Quantum computing for chemical and biomolecular product design

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Martin P Andersson¹, Mark N Jones¹,², Kurt V Mikkelsen³, Fengqi You⁴ and Seyed Soheil Mansouri¹

Chemical process design has for long been benefiting from computer-aided methods and tools to develop new processes and services that can meet the needs of society. Chemical and biomolecular product design could also benefit from the use of computer-aided solution strategies and computational power to efficiently solve the problems at various scales as the complexity and size of problems grow. In this context, new modes of computation such as quantum computing are receiving increasing attention. While quantum computing has been in development for quite some time, the development of the technology to the point of making commercial use of such resources is quite recent, and still quite limited in scope. However, projections point to a rapid development of quantum computing resources becoming available to academia and industry, which opens potential application areas in chemical and biomolecular product design. With the advent of hybrid algorithms that are able to take advantage of both classical computing and quantum computing resources, as quantum computing grows, more and more problems relevant for chemical product design will become solvable. In this paper, some perspectives are given by identifying a set of needs and challenges for a selected set of opportunities, such as quantum chemistry-based property prediction, protein folding, complex multi-step chemical reactions, and molecular reaction dynamics.

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Introduction
Chemical product design involves generation of numerous candidates and their evaluation and screening to fulfill consumer, service and/or process needs. Computer-aided product and process design has been for many years, the focus of many scholarly works, predominantly within the process systems engineering discipline since it requires the integrated use of different tools and data (predicted or experimental). Gani [1**] has illustrated the requirements for computer-aided product design, the associated processes to develop products and challenges and opportunities that they provide. It is emphasized, that the challenges and opportunities are in terms of the needs for multi-scale modeling with focus on property models that are suitable for computer-aided applications, solution strategies that can solve a large range of chemical product design problems and, a chemical product design framework with the overall objective to reduce the time and cost to market a new or improved product. Furthermore, the search for novel, innovative, and sustainable solutions need to consider issues related to the multidisciplinary nature of problems, the lack of data (knowledge) needed for model development, solution strategies that incorporate multiscale options, and reliability versus predictive power [2]. One crucial aspect needed to enable product and/or process design is the availability of relevant chemical and physical properties of the involved materials and molecules. These properties range from the molecular scale (such as catalyst activity of a material) up to macroscopic scale (such as vapor pressure of a molecule). In many instances, especially in novel designs, the necessary high-quality experimental data might not be available. Therefore, to manage the complexity associated with solution strategies to design novel products, there have been efforts to take advantage of molecular scale modeling, and computational chemistry approaches for product design as listed in Table 1. An elaborate discussion on the use of approaches such as COSMO-RS for fluid phase thermodynamics and drug design has been reported by Klamt [3]. As listed in Table 1, it is important to note that application of quantum chemistry in product and process design is currently already being explored by the process systems engineering community. With the development of classical computers over many decades, computational theoretical predictions of several molecular scale properties have become possible, including use of first-principles calculations in quantum chemistry. Examples of
### Table 1

<table>
<thead>
<tr>
<th>Work</th>
<th>Product design problem</th>
<th>Molecular scale modeling approach</th>
<th>Tool</th>
<th>Case studies</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fleitmann et al. [11]</td>
<td>Environmental assessment and design of solvents</td>
<td>COSMO-RS</td>
<td>COSMO-susCAMPD</td>
<td>Designing solvents in a hybrid extraction-distillation process</td>
</tr>
<tr>
<td>Gertig et al. [12]</td>
<td>In-silico design of catalysis and process optimization</td>
<td>COSMO-RS</td>
<td>CAT-COSMO-CAMPD</td>
<td>Diels-Alder reaction, Meuselmeier reaction</td>
</tr>
<tr>
<td>Liu et al. [13]</td>
<td>Reaction solvent and mixture design</td>
<td>GC-COSMO/GC</td>
<td>OptCAMD (ProCAPD)</td>
<td>Liquid solubility, fuel blends, solvents</td>
</tr>
<tr>
<td>Kalakul et al. [14]</td>
<td>Wide range of problems</td>
<td>Wide range of models</td>
<td>ProCAPD</td>
<td>Hydrogen recovery and conversion from an aqueous alkylamine solution to value-added products</td>
</tr>
<tr>
<td>Pudi et al. [15,16]</td>
<td>Phase transfer catalysis design</td>
<td>COSMO-RS</td>
<td>–</td>
<td>Ionic liquid-based gas separation processes</td>
</tr>
<tr>
<td>Liu et al. [17]</td>
<td>Ionic liquids</td>
<td>COSMO-RS and UNIFAC</td>
<td>ICAS — ILPro</td>
<td>Value-added products</td>
</tr>
</tbody>
</table>

