this model gradually decreased. From 2004 to 2011, measurement-based models were consistently at the top
of the chart. Currently, the number of publications on topological quantum models and measurement-based models are
ahead. In the last decade, 1,639 articles were published, of which 588 articles relate to the measurement-based model,
562 articles to the topological models, 282 to the adiabatic model and 197 to gate-based models.

Figure [8] illustrates a quantitative analysis for identifying trends throughout the years for two main types of qubit
technology, trapped ion and superconducting qubit technology. The vertical axis shows the number of publications and
the horizontal axis shows years, from 1997 to 2020. The figure is based on a list of composite keywords:

- (“Quantum Computing” OR “Quantum Computation”) AND “Superconducting”
- (“Quantum Computing” OR “Quantum Computation”) AND (“Trapped ion”)

The figure contains two lines such that each line shows one of the models described in Section 2. In total, 872
publications were found, of which 356 articles belong to trapped ion technology and 516 articles to superconducting
qubits.

Figure [10] shows the result of the search in topics from 1997 to 2020. This figure illustrates the number of papers
that are related to the sub-fields of chemical engineering (heat transfer, mass transfer, material science, membrane
process, nanotechnology, natural environment, process control, thermodynamics) and QC. In total, 923 papers were
Figure 7: Search in topics from 1993 to 2021. Topics contain “quantum computing OR quantum computation” AND the keywords that are in the legend. These keywords are related to the various types of quantum models.

Figure 8: Search in topics from 1997 to 2020. Topics contain “quantum computing/computation” AND the keywords that are in the legend. These keywords are related to the various types of qubit technologies.
Figure 9: Search in topics from 1992 to 2020. Topics contain “quantum computing” OR ”quantum computation” AND the keywords that are in the legend. These keywords are related to the various fields of chemical engineering part 1.

Figure 10: Search in topics from 1995 to 2020. Topics contain “quantum computing/computation” AND the keywords that are in the legend. These keywords are related to the various fields of chemical engineering part 2.
found, of which 444 belong to the field of thermodynamics, 369 to nanotechnology, 62 to material science, 36 to heat transfer, 7 to process control, 2 to natural environment, 2 to membrane process, and 1 to mass transfer. In 1997, four papers were published, all with respect to nanotechnology. [Young and Sheu 1997, Porod 1997, Drăgănescu 1997, Bandyopadhyay and Roychowdhury 1997] The first paper in the thermodynamics field was published in 1998. [Ulyanov et al. 1998] The authors tried to describe the principles of quantum computing and quantum search algorithms by considering new informational technologies and modern physics. "Modern physics" (at that time) is described in two main sections. The first section is quantum information theory and the second is non-equilibrium thermodynamics and quantum mechanics. Figure 12 represents the country related distribution of QC related publication data in chemical and biochemical engineering. The data is collected based on the number of publications from 2012 to 2020. The keywords used are:

- ("Quantum Computing" OR "Quantum Computation") AND ("chemistry" OR "chemical" OR "biochemical").

Overall, 1157 articles were found. The top 10 countries based on the number of publications are the USA (483 articles), China (257), Germany (125), England (101), Japan (81), Canada (67), Australia (61), France (53), Spain (46), and Switzerland (46).

The assessment of the bibliography analysis represents that the application of QC in thermodynamics, biomedical, and biochemical are the most explored. These fields have moved beyond the testing phase, and practical applications are becoming more common. There is also a clear trend in qubit technologies (superconducting and trapped-ion), measurement-based model, and topological quantum modelling.

5 Quantum computing in chemical and biochemical engineering

Chemical and biochemical engineering C&B intersect the topics of chemistry, physics, biology and mathematics to serve the societal need of delivering industrial scale solutions to manufacture products and to generate energy carriers. QC will serve as a computing architecture to improve on existing methods to model quantum mechanical systems and solve them more efficiently and accurately in combination with classical algorithms. QC will allow specific optimization problems to be solved with exponential speed up in comparison to existing classical algorithms when the problem scales in size and lies within the NP complexity class and the bounded-error quantum polynomial time (BQP) class. Within the multi-scale layer concept of C&B and process systems engineering (PSE), quantum mechanical calculations can be applied for predicting the properties of chemical compounds and the kinetics of reaction networks. The prediction values are needed to design products and processes. QC can potentially also contribute to the calculation of transport phenomena and fluid dynamics. [Gaitan 2020, Budinski 2021, Ray et al. 2019] This would lead to generating results faster since fluid dynamic problems can take weeks to solve on high performance computing platforms. Finally, it would be remiss not to consider the logistics for C&B products in the post-production stage. Here, channeling the right product to the right destination, in the right quantities at the right time, is necessary to prevent disruptions in a distribution chain. These kind of supply chain optimization problems can also be solved efficiently with
Figure 12: Search distribution world-wide from 2012 to 2020. Search contains (“quantum computing OR computation”) AND (“chemical” OR “chemistry” OR "biochemical")

The current authors have taken the multi-layer view of C&BC proposed by [Gani et al., 2020] and reduced it to a simplified model (Figure 13) for the purpose of the current discussion.

The final derived model (Figure 14) illustrates the relationship between five distinct classes which can be summarized under the headings:

- Resources
- Knowledge & work force
- Quantum technologies
- Products & services
- Market

Further, each class can be utilized in the creation of a landscape for QC in C&BC, where QC itself is an instance situated in the quantum technologies class. Resources are needed in form of materials, compute power (sustained by electricity and cooling) and documented knowledge repositories. These resources are needed to develop quantum technologies, run the developed hardware for market usage and to educate students with the needed knowledge to perform research or work in the quantum technology domain.

Figure 15 depicts the impact which quantum technologies and QC will have on sustainable technologies and how this will affect our societies in the world. Near term quantum computing applications such as quantum machine learning, quantum chemistry and quantum Monte Carlo simulations will allow to accelerate the development of digital solutions and new materials such as catalysts or pharmaceutical drug compounds. We expect that quantum computing will contribute to improved energy efficiencies with respect to less electricity consumption of machine learning and optimisation algorithms. This leads consequently to a reduced carbon emission footprint. Further, the QC enhanced design of sustainable materials, processes and products will also have a beneficial impact on carbon emissions and other societal needs. The sections that follow will explore the opportunities for QC in the field of C&BC and its’ applications within the following:

- Pharmaceutical applications
- Biochemical applications
- Solid material applications
- Process & product design, optimization, monitoring & control
- Supply chain optimization
Figure 13: Simplification of C&BC multi-layer view by Gani et al.