The nature of quantum computers is better suited to solve the Schrödinger equation in quantum chemistry than classical computers, at least from a conceptual point of view. A classical computer needs to use various approximate methods to solve a real multi-electron molecular system Schrödinger equation, as it cannot be solved analytically. That approximation is inherently limited in accuracy but can be solved exactly. A classical computer and a quantum computer both approximate the real solution of a quantum mechanical system, but the nature of the approximation is quite different. The most accurate quantum chemical methods scale very steeply with system size, up to N^2, where N is the number of atoms for which the Schrödinger equation needs to be solved. Therefore, approximations such as density functional theory are used instead, which scale roughly as N^3. For example, the number of bits required to describe the caffeine molecule (C_8H_10N_4O_2, CAS 50-06-2) exactly is 1048, which is ~1035 TB [18]. The number of qubits (a quantum bit) required to store that same data during computation is roughly 160 [18], which is on IBM’s roadmap to be reached already in 2022 [19].

Quantum computing in relation to computer-aided product design is discussed in this work. First, an overview of evolution of computations and status of quantum computing (QC) is given. Next, the needs and challenges of using QC in chemical product design are highlighted. Next, perspectives of QC in relation to specific chemical product design applications such as, property prediction, protein structure prediction, micellar chemo-catalysis and/or bio-catalysis, and, molecular reaction dynamics, are given before concluding statements on QC and its future.

**What is a quantum computer and how does it work?**

Quantum computing, a new model of computation based on properties of quantum physics, has been an active area of research since the 1980s and has intensified greatly with a) the discovery of QC algorithms providing exponential or quadratic speedups in computational times, and b) the advent of physical, operational QC devices in the past decade [20].

To understand what makes a quantum computer so special, it is important to understand how it differs from classical computers. Computer information technology is based on bits, a binary system which can store information.
in one of two states, ‘0’ or ‘1’. These are the so-called logical bits and are represented by transistors in a computer. The transistors can be seen as a light switching on and off, hence ‘0’ and ‘1’. Many calculations can be done very quickly on existing computers and supercomputers, but they still have their limitations with respect to the binary state space calculations they can perform. This entails a limitation in speed, as the time required for large calculations becomes infeasible on classical computers.

A quantum bit, commonly known as a qubit, is represented by a physical system in between two states. Some examples are the spin of an electron, the two different polarizations of a photon and the energy states of an atom in its ground state and its excited state. Considering the spin of an electron, the qubit can therefore be either spin up or spin down, or a linear combination of the two. This physical phenomenon is called superposition, and it is the expanded state space of performing calculations on a quantum computer that makes it different than a classical computer. According to Aaronson [21] ‘What superposition really means is ‘complex linear combination’’. Here, the term ‘complex’ is not used in the sense of ‘complicated’ but in the sense of a real plus an imaginary number, while ‘linear combination’ means addition of different multiples of states. Therefore, a qubit is a bit that has a complex number called an amplitude attached to the possibility that, it is 0, and a different amplitude attached to the possibility that, it is 1. These amplitudes are closely related to probabilities, in that the further some outcome’s amplitude is from zero, the larger the chance of seeing that outcome; more precisely, ‘the probability equals the distance squared’.

Amongst the first ideas of a quantum computer is that of Richard Feynman [22] who pointed out that QC was not able to extend the computational model of classical computers, but could potentially run simulations in practical time that would be impractical (but not impossible) by classical computers. Over the next twenty years, different quantum computer technology concepts were explored, both physical requirements and how they could be used. In 2001, the Shor algorithm [24] was realized with the help of a nuclear magnetic resonance (NMR) system and over the next 15 years, quantum computing technology developed and improved to the point where commercial availability of resources began to emerge [23]. D-Wave started producing quantum annealing computers in 2010; however, until today these kinds of hardware cannot implement most quantum algorithms, including Shor’s algorithm [24]. In 2013, Google claimed that when QC was used to test a specific algorithm, it could solve the problem 100 million times faster than a classical computer. Note however, it was compared against a single algorithm (simulated annealing) using a single thread [25]. In fact, such speedups are deceiving and have been speculated ever since in the literature, see, for example, Mandra et al. [26]. In 2016, IBM launched their quantum experience program, allowing public to use their Quantum Cloud Services to run their algorithms on IBM’s quantum processor from their own computers. Also in 2016, Google successfully simulated the energy levels of the H₂ molecule, demonstrating the enormous potential of QC in the field of quantum chemistry [27]. Smaller quantum systems have been developed since 2016, with IBM developing both 5-qubit and 27-qubit processors and in 2019 and Google announcing the development of a 53-qubit system. Accordingly, the currently available quantum computers should be able to solve a problem that would take a supercomputer 10 000 years in only 3 min [28]. The competition in this emerging field is strong and just in September 2020, IBM also released the 65-qubit IBM Quantum Hummingbird processor. With IBM’s promises of a 127-qubit processor in 2021, a 433-qubit processor in 2022 and a 1121-qubit processor in 2023, quantum computing is a field that may grow significantly in the next few years [19].

Needs and challenges for using QC in product design

If the goal of the calculation in each product design problem is to capture major trends or to produce semi-quantitative results, then even rather simple approximate solutions to the Schrödinger equation tend to give results with acceptable accuracy. This is especially true for well-behaved systems, from a quantum mechanical point of view. Examples include non-transition metal containing insulating materials, simple organic molecules, and systems without unpaired d-electrons. A frequently used method for approximating a quantum mechanical system for such systems is density functional theory, which favorably balances accuracy with computational effort. Even rather large systems can be studied, which has enabled prediction of catalytic activity [29] as well as material electrical and mechanical properties [30], all of which can be relevant properties for optimal product and/or process design. In the text below, chemical product design problems involving different types of systems are highlighted together with their design methods.

Chemical and biological products

(Bio)catalysts

Organic synthesis using enzyme catalysis offers some distinct advantages over conventional transition metal catalysis, such as high activity, superb selectivity and increased sustainability using aqueous solvent systems [31]. The use of water as solvent for enzyme catalysis is also the source of some drawbacks preventing widespread industrial implementation. Drawbacks include low total turnovers because of low reactant and/or product solubility in water as well as the much more limited scope of chemical transformations that can be achieved, as enzymes for the desired reaction may not yet exist.
Enzymes are complex biomolecules which are ‘difficult’ systems, with many atoms and often with a transition metal in the active site. Transition metal containing systems often require advanced approximate methods for treating electron correlation on a classical computer and choosing inappropriate computational methods can lead to large and significant errors. This is particularly true for open shell systems that contain unpaired electrons at the metal site. Quantum computing could potentially help solving such difficult systems [32,33]. At the heart of biomanufacturing are entities such as enzymes to catalyze the required chemical couplings in manufacturing processes. To better understand and optimize such processes, the quantum chemical properties (if known well enough) can facilitate process and product design. Full quantum chemical calculations for whole enzymes are not likely to come within reach even for quantum computers in the coming years. The scaling of computational time with system size is very unfavorable for classical computers (except particular properties achievable using linear scaling density functional theory methods, e.g. Ref. [33],) and the number of qubits in quantum computers is still insufficient. Various forms of hybrid implementations can at least partially overcome this limitation. Hybrid methods are standard for quantum chemical calculations on enzymes, using different methods for different parts of the system. One example is the combined use of quantum mechanics (QM) for the active site and molecular mechanics (MM) using simple analytic force fields for the remainder of the biomolecule [34,35]. New hybrid methods for combining classical computers and quantum computers to different aspects of the overall quantum chemical calculation are emerging.