Figure 14: Relationship diagram for quantum technologies
5.1 Pharmaceutical applications

The development of a market ready pharma product can take up to 12 years or longer [Gaudelet et al., 2021], and is characterized by tedious lab (in-vitro and in-vivo) experiments thus leading to high time investment and costs. Especially in the last decade in-silico experiments have been more and more integrated in the drug discovery pipeline due to the availability of high-quality structured data, next-generation sequencing technology, advances in quantitative biology and increased computer power. [Sormanni et al., 2018, Ringel et al., 2020]

Especially the drug discovery and pre-clinical research phases can benefit from quantum computing enhanced quantum chemistry calculations. [Lam et al., 2020, Zinner et al., 2021, Cova et al., 2022] Amongst the recent developments in this area are big-pharma collaborations with quantum computing software and algorithm developers. For example Roche and Cambridge Quantum Computing (CQC), a UK-based developer of quantum computing software, are collaborating on designing quantum algorithms for early-stage drug discovery and development. [Darroch, 2021] A partnership between Seeqc and Merck has been formed to develop hybrid quantum-classical algorithms for commercial scale development. [Castellanos, 2020] Zapata Computing is a Boston based startup which has successfully attracted an investment from BASF to assist in the development and discovery of new chemicals, pharmaceuticals and materials using QC. [Nelson, 2020] These are only a selection of many examples to show that QC has attracted great interest in industry and several other announcements have been made between specialized quantum computing SMEs and big pharma companies.

According to an article in C&EN News, big pharma executives are discussing QC for drug discovery on a landscape where data-dependent discovery is dominating. [Mullin, 2020] The start-up MentenAI has focused for example on accelerating protein design with machine learning and quantum computing on the D-Waves architecture. [Maguire et al., 2021] Other use-cases in the drug discovery area can be found with respect to the modelling of chemical reactions and understanding how pharmaceutical drugs interact with proteins and enzymes in the human body. [Cao et al., 2018]

Given all these developments, there still exist a great opportunity for exploring the application of QC where chemical engineers possess extensive know-how, namely pharmaceutical process development, control, optimization and monitoring. These areas involve a combination of skills within process systems engineering. Thus, QC will have an important contribution in multi-scale and enterprise-wide developments for integrated product-process development as further elaborated in section 5.4.

Quantum machine learning can contribute to reducing the energy footprint of artificial intelligence (AI) and machine learning (ML) models based on neural networks. [Andersson et al., 2022] Here, the training of these model can take several weeks and consume a high amount of electricity and thus contribute to CO2 emissions. Studies show that the training of a natural language processing (NLP) model emits more CO2 than the average of two US American citizens.
produce per year [Strubell et al., 2020], and the breakthrough Alpha Fold 2 model had to be trained for three weeks to win the protein folding contest CASP14 [Jumper et al., 2021]. Ising models and thus quantum annealing can be applied to speed up various algorithms and it has been mathematically proven that convolutional neural networks can benefit from being trained on quantum computer devices with large data sets [Lucas, 2014b; Pesah et al., 2021]. In molecular design, a quantum computer can be used to design molecules and solid materials by considering specific properties, which leads to reduced lab work. Prediction of the molecular properties is one of the significant parts in molecular design. As C&BC deals with the atomic scale, interactions are applied by the quantum behavior of nuclei and electrons. It is very hard for classical computers to model the quantum mechanical systems accurately enough because the interactions between particles are increasing very quickly as the system becomes more complex. [Aaronson 2009] There are many computational tools that are being used by researchers for chemical computations, such as density functional theory (DFT) [Geerlings et al., 2003], which provides an approximation of molecular systems. However, these tools are effective for small molecules and have some limitations when dealing with large molecules such as proteins. But quantum algorithms have already been implemented as proof of concepts such as protein folding to be applied when the number of available qubits is large enough for real use-case problems. [Perdomo-Ortiz et al., 2012]

To conclude, plenty applications of QC in chemical engineering exist with respect to pharmaceutical applications.

5.2 Biochemical applications

One of the very popular examples being mentioned in general articles about quantum computing applications is unveiling the detailed bio-synthetic reduction mechanism of dinitrogen to two ammonia molecules by the Mo-dependent nitrogenase enzyme, a complex metalloprotein. The most active site of this metalloprotein is the iron-molybdenum cofactor (FeMo-co). [Reiher et al., 2017] A Fe and the MoFe protein form the pocket in nitrogenase where FeMo-co is contained. [Seefeldt et al., 2009] This enzymatic process takes place at ambient pressure and temperature and if decoded could substitute the energy intensive Haber-Bosch process. Reiher et al. [Reiher et al., 2017] propose to calculate the reaction mechanisms by implementing a multi-configurational wave function as a sub-model to be solved on a quantum computer to improve/enhance classical methods such as density functional theory (DFT). Apart from enzyme design, Cheng et al. [2020], these kind of computational studies of reaction mechanisms and kinetics can be found for a wide area of high impact applications such as green catalysis of the Mannich reaction [Stevens, 2017], biochemical redox reactions [Jinich et al., 2019] and calculating uncertainties in microkinetic models [Becerra et al., 2021].

5.3 Solid material applications

Quantum computing could benefit combined ML and DFT models to for example analyze new battery materials where oxidation potentials have to be analyzed via high throughput screening. [Doan et al., 2020] As already stated before machine learning itself can profit from quantum computing [Zlokapa et al., 2021], and further improve quantum chemistry calculations with ML approaches such as presented with FermiNet [Pfau et al., 2020] or PauliNet [Hermann et al., 2020]. With respect to quantum chemistry calculations being one of the first domains to be applied on NISQ devices, novel battery systems such as calcium battery electrolytes can be analyzed more accurately and efficiently. [Araujo et al., 2021] Screening for synthetic catalysts can also be achieved by applying a hybrid classical-quantum algorithm where the free energies of all species in a reaction scheme are calculated on a quantum computer. This iterative process of providing initial parameter values of the Hamiltonian to the quantum computer to calculate the free energies for reaction pathway analysis will allow to modify the catalyst structure in each step to identify the most thermodynamic favorable reaction route. [von Burg et al., 2021] The analysis of polymeric structures allows to design more efficient plastic manufacturing and recycling processes [Walker et al., 2020; Sánchez-Rivera et al., 2021], and the design of novel bio-degradable polymers via redox switchable catalysis for example, [Upton et al., 2014]; [Deng and Diaconescu, 2021] These topics can be tackled with quantum chemistry and quantum computing in the future with highly automated algorithms. [Deglmann et al., 2015]