For solid catalyst design, QC is expected to become beneficial for solving the Schrödinger equation for materials with complex electronic structures, where conventional methods like density functional theory have difficulties. Examples include strongly correlated materials, like metal oxides.

**Protein folding**

Protein structure prediction is currently a major problem in computational biology [36]. Solving this problem can provide many benefits in molecular engineering and drug discovery. That is, better understanding of these structures would both serve to develop new products as well as efficient processes for their purification. According to the funnel hypothesis of protein folding, the native structure of a protein is believed to be the global minimum of its free energy [37,38]. Given the vast conformational space available to even small peptides, exhaustive classical simulations are intractable. However, many have wondered if quantum computing may be able to assist this problem. Therefore, the main aspect in designing proteins and solving protein structure problems is finding the lowest-energy conformation of a lattice model, which is an NP-hard (non-deterministic polynomial-time) problem [39,40], meaning that under standard hypotheses, no polynomial-time classical algorithm for this problem exists. Furthermore, it is currently believed that quantum computers cannot offer an exponential speedup to NP-complete and harder problems [41], although they can offer scaling advantages that have been known in the literature as ‘limited quantum speedup’ [41].

**Product design approaches**

One application that is being heavily investigated for use with QC is mathematical programming optimization. Optimization is required in a wide variety of fields, such as process systems (synthesis, design, intensification, and supply chain), chemical and biochemical product design, and environmental modeling. There have been works in developing optimization-based frameworks for product design such as in the works of Liu et al. [13] where an MINLP (mixed-integer nonlinear program) model for computer-aided molecular design is established to design different kinds of chemical products simultaneously. Moreover, an overview of computer-aided product design approaches are given and perspectives on hybrid knowledge-based and data-driven approaches are provided by Alshehri et al. [42]. The promise of exponential speedups is related to complexity classes (binary quadratic problems) that have been proved are subcases of NP (nondeterministic polynomial). Many such problems are so-called NP-hard problems, meaning that they scale very poorly on classical systems, making them prime targets for quantum advancements [43]. Apart from being very practical, certain phenomena of quantum physics apply well to some common aspects of many optimization problems. For example, one of the hallmarks of optimization problems is the presence of highly interconnected decision variables. Entanglement, the phenomenon in which the state of two quantum particles can be connected, can give quantum devices an edge on heavily connected problems [44]. In this work, we point out a few emerging application areas where we see QC as an upcoming useful technology for chemical and biomolecular product and process design.

**Perspectives**

**Property prediction using quantum chemistry**

Quantum chemistry has been used as a key component in many aspects of product design, where data acquisition by experiments is too expensive, difficult and/or impossible to predict for properties required in product design. Two examples are catalyst design and solvent design.

For computational catalyst design, the correct molecular scale properties need to be known and predicted with reasonable accuracy. In principle, this means that for a given catalyzed reaction, all stable reaction intermediates and transition states along the reaction coordinate(s) need to be known or estimated. Computational design of both molecular scale catalysts [45,46] and heterogeneous
catalysts (see, for example, Refs. [4,29**,47]) have been successful, demonstrating the viability and power of computer-aided design. The design of molecular organo-metallic catalysts to desired yield, rate and selectivity requires the proper combination of metal ion and organic ligands to tune reactivity and selectivity (steric and electronic effects dominate) [48]. In heterogeneous catalysis, solid materials structure and chemistry are the main contributors to catalyst activity and selectivity.

These molecular scale properties can be combined with other system parameters such as concentrations in solution or solid catalyst area to obtain the desired macroscopic properties including catalyst activity and selectivity as function of temperature and pressure, that is, parameters that are controllable during the process. In this respect, tailor-made computer-aided design of solvents to enhance the reaction rate can play an important role. One example of solvent design from quantum chemistry is that BASF designed a solvent using COSMO-RS to optimize a polymerization process [49**]. Improved design of solvents is possible by applying an integrated solvent and process design, as opposed to separate optimizations [50].

Any relevant application towards product design using quantum chemistry requires that the quality of the predictions is high enough, and as is often the case with any computer aided design problem, the main limitation is the computing power. Therefore, density functional theory has completely overtaken theoretical heterogeneous catalysis — no other method can provide enough accuracy for a large enough system to be relevant. That is also the reason why scaling relations between adsorbed reaction intermediates have been introduced to reduce time for screening for new materials [47,51]. While in principle molecular scale details are required, with proper assumptions some can be replaced with descriptors like the scaling relations, and in some cases even estimated via data-driven machine learning-based methods. Thereby, the following are potentially focus areas for QC in relation to property prediction:

- Combining molecular scale properties with process scale models in an integrated product-process design problem [52].
- Obtaining high quality data by solving selected, difficult quantum chemistry problems with quantum computing.
- Integration of machine-learning and data-driven approaches to combine the abilities of QC for faster and more efficient property model development.

Protein structure prediction
Protein folding has been regarded as one of the most difficult problems to solve within the biotech domain for more than 50 years [53,54]. Protein folding is a central challenge in computational biology, as a hard combinatorial optimization problem, it has been studied as a potential target problem for quantum annealing. Although several experimental implementations have been discussed in the literature, the computational scaling of these approaches has not been elucidated [55].

The bi-annual ‘Critical Assessment of protein Structure Prediction’ (CASP) competition has been won by the company DeepMind at CASP13 (2018) and CASP14 (2020) with the submitted algorithm AlphaFold [56], benchmarking against the competition with a score of 58.9% for the global distance test (GDT), which depicts the degree of similarity to the set of experimentally analyzed protein structures. With a score of 92.4%, AlphaFold 2 [57] achieved an impressive improvement to the GDT score. It is evident that the predictive capabilities of deep neural networks have advanced the efforts to tackle protein folding significantly.

One open question we find worthwhile to ask is whether quantum computing can even enhance deep neural networks by combining quantum hardware with the use of graphical processing units (GPUs), field programmable gate arrays (FPGAs) or application-specific integrated circuits (ASICs) such as Alphabet’s proprietary TPU architecture. The trained AlphaFold 2 network relied on large computing power (16 TPUs vs equivalent to 128 TPUs) and approximately comparable to the power of 100–200 GPUs [57] and would cost research groups a considerable financial budget (with 2.64 USD/hour pre-emptible price per TPU vs resulting in 2.64 USD/hour × 16 × 128 × 21 days × 24 hour/day = 2724 986 USD) to implement and perform such neural network training algorithms. Also, researchers would probably re-train the model several times to explore new ideas, debug the code, and so on. This means that such kind of research would cost millions of USD. Thus, we believe that quantum machine learning (QML) can provide a way to circumvent such large-scale computing power issues and QML is also an active area of research where for example feed-forward neural networks have been trained via a quantum algorithm and achieved exponential speedup over gradient-descent [58]. Other approaches to solving the protein folding problem with quantum devices have been applied with different kinds of variational quantum eigensolvers [59], such as the Conditional Value-at-Risk Variational Quantum Eigensolver (CVaR-VQE) [60], or with quantum walks [61]. The question here is, whether quantum computers will be able to solve this problem more efficiently than classical AI implementations. Whether any of these hybrid classical–quantum computing algorithms will be able to outperform classical deep neural networks still needs to be studied. Thereby, the following are potentially focus areas for QC in relation to protein structure property prediction:

- There have been efforts in solving problems to predict protein structures with QC. However, work needs to be
done to develop more efficient solution strategies as quantum computers scale up.

**Sustainable micellar chemo-catalysis and bio-catalysis**

With the emerging use of designer surfactants in water, which can act as reaction medium for simultaneous enzyme catalysis and chemo-catalysis [62**] a more sustainable process for fine chemicals production can begin to be designed. Biocatalysis can then be naturally phased into multistep synthesis routes whenever a reaction step using an enzyme is superior to a conventional catalyst. Ideally, such combinations should be possible even without extraction and change of solvent.