5.4 Process and product design, fault-diagnosis and logistics optimization

One important aspect worth highlighting is that knowledge transfer from different disciplines and application fields within quantum computing will become an important part of future research to identify novel solutions within manufacturing. One example is the work by Castaldo et al. where the optimal control in laser-induced population transfer is studied on the molecule cyanidin. [Castaldo et al., 2021] This kind of work is important e.g. for dye-sensitized solar cells where the efficiency and stability of photovoltaic materials is still undergoing a phase of improvement before market readiness. [Castillo-Robles et al., 2021] Castaldo et al. developed a hybrid quantum-classical algorithm involving also machine learning to simulate and control a ultra-short laser pulse directed at a cyanidin molecule to study the time-evolution of its state. Different algorithms were benchmarked and involved Broyden–Fletcher–Goldfarb–Shanno (BFGS), a genetic algorithm (GA) and Nelder–Mead (NM) methods combined with a quantum routine. These hybrid
algorithms were compared against the classical Rabitz algorithm. This quantum optimal control theory (QOCT) example shows that quantum computing can tackle use-cases and implement algorithms which intersect material/product design, control, monitoring, optimization and in the end can also contribute to needed knowledge of designing or modifying a manufacturing process. To leverage the potential of quantum computing, chemical engineers have to be involved to apply their systems thinking approach with the expertise of quantum physicists while abstractions have to be made so that all engineering disciplines are able to make use of quantum computers.

First-principle models are important to design processes or products to accommodate the next industrial shift to Industry 5.0 applications. Industry 5.0 envisions a connection between customer defined products and the possibility that manufacturing plants are able to produce the defined product specification of the customer. Here we see the potential that materials can be designed via hybrid classical-quantum algorithms and manufacturing processes will be set with the specific process parameters to produce the specified product. Quantum computing can enhance process and product design pipelines which combine various computational models ranging from the property prediction layer to process and products models such as unit operation models or product formulation models.

One such example, is designing solvents for various applications. Solvents are used in abundance in the chemical and biochemical industry. The use of efficient model-based solvent selection techniques is an option worth considering for rapid identification of candidates with better economic, environment and human health properties. The underlying solvation models which make use of quantum chemical calculations can benefit from quantum computing when methods have been developed to map such calculations to a quantum computer. For example, several research publications have developed frameworks combining machine-learning and computer-aided molecular design (CAMD) where machine learning algorithms have been combined with molecular descriptor packages while quantum chemical calculations were performed with DFT and solvation models. In these frameworks, solving the density functional theory calculations using quantum computing can improve the accuracy and computational efficiency of these frameworks in the future.

Several research papers have been published on the topics of manufacturing operations management, fault diagnosis, scheduling, logistics, and optimization of energy systems. In order to address the computational challenges, hybrid QC-based algorithms are proposed in the referenced literature and extensive computational experimental results are presented to demonstrate their applicability and efficiency.

Navigation-type and scheduling-type problems have been tackled with the D-Waves quantum computer by Rieffel et al. The authors took two approaches to tackle these kind of problems: (I) to map from general classical planning problem formulations to QUBO form; (II) to look at the problems specifically and perform a direct mapping to QUBO form. The general mapping was performed with two variants: a conjunctive normal form (CNF) instance and a time-slice instance adapted from Smelyanskiy et al. Direct mapping of graph coloring and direct mapping of Hamiltonian path formulations to the QUBO formulation were performed for the individual problem types. The direct mapping schemes have shown better performance than the more general undirected graph mapping scheme. The conclusion is that direct mapping schemes for the individual specific problem at hand (navigation-type, scheduling-type) will outperform general-purpose mapping methods which try to cover multiple problems. Thus, the most beneficial would be to develop a methodology or framework which applies direct mapping schemes for specific planning (navigation-type, scheduling-type) problems.

The attempts on tackling dynamic optimization and process monitoring by combining deep learning approaches and QC, a deep learning based fault diagnosis method and its application on selected problems such as continuous stirred tank reactors (CSTRs) and the Tennessee Eastman process has been proposed. This is a domain where hybrid machine-learning and quantum assisted algorithms can be developed for process monitoring, fault diagnosis and control. However, to date such approaches have been only applied to benchmark simulation models and their real use-case application in this sector requires further research.

A tree-search based quantum-classical algorithm has been implemented to solve a scheduling problem by dissecting the problem into a master formulation and multiple sub-problems. The master formulation was implemented on the quantum computer while the global tree search algorithm and the sub-problems were run on a classical device. This kind of concept bears similarity to the formulation of a molecular conformation search problem where also this kind of hybrid split up between master and sub-routines between quantum and classical devices has been performed. A flexible job shop scheduling problem has been developed with a quantum-inspired quantum annealer and digital annealer algorithms. The quantum annealer algorithm was implemented as a time-indexed QUBO problem derived from a makespan-minimization problem formulation. The digital annealer implementation extends the before mentioned QUBO formulation with a penalty term to adjust for shorter makespans in the schedule. The computational power plays a significant role in scheduling and logistics applications, especially when applying machine learning and considering multiple variables. The number of variables can increase because of real-time applications and market demands. For example, the number of constraints on the system can be affected by the
out-of-stock products or fleet breakdown. Decision making is at the core of such supply chain systems to reduce operational costs. [Roman Malina, 2019] Fujitsu and Toyota proposed optimizing supply chain and logistic network operations using Fujitsu’s quantum-inspired digital annealer computing solution. [Toyota Systems, 2020] The results showed that it takes 30 minutes to determine an optimal route that can reduce the logistics cost by about 2 to 5 percent. Not too much work has been published yet specifically dealing with process control theory and quantum computing. But we expect in the upcoming years that more hybrid classical-quantum deep/machine learning algorithms will be applied to controlling unit operations or entire processes. Ajagekar et al. [Ajagekar and You, 2020] have developed a deep learning algorithm to control a CSTR and the Tennessee Eastman process. Restricted boltzmann machines (RBMs) were implemented to generate via quantum sampling the run data for the quantum annealer which delivers then the expectation values to set the model parameters. The CSTR fault diagnosis problem shows improved performance with the QC algorithm with respect to fault detection rates. In case of the Tennessee Eastman process the deep learning algorithm adapted from [Zhang and Zhao, 2017] showed superior performance over the principal component analysis (PCA) algorithm whereas the QC adapted deep learning algorithm showed better fault detection rates for some individual detected faults and some for rates equal to 0 for the classical deep learning algorithm. We also expect that quantum machine learning (QML) will have an impact on chemical and biochemical process control applications since many machine learning algorithms are being developed for process control. Important for QML algorithms is the storage of the input data on the random access memory (RAM) of the quantum device termed QRAM. And research has already been performed to implement quantum-inspired regression to benchmark against quantum algorithms. [Gilyén et al., 2020] It was also shown under which practical conditions quantum-inspired and quantum algorithms can achieve practical results. [Arrazola et al., 2020] Quantum-inspired machine learning is suitable for input matrices with a low rank, low condition number and a very large dimension whereas quantum machine learning algorithms can be fed with sparse matrices of a high rank. Further to highlight with respect to QML is that a mathematical proof has been delivered showing that convolutional neural networks (CNNs) can be solved at scale with large data sets as a quantum CNN (QCNN) in contrast to classical CNN implementations. [Pesah et al., 2021] Ajagekar et al. [Ajagekar and You, 2019, Ajagekar et al., 2020] have solved unit commitment, facility-location, and heat exchanger networks problems using QC. In their work, they have concluded that the current capacity of quantum computers negatively affects the quality of solutions obtained for large-scale problems. However, this can be overcome in the next few years as the number of available qubits will increase and error-correction approaches will increase the performance of quantum computers.

6 Conclusion

This paper summarizes the fundamentals of QC, quantum computers, the application of QC in C&BC engineering and future progress directions. The main goal of this paper is to provide an overview to chemical and biochemical researchers and engineers who are not yet familiar with quantum computation.

Numerous articles were dedicated to the different applications of QC in C&BC engineering. The result of the bibliography analysis showed a 10.29 percent growth in 2020. These statistics in chemical and biochemical topics equal 1,010 papers out of 34,698 with 43.51 average citations per paper, where the average citation per year equals 1569.64. The paper provides a detailed view into quantum computing hardware and conducted research in C&BC engineering. The intention is that the reader picks up an interest to read up on one of the applications or quantum hardware devices and hopefully starts re-implementing their own algorithms and further develop them.

References

Paul Benioff. The computer as a physical system: A microscopic quantum mechanical hamiltonian model of computers as represented by turing machines. *Journal of statistical physics*, 22(5):563–591, 1980.

Gilles Brassard. Brief history of quantum cryptography: A personal perspective. In *IEEE Information Theory Workshop on Theory and Practice in Information-Theoretic Security*, 2005., pages 19–23. IEEE, 2005.

Whitfield Diffie and Martin Hellman. New directions in cryptography. *IEEE transactions on Information Theory*, 22(6): 644–654, 1976.

Charles H Bennett, Gilles Brassard, Claude Crépeau, Richard Jozsa, Asher Peres, and William K Wootters. Teleporting an unknown quantum state via dual classical and einstein-podolsky-rosen channels. *Physical review letters*, 70(13): 1895, 1993.

Charles H Bennett, Gilles Brassard, Sandu Popescu, Benjamin Schumacher, John A Smolin, and William K Wootters. Purification of noisy entanglement and faithful teleportation via noisy channels. *Physical review letters*, 76(5):722, 1996.
Charles H Bennett, Ethan Bernstein, Gilles Brassard, and Umesh Vazirani. Strengths and weaknesses of quantum computing. *SIAM Journal on Computing*, 26(5):1510–1523, 1997.

Charles H Bennett, Gilles Brassard, and Artur K Ekert. Quantum cryptography. *Scientific American*, 267(4):50–57, 1992.

David Deutsch. Quantum theory, the church–turing principle and the universal quantum computer. *Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences*, 400(1818):97–117, 1985.

John Preskill. Quantum computing and the entanglement frontier. *arXiv preprint arXiv:1203.5813*, 2012.

Frank Arute, Kunal Arya, Ryan Babbush, Dave Bacon, Joseph C Bardin, Rami Barends, Rupak Biswas, Sergio Boixo, Fernando GSL Brandao, David A Buell, et al. Quantum supremacy using a programmable superconducting processor. *Nature*, 574(7779):505–510, 2019.

et al Edwin Pednault. Quantum supremacy. *IBM website*, 2019. URL [https://www.ibm.com/blogs/research/2019/10/on-quantum-supremacy.html](https://www.ibm.com/blogs/research/2019/10/on-quantum-supremacy.html).

Jacob West. The quantum computer. *Retrieved December, 1:2002*, 2000.

Tosio Kato. On the adiabatic theorem of quantum mechanics. *Journal of the Physical Society of Japan*, 5(6):435–439, 1950.

Jérémie Roland and Nicolas J Cerf. Quantum search by local adiabatic evolution. *Physical Review A*, 65(4):042308, 2002.

Lov K Grover. A fast quantum mechanical algorithm for database search. In *Proceedings of the twenty-eighth annual ACM symposium on Theory of computing*, pages 212–219, 1996.

Tadashi Kadowaki and Hidetoshi Nishimori. Quantum annealing in the transverse ising model. *Physical Review E*, 58(5):5355, 1998.

Richard Harris, Mark W Johnson, T Lanting, AJ Berkley, J Johansson, P Bunyk, E Tolkacheva, E Ladizinsky, N Ladizinsky, T Oh, et al. Experimental investigation of an eight-qubit unit cell in a superconducting optimization processor. *Physical Review B*, 82(2):024511, 2010.

Andrew Lucas. Ising formulations of many np problems. *Frontiers in physics*, 2:5, 2014a.

Robert Raussendorf and Hans J Briegel. A one-way quantum computer. *Physical Review Letters*, 86(22):5188, 2001.

Wolfgang Pfaff, Tim H Tamiaiau, Lucio Robledo, Hannes Bernien, Matthew Markham, Daniel J Twitchen, and Ronald Hanson. Demonstration of entanglement-by-measurement of solid-state qubits. *Nature Physics*, 9(1):29–33, 2013.