While computational chemistry has been successfully utilized to better understand conventional chemo-catalysis (for example, see Ref. [63]), only some work has been done on chemo-catalysis in micelles [64], and none on enzyme catalysis in micelles. With many new opportunities opening when combining the biocatalysis and chemo-catalysis, any optimization and fundamental understanding becomes combinatorically more difficult than either case on its own. The complexity is simply too great in a system with transition metal catalysts, surfactant micelles, enzyme catalyst, reactants, and products, some of which can change along the multiple reaction steps. The vast number of computations necessary to completely describe such a complex system is beyond classical computers and the associated solution strategies, but the use of quantum computing holds a potential key to success, not least because of the possibility to hold more data during the computations. The discussions in previous examples hint at possibilities to optimize reaction activity and selectivity across multiple steps via more accurate activation energies, also considering the necessary conformational degrees of freedom of both surfactant micelles and enzymes. A conceptual visualization of such an integrated approach is shown in Figure 1. The real experimental system is shown in the central tank, and property predictions for key molecular and process properties are done using an appropriate hybrid approach between a quantum computer and a ‘normal’ supercomputer.

Using micelles as reaction media has numerous benefits. Chemo-catalysis becomes more efficient, uses less catalyst, requires little to no organic solvent, and often requires only mild heating, if any [65,66]. The biocatalytic reaction has a higher yield and becomes less susceptible both to pH and temperature effects [62**]. The use of designer surfactants in water thus has strong synergistic effects on both processes, allowing them to run simultaneously in the same reaction vessel. The potential gains are tremendous, but the main hurdle is that the added complexity makes progress difficult, particularly any attempts at rational product and reaction design.

An aqueous micellar solution is a multi-component system in which co-location of reactants is required for the reaction to run. In order to satisfy the design requirements for separation/recycling and control over unwanted physical phenomena, preferential control over partitioning of the various components is required, including potential physical transformations, such as solid precipitation. Ideally, both the kinetic parameters from transition state calculations for catalysts as well as physicochemical properties of the surfactants and all components in the system should be available.

To fully design processes for sustainable micelle-based synthetic routes, the ability to predict certain key properties are required, which could benefit from QC:

- Catalyst activity, selectivity, and compatibility with the micellar environment. This would require molecular property prediction for formulations, enzymes and organometallic catalysts.
- Efficient recovery and purification of the product — essentially an integrated surfactant, catalyst, solvent, and process optimization.

**Quantum computers and molecular reaction dynamics**

The optimization of chemical processes to yield desired products often requires knowing the reaction dynamics and finding energy efficient reaction routes, for example, by using proper catalysts. The core of reaction dynamics is the dynamics of processes involving breaking and formation of chemical bonds, transfer of electrons and protons along with photoinduced processes involving the interactions between electromagnetic radiation and molecular systems [67,68].

Several of these processes involve nonadiabatic operations that involve investigations of the electron-nuclear dynamics that goes beyond the Born-Oppenheimer approximation. This is a very difficult problem to solve using conventional methods because it would be a problem that is efficiently solved using quantum computers and finding new methods using quantum algorithms for the description of nonadiabatic phenomena involved in photoinduced reactions. One key aspect for why quantum computers could help solve the problem is the conceptual advantage of using qubits as opposed to bits, with the capability of storing a much larger amount of data during the computations. The dynamics of the chemical processes involve the determination of thermal and vibrational relaxation rates of the ground and electronically excited states, and accurate assessments of these rates will provide an unprecedented understanding of how to control and exploit the chemical processes. Reaction dynamics involving nuclear tunneling would be an attractive undertaking for quantum computer algorithms since this problem can be investigating using boson algebra for the
nuclear tunneling dynamics and go beyond the conventional semiclassical approximations [67–69].

The understanding of chemical reactions in the atmosphere is crucial for evaluating the future of climate change and how atmospheric pollution, for example, from use of chemical products and operation of industrial chemical processes, affects human health. A full understanding of the complicated reaction mechanisms of atmospheric chemical reactions involves determinations of elementary rate constants along with the crucial and relevant chemical mechanisms. This involves including spin-orbit, relativistic effects and nonadiabatic effects in the quantum calculations of relevant atmospheric chemical rate constants [67].

Furthermore, reaction dynamics investigations of thermal reactions, such as involved in chemical weapons and/or explosives, can be described by quantum-based reaction molecular dynamics simulations. Based on these methods, it is possible to provide data on impact sensitivity and safety handling of the explosives, both important aspects of product design.