David Gross, Steve T Flammia, and Jens Eisert. Most quantum states are too entangled to be useful as computational resources. *Physical Review Letters*, 102(19):190501, 2009.

Tomoyuki Morimae. Finding resource states of measurement-based quantum computing is harder than quantum computing. *Physical Review A*, 96(5):052308, 2017.

Tomoyuki Morimae. Measurement-based quantum computation cannot avoid byproducts. *International Journal of Quantum Information*, 12(05):1450026, 2014.

Mikkel V Larsen, Xueshi Guo, Casper R Breum, Jonas S Neergaard-Nielsen, and Ulrik L Andersen. Deterministic generation of a two-dimensional cluster state. *Science*, 366(6463):369–372, 2019.

Anne Broadbent, Joseph Fitzsimons, and Elham Kashefi. Universal blind quantum computation. In *2009 50th Annual IEEE Symposium on Foundations of Computer Science*, pages 517–526. IEEE, 2009.

Joseph F Fitzsimons. Private quantum computation: an introduction to blind quantum computing and related protocols. *npj Quantum Information*, 3(1):1–11, 2017.

Tzu-Chieh Wei. Measurement-based quantum computation. *Oxford Research Encyclopedia of Physics*, Mar 2021. doi:10.1093/acrefore/9780190871994.013.31

Hans J Briegel, David E Browne, Wolfgang Dür, Robert Raussendorf, and Maarten Van den Nest. Measurement-based quantum computation. *Nature Physics*, 5(1):19–26, 2009.

Dan Browne and Hans Briegel. One-way quantum computation. *Quantum Information: From Foundations to Quantum Technology Applications*, pages 449–473, 2016.

Torsten Karzig, William S. Cole, and Dmitry I. Pikulin. Quasiparticle poisoning of majorana qubits. *Phys. Rev. Lett.*, 126:057702, 2021. doi:10.1103/PhysRevLett.126.057702 URL [https://link.aps.org/doi/10.1103/PhysRevLett.126.057702](https://link.aps.org/doi/10.1103/PhysRevLett.126.057702).

Ady Stern. Non-Abelian states of matter. *Nature*, 464(7286):187–193, 2010. ISSN 0028-0836. doi:10.1038/nature08915
Frank Wilczek. Majorana returns. *Nature Physics*, 5(9):614–618, 2009. ISSN 17452481. doi:10.1038/nphys1380

H. Bartolomei, M. Kumar, R. Bisognin, A. Marguerite, J. M. Berroir, E. Bocquillon, B. Plaçais, A. Cavanna, Q. Dong, U. Gennser, Y. Jin, and G. Fève. Fractional statistics in anyon collisions. *Science*, 368(6487):173–177, 2020. ISSN 10959203. doi:10.1126/science.aaz5601 URL http://science.sciencemag.org/

James Nakamura, Shuang Liang, Geoffrey C. Gardner, and Michael J. Manfra. Direct observation of anyonic braiding statistics at the v=1/3 fractional quantum Hall state. *Nature Physics*, 16:931–936, 2020. URL http://arxiv.org/abs/2006.14115

Roman M Lutchyn, Erik PAM Bakkers, Leo P Kouwenhoven, Peter Kroegstrup, Charles M Marcus, and Yuval Oreg. Majorana zero modes in superconductor-semiconductor heterostructures. *Nature Reviews Materials*, 3(5):52–68, 2018.

Roman M. Lutchyn, Jay D. Sau, and S. Das Sarma. Majorana fermions and a topological phase transition in semiconductor-semiconductor heterostructures. *Physical Review Letters*, 105(7), 2010. ISSN 00319007. doi:10.1103/PhysRevLett.105.077001

Yuval Oreg, Gil Refael, and Felix Von Oppen. Helical liquids and Majorana bound states in quantum wires. *Physical Review Letters*, 105(17), 2010. ISSN 00319007. doi:10.1103/PhysRevLett.105.177002

Torsten Karzig, Christina Knapp, Roman M. Lutchyn, Parsa Bonderson, Matthew B. Hastings, Chetan Nayak, Jason Alicea, Karsten Flensberg, Stephan Plugge, Yuval Oreg, Charles M. Marcus, and Michael H. Freedman. Scalable designs for quasiparticle-poisoning-protected topological quantum computation with Majorana zero modes. *Physical Review B*, 95(23), 2017. ISSN 24699969. doi:10.1103/PhysRevB.95.235305

A. Yu Kitaev. Fault-tolerant quantum computation by anyons. *Annals of Physics*, 303(1):2–30, 2003. ISSN 00034916. doi:10.1016/S0003-4916(02)00018-0.

Morten Kjaergaard, Mollie E Schwartz, Jochen Braunmüller, Philip Krantz, Joel I-J Wang, Simon Gustavsson, and William D Oliver. Superconducting qubits: Current state of play. *Annual Review of Condensed Matter Physics*, 11:369–395, 2020.

Fei Yan, Simon Gustavsson, Archana Kamal, Jeffrey Birenbaum, Adam P Sears, David Hover, Ted J Gudmundsen, Danna Rosenberg, Gabriel Samach, Steven Weber, et al. The flux qubit revisited to enhance coherence and reproducibility. *Nature communications*, 7(1):1–9, 2016.

Jens Koch, M Yu Terri, Jay Gambetta, Andrew A Houck, DI Schuster, J Majer, Alexandre Blais, Michel H Devoret, Steven M Girvin, and Robert J Schoelkopf. Charge-insensitive qubit design derived from the cooper pair box. *Physical Review A*, 76(4):042319, 2007.

Matthias Steffen, Shwetank Kumar, David P DiVincenzo, JR Rozen, George A Keefe, Mary Beth Rothwell, and Mark B Ketchen. High-coherence hybrid superconducting qubit. *Physical review letters*, 105(10):100502, 2010.

Juan I Cirac and Peter Zoller. Quantum computations with cold trapped ions. *Physical review letters*, 74(20):4091, 1995.

Colin D Bruzewicz, John Chiaverini, Robert McConnell, and Jeremy M Sage. Trapped-ion quantum computing: Progress and challenges. *Applied Physics Reviews*, 6(2):021314, 2019.

Andrew W Cross, Lev S Bishop, Sarah Sheldon, Paul D Nation, and Jay M Gambetta. Validating quantum computers using randomized model circuits. *Physical Review A*, 100(3):032328, 2019.

Nati Katz. Honeywell and cambridge quantum reach new milestones, 2021. URL https://www.honeywell.com/us/en/press/2021/07/honeywell-and-cambridge-quantum-reach-new-milestones

Jonathan M Kindem, Andrei Ruskuc, John G Bartholomew, Jake Rochman, Yan Qi Huan, and Andrei Farao. Control and single-shot readout of an ion embedded in a nanophotonic cavity. *Nature*, 580(7802):201–204, 2020.

Boris B Blinov, Dietrich Leibfried, C Monroe, and David J Wineland. Quantum computing with trapped hyperfine qubits. *Quantum Information Processing*, 3(1):45–59, 2004.

Natalie C Brown and Kenneth R Brown. Comparing zeeman qubits to hyperfine qubits in the context of the surface code: Yb+ 174 and yb+ 171. *Physical Review A*, 97(5):052301, 2018.

Sergei Slussarenko and Geoff J Pryde. Photonic quantum information processing: A concise review. *Applied Physics Reviews*, 6(4):041303, 2019.

Fulvio Flamini, Nicolo Spagnolo, and Fabio Sciarrino. Photonic quantum information processing: a review. *Reports on Progress in Physics*, 82(1):016001, 2018.

Daniel B Higginbottom, Lukáš Slodička, Gabriel Araneda, Lukáš Lachman, Radim Filip, Markus Hennrich, and Rainer Blatt. Pure single photons from a trapped atom source. *New Journal of Physics*, 18(9):093038, 2016.
Julia Benedikter, Hanno Kaupp, Thomas Hümmer, Yuejiang Liang, Alexander Bommer, Christoph Becker, Anke Krueger, Jason M Smith, Theodor W Hänsch, and David Hunger. Cavity-enhanced single-photon source based on the silicon-vacancy center in diamond. *Physical Review Applied*, 7(2):024031, 2017.

Peter Lodahl. Quantum-dot based photonic quantum networks. *Quantum Science and Technology*, 3(1):013001, 2017.

Ravitej Uppu, Hans T Eriksen, Henri Thyrrestrup, Ash D Uğurlu, Ying Wang, Sven Scholz, Andreas D Wieck, Arne Ludwig, Matthias C Löbl, Richard J Warburton, et al. On-chip deterministic operation of quantum dots in dual-mode waveguides for a plug-and-play single-photon source. *Nature communications*, 11(1):1–6, 2020.

Łukasz Dusanowski, Soon-Hong Kwon, Christian Schneider, and Sven Höfling. Near-unity indistinguishability single photon source for large-scale integrated quantum optics. *Physical review letters*, 122(17):173602, 2019.

Lucia Caspani, Chunle Xiong, Benjamin J Eggleton, Daniele Baijoni, Marco Liscidini, Matteo Galli, Roberto Morandotti, and David J Moss. Integrated sources of photon quantum states based on nonlinear optics. *Light: Science & Applications*, 6(11):e17100–e17100, 2017.

Kumel H Kagalwala, Giovanni Di Giuseppe, Ayman F Abouraddy, and Bahaa EA Saleh. Single-photon three-qubit quantum logic using spatial light modulators. *Nature communications*, 8(1):1–11, 2017.

Michael A Nielsen. Optical quantum computing using cluster states. *Physical review letters*, 93(4):040503, 2004.

Warit Asavanant, Yu Shiozawa, Shota Yokoyama, Baramee Charoensombutamon, Hiroki Emura, Rafael N Alexander, Shunarto Takeda, Jun-ichi Yoshikawa, Nicholas C Menicucci, Hidehiro Yonezawa, et al. Generation of time-domain-multiplexed two-dimensional cluster state. *Science*, 366(6463):373–376, 2019.

Elena Ferraro and Enrico Prati. Is all-electrical silicon quantum computing feasible in the long term? *Physics Letters A*, 384(17):126352, 2020.
Sébastien Pezzagna and Jan Meijer. Quantum computer based on color centers in diamond. Applied Physics Reviews, 8 (1):011308, 2021.

Loïc Henriet, Lucas Beguin, Adrien Signoles, Thierry Lahaye, Antoine Browaeys, Georges-Olivier Reymond, and Christophe Jurczak. Quantum computing with neutral atoms. Quantum, 4:327, 2020.

Mark Saffman. Quantum computing with neutral atoms. National Science Review, 6(1):24–25, 2019.

Takashi Mizutani. Novel quantum effect devices for future functional logic gates. In ESSDERC ’93: 23rd European Solid State Device Research Conference, pages 745–752. IEEE, 1993.

Giuseppe Castagnoli and David Ritz Finkelstein. Theory of the quantum speed-up. Proceedings of the Royal Society of London. Series A: Mathematical, Physical and Engineering Sciences, 457(2012):1799–1806, 2001.

G Castagnoli and M Rasetti. The notions of symmetry and computational feedback in the paradigm of steady, simultaneous quantum computation. International Journal of Theoretical Physics, 32(12):2335–2347, 1993.

Lance Fortnow and John Rogers. Complexity limitations on quantum computation. Journal of Computer and System Sciences, 59(2):240–252, 1999.

Giuseppe Castagnoli. Quantum computation based on retarded and advanced propagation. Physica D: Nonlinear Phenomena, 120(1-2):48–61, 1998.

Arpad Csurgay and Wolfgang Porod. Toward nanoelectronic systems integration. In 2000 IEEE International Symposium on Circuits and Systems (ISCAS), volume 1, pages 1–4. IEEE, 2000.

Tomohiro Yamasaki, Hirotada Kobayashi, Yuuki Tokunaga, and Hiroshi Imai. One-way probabilistic reversible and quantum one-counter automata. In International Computing and Combinatorics Conference, pages 436–446. Springer, 2000.

Andris Ambainis, Michele Mosca, Alain Tapp, and Ronald De Wolf. Private quantum channels. In Proceedings 41st Annual Symposium on Foundations of Computer Science, pages 547–553. IEEE, 2000.

Peter H Handel. Quantum 1/f effect in spin decoherence rates and quantum computing. In AIP Conference Proceedings, volume 573, pages 156–165. American Institute of Physics, 2001.