The dynamics and energy transfer undergoing the excitations of vibrational molecular modes are crucial for determining the products formed during chemical reactions, either thermally activated or by interactions with electromagnetic radiation fields. The mechanisms for vibrational dynamics are crucial for understanding the effects of vibrational excitations on selective bonds and how the dissociation processes evolve with time and surplus of energy. Being able to predict photoinduced chemical reactions could help identify new and more efficient reaction routes, making production of key chemicals more energy efficient and enabling new target molecules to be produced at scale. The following can be potentially achieved with quantum computing and algorithms:

- Quantum algorithms for simulating molecular vibrational excitation would be a relevant avenue within the area of quantum computing [69–71].
- Quantum algorithms would be able to provide crucial insight into the relevant mechanisms of delay times, energy impact, pressure changes and how to prevent unsafe explosions [67,68].

Conclusions
Quantum computing is already being realized across many different fields, despite being an emerging technology in its early stages of development and requiring far more development in terms of hardware capacity, adapting solution strategies to exploit its capabilities, and solving real-world problems. In this work, the connection between chemical and biomolecular product design and quantum computing has been discussed. Chemical and biomolecular product design has largely benefited from computer-aided methods and tools using classical computers. However, some emerging applications towards developing novel products associated with more sustainable processes (green solvents, more efficient process design, integrated process-product design, and new drug developments or vaccines for a future pandemic) can benefit from emerging computational tools such as quantum computing. There are prospects for its application in process design, process control and monitoring as well. Several needs and challenges have been identified and specific perspectives on how to utilize quantum computing in this context have been provided. We foresee ample opportunities for taking advantage of quantum computing for developing and designing more efficient, economic, and sustainable products and chemical processes in the not-too-distant future. To conclude we find the following areas relevant for future use of quantum computing for applications related to chemical product-process design:

- Hybrid QC methods are likely to play an important role also, as many multivariable problems will be optimally solved through a combination of ‘expensive’ QC resources and ‘cheap’ classical computing power. Front-end applications that can optimize the ratio of QC and classical computing resources that are applied for a given problem are likely also to be of utility. Training and educational initiatives that can support this will also play an important role.
- Identifying relevant problems that can appropriately be formulated as optimization problems to solve with quantum computers. Quantum computers are not supposed to replace ‘all’ existing modes of computations.
- Using quantum computing (hybrid or stand-alone) combined with machine-learning approaches can provide significant advantages through the development of multi-variate statistical process monitoring and fault-diagnosis systems.
- Computational modeling of quantum-mechanical systems such as molecules, including predictions of their
properties, structure, and reactivity, is likely to be much more precise using quantum computing, and this will directly impact areas such as pharmaceutical drug discovery and specialty chemical material design.

Conflict of interest statement
Nothing declared.

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References and recommended reading

Papers of particular interest, published within the period of review, have been highlighted as:
• of special interest
•• of outstanding interest


23. This reference provides the first ideas around formation of quantum computers by R Feynman.


This reference serves as an excellent review over how density functional theory has been and is being used to identify key trends in materials properties. The authors then demonstrate how to calculate the activity and selectivity of new catalyst materials and how to use quantum chemistry as a computational screening tool.


This reference demonstrates how a quantum computer could be used together with classical computers to solve the Schrödinger equation for a large system with complex electronic structure, nitrogenase, a biocatalytic system with a transition metal center. This would lead to more accurate activation energies, beyond what classical method alone can achieve.


The review article presents a detailed discussion of the current perspectives and challenges of knowledge-based and data-driven CAMD and identifies key areas for future research directions.


This reference showcases how a proper combination of different, complimentary quantum chemical methods can accurately predict reaction pathways and dynamics for an industrially relevant polymerization reaction. COSMO-RS was used to model solvent effects, while higher level ab initio methods was used to model the reaction energy.


This reference demonstrates how chemocatalysis can be used together with biocatalysis in a multi-step reaction, enabled by the aqueous micellar solution medium. It showcases that added apparent complexity can in fact reduce the number of separate reaction steps and lead to an overall more efficient intensified process.