Rocco A Servedio. Separating quantum and classical learning. In International Colloquium on Automata, Languages, and Programming, pages 1065–1080. Springer, 2001.

Michael H Freedman. P/np, and the quantum field computer. Proceedings of the National Academy of Sciences, 95(1):98–101, 1998.

Wayne C Young and Bing J Sheu. Unraveling the future of computing. IEEE Circuits and Devices Magazine, 13(6):14–21, 1997.

Wolfgang Porod. Quantum-dot devices and quantum-dot cellular automata. Journal of the Franklin Institute, 334(5-6):1147–1175, 1997.

Mihai Drăgănescu. From solid state to quantum and molecular electronics, the deepening of information processing. In 1997 International Semiconductor Conference 20th Edition. CAS’97 Proceedings, volume 1, pages 5–21. IEEE, 1997.

S Bandyopadhyay and VP Roychowdhury. Switching in a reversible spin logic gate. Superlattices and microstructures, 22(3):411–416, 1997.

SV Ulyanov, G Degli Antoni, K Yamafuji, T Fukuda, GG Rizzotto, and I Kurawaki. Physical limits and information bounds of micro control. part 2: Quantum soft computing and quantum searching algorithms. In Proc., page 217, 1998.

Frank Gaitan. Finding flows of a navier–stokes fluid through quantum computing. Npj Quantum Information, 6(1), 2020. doi:10.1038/s41534-020-00291-0, 10.1038/41534.2056-6387

Ljubomir Budinski. Quantum algorithm for the navier-stokes equations, 2021.

Navamita Ray, Tirtha Banerjee, Balasubramanya Nadiga, and Satish Karra. Towards solving the navier-stokes equation on quantum computers, 2019.

Rafiqul Gani, Jerzy Baldyga, Béatrice Biscans, Elisabetta Brunazzi, Jean-Claude Charpentier, Enrico Drioli, Hermann Feise, Andrew Furlong, Kevin M. Van Geem, Jean-Charles de Hemptinne, Antoon J.B. ten Kate, Georgios M. Kontogeorgis, Flavio Manenti, Guy B. Marin, Seyed Soheil Mansouri, Patrick M. Piccione, Ana Povoa, Manuel Andres Rodrigo, Bent Sarup, Eva Sorensen, Isuru A. Udugama, and John M. Woodley. A multi-layered view of chemical and biochemical engineering. Chemical Engineering Research and Design, 155:A133–A145, 2020. doi:https://doi.org/10.1016/j.cherd.2020.01.008
Thomas Gaudelet, Ben Day, Arian R Jamasb, Jyothish Soman, Cristian Regep, Gertrude Liu, Jeremy B R Hayter, Richard Vickers, Charles Roberts, Jian Tang, David Roblin, Tom L Blundell, Michael M Bronstein, and Jake P Taylor-King. Utilizing graph machine learning within drug discovery and development. *Briefings in Bioinformatics*, 22(6), 05 2021. doi:10.1093/bib/bbab159

Pietro Sormanni, Francesco A. Aprile, and Michele Vendruscolo. Third generation antibody discovery methods: in silico rational design. *Chem. Soc. Rev.*, 47:9137–9157, 2018. doi:10.1039/C8CS00523K

Michael S Ringel, Jack W Scannell, Mathias Baedecker, and Ulrik Schulze. Breaking eorum’s law. *Nature Reviews. Drug Discovery*, 19(12):833–834, 2020. doi:10.103841573-020-00059-3

Yu-hong Lam, Yuriy Abramov, Ravi S. Ananthula, Jennifer M. Elward, Lori R. Hilden, Sten O. Nilsson Lill, Per-Ola Norrby, Antonio Ramirez, Edward C. Sherer, Jason Mustakis, and Gerald J. Tanoury. Applications of quantum chemistry in pharmaceutical process development: Current state and opportunities. *Organic Process Research & Development*, 24(8):1496–1507, 2020. doi:10.1021/acs.oprd.0c00222

Maximillian Zinner, Florian Dahlhausen, Philip Boehme, Jan Ehlers, Linn Bieske, and Leonard Fehring. Toward the institutionalization of quantum computing in pharmaceutical research. *Drug Discovery Today*, 2021. doi:https://doi.org/10.1016/j.drudis.2021.10.006

Tânia Cova, Carla Vitorino, Márcio Ferreira, Sandra Nunes, Paola Rondon-Villarreal, and Alberto Pais. *Artificial Intelligence and Quantum Computing (QC) as the Next Pharma Disruptors*, pages 321–347. Springer US, New York, NY, 2022. ISBN 978-1-0716-1787-8. doi:10.1007/978-1-0716-1787-8_14

Gordon Darroch. Cambridge quantum to develop quantum algorithms with roche for drug discovery and development, 2021. URL https://cambridgequantum.com/cambridge-quantum-roche-drug-discovery/

Sara Castellanos. Merck venture arm invests in quantum computing startup seeqc, 2020. URL https://www.wsj.com/articles/merck-venture-arm-invests-in-quantum-computing-startup-seeqc-11586454285

Anya Nelson. Zapata computing announces $38 million funding for series b financing to accelerate the commercial adoption of quantum computing technologies and applications, 2020. URL https://www.basf.com/global/en/who-we-are/organization/group-companies/BASF_New-Business-GmbH/news/press-releases/2020/zapata-computing.html

Rick Mullin. Let’s talk about quantum computing in drug discovery, 2020. URL https://www.cen.acs.org/business/informatics/Lets-talk-quantum-computing-drug/98/i35

Jack B. Maguire, Daniele Grattarola, Eugene Klyshko, Vikram Khipple Mulligan, and Hans Melo. Xenet: Using a new graph convolution to accelerate the timeline for protein design on quantum computers. *bioRxiv*, 2021. doi:10.1101/2021.05.05.442729

Yudong Cao, Jhonathan Romero, and Alán Aspuru-Guzik. Potential of quantum computing for drug discovery. *IBM Journal of Research and Development*, 62(6):6–1, 2018.

Martin P Andersson, Mark N Jones, Kurt V Mikkelsen, Fengqi You, and Seyed Soheil Mansouri. Quantum computing for chemical and biomolecular product design. *Current Opinion in Chemical Engineering*, 36:100754, 2022. ISSN 2211-3398. doi:https://doi.org/10.1016/j.coche.2021.100754

Emma Strubell, Ananya Ganesh, and Andrew McCallum. Energy and policy considerations for modern deep learning research. *Proceedings of the AAAI Conference on Artificial Intelligence*, 34(09):13693–13696, Apr. 2020. doi:10.1609/aaai.v34i09.7123

John Jumper, Richard Evans, Alexander Pritzel, Tim Green, Michael Figurnov, Olaf Ronneberger, Kathryn Tunyasuvunakool, Russ Bates, Augustin Žídek, Anna Potapenko, Alex Bridgland, Clemens Meyer, Simon A A Kohl, Andrew J Ballard, Andrew Cowie, Bernardino Romera-Paredes, Stanislav Nikolov, Rishub Jain, Jonas Adler, Trevor Back, Stig Petersen, David Reiman, Ellen Clancy, Michal Zieinski, Martin Steinegger, Michalina Pacholska, Tamas Berghammer, Sebastian Bodensteiner, David Silver, Oriol Vinyals, Andrew W Senior, Koray Kavukcuoglu, Pushmeet Kohli, and Demis Hassabis. Highly accurate protein structure prediction with alphafold. *Nature*, 596(7873):583–589, 2021. doi:10.1038/s41586-021-03819-2

Andrew Lucas. Ising formulations of many np problems. *Frontiers in Physics*, 2:5, 2014b. doi:10.3389/fphy.2014.00005 URL https://www.frontiersin.org/article/10.3389/fphy.2014.00005

Arthur Pesah, M. Cerezo, Samson Wang, Tyler Volkoff, Andrew T. Sornborger, and Patrick J. Coles. Absence of barren plateaus in quantum convolutional neural networks. *Phys. Rev. X*, 11:041011, Oct 2021. doi:10.1103/PhysRevX.11.041011

Scott Aaronson. Why quantum chemistry is hard. *Nature Physics*, 5(10):707–708, 2009.
Paul Geerlings, F De Proft, and W Langenaeker. Conceptual density functional theory. *Chemical reviews*, 103(5):1793–1874, 2003.

Alejandro Perdomo-Ortiz, Neil Dickson, Marshall Drew-Brook, Geordie Rose, and Alán Aspuru-Guzik. Finding low-energy conformations of lattice protein models by quantum annealing. *Scientific Reports*, 2(1):571, 2012. doi:10.1038/srep00571

Markus Reiher, Nathan Wiebe, Krysta M. Svore, Dave Wecker, and Matthias Troyer. Elucidating reaction mechanisms on quantum computers. *Proceedings of the National Academy of Sciences*, 114(29):7555–7560, 2017. doi:10.1073/pnas.1619152114

Lance C Seefeldt, Brian M Hoffman, and Dennis R Dean. Mechanism of Mo-dependent nitrogenase. *Annual Review of Biochemistry*, 78(1):701–22, 2009. doi:10.1146/annurev.biochem.78.070907.103812

Jonathan Stevens. Virtually going green: The role of quantum computational chemistry in reducing pollution and toxicity in chemistry. *Physical Sciences Reviews*, 2(7):20170005, 2017. doi:10.1515/psr-2017-0005

Adrian Jinich, Benjamin Sanchez-Lengeling, Haniu Ren, Rebecca Harman, and Alán Aspuru-Guzik. A mixed quantum chemistry machine learning approach for the fast and accurate prediction of biochemical redox potentials and its large-scale application to 315000 redox reactions. *Acs Central Science*, 5(7):1199–1210, 2019. doi:10.1021/acscentsci.9b00297

Alexander Zlokapa, Anand Prabhu, Mary Sharmila Rongali, Sri Charan Simha Velpur, Bert Debusschere, and Eric A Walker. How a quantum computer could quantify uncertainty in microkinetic models. *Journal of Physical Chemistry Letters*, 12(29):6955–6960, 2021. doi:10.1021/acs.jpclett.1c01917

Hieu A. Doan, Garvit Agarwal, Hai Qian, Michael J. Counihan, Joaquin Rodriguez-Lopez, Jeffrey S. Moore, and Rajeev S. Assary. Quantum chemistry-informed active learning to accelerate the design and discovery of sustainable energy storage materials. *Chemistry of Materials*, 2020. doi:10.1021/acs.chemmater.0c00768

Alexander Zlokapa, Hartmut Neven, and Seth Lloyd. A quantum algorithm for training wide and deep classical neural networks, 2021.
Davide Castaldo, Marta Rosa, and Stefano Corni. Quantum optimal control with quantum computers: A hybrid algorithm featuring machine learning optimization. *Physical Review A*, 103(2), Feb 2021. doi:10.1103/physreva.103.022613.

José A. Castillo-Robles, Enrique Rocha-Rangel, José A. Ramírez-de León, Frida C. Caballero-Rico, and Eddie N. Armendáriz-Mireles. Advances on dye-sensitized solar cells (dsscs) nanostructures and natural colorants: A review. *Journal of Composites Science*, 5(11), 2021. doi:10.3390/jcs5110288.

Qilei Liu, Lei Zhang, Kun Tang, Linlin Liu, Jian Du, Qingwei Meng, and Rafiqul Gani. Machine learning-based atom contribution method for the prediction of surface charge density profiles and solvent design. *AIChE Journal*, 67(2):e17110, 2021. doi:https://doi.org/10.1002/aic.17110.

Eleanor G. Rieffel, Davide Venturelli, Bryan O’Gorman, Minh B. Do, Elicia M. Prystay, and Vadim N. Smelyanskiy. A case study in programming a quantum annealer for hard operational planning problems. *Quantum Information Processing*, 14(1):1–36, Dec 2014. doi:10.1007/s11128-014-0892-x.

Akshay Ajagekar and Fengqi You. Quantum computing assisted deep learning for fault detection and diagnosis in industrial process systems. *Computers & Chemical Engineering*, 143:107119, 2020. doi:https://doi.org/10.1016/j.compchemeng.2020.107119.

Eleanor G. Rieffel, Davide Venturelli, Bryan O’Gorman, Minh B. Do, Elicia M. Prystay, and Vadim N. Smelyanskiy. A near-term quantum computing approach for hard computational problems in space exploration, 2012.

Davide Venturelli, Dominic J. J. Marchand, and Galo Rojo. Quantum annealing implementation of job-shop scheduling, 2016.