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Introduction to “Quantum computing for chemistry, material science and biotechnology”

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Quantum computing is a new computational paradigm that is making waves in the scientific community as well as the business world. The best possible scenario of an exponential speedup for some algorithms makes this technology enticing for application areas that are currently limited in their speed and efficiency by computational resources. The chemical industry, materials development and biotechnology are prime examples that would benefit from larger and more accurate simulations to unlock progress. As it stands, determining the most promising application and the most advantageous algorithms is still a very active area of research. This themed collection was conceived to highlight developments in research that bring practical quantum computations closer to reality. It coincides with the United Nations “International Year of Quantum” and aligns well with its intention to raise awareness about quantum science and technology.

At the time of publication, the first practical implementations of error correction codes are being executed on hardware. The quantum computing community is experiencing a transition from noisy intermediate scale quantum computing (NISQ) to fault-tolerant quantum computing (FTQC). A timely topic of this collection concerns techniques to extend the capabilities of noisy devices before error correction becomes a reality. One strategy is to counteract noise by learning its properties for

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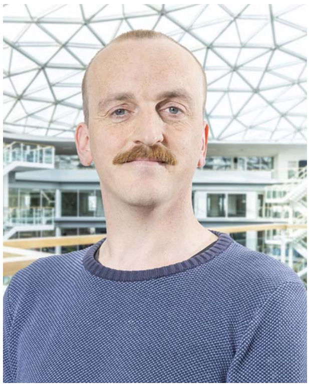

Matthias Degroote

Dr Matthias Degroote investigates the application of quantum computers in drug design at Boehringer Ingelheim. He is a quantum chemist who has approached the quantum many-body problem from the classical and quantum computing sides. Degroote received a PhD in physics from Ghent University working on Green’s functions and has gone on from there to do postdoctoral research in method development at Ghent University and Rice University. Since 2018 he is interested in the application of quantum computers on which he has done research at Harvard University and University of Toronto. Degroote is also an associate editor at the Royal Society of Chemistry for the journal Digital Discovery.

Joonho Lee

Dr Joonho Lee is an assistant professor in the Department of Chemistry and Chemical Biology at Harvard University. His group’s research focuses on developing advanced electronic-structure methods for complex materials and chemical systems. His work spans ab initio many-body approaches, electron–phonon interactions, polarons, and electrochemical simulations, with an emphasis on building accurate and scalable theoretical tools that connect fundamental quantum theory to real materials problems. He has also worked on methods related to auxiliary-field quantum Monte Carlo, variational approaches to coupled electron-nuclear dynamics, and constant-potential density functional theory for condensed-phase and interfacial systems.

a selected set of states. Expanding this set of states from a single reference to the multi-reference case[1] significantly improves the performance of NISQ devices for initial state preparation. As longer circuits become available in the early fault-tolerant regime, subspace diagonalization methods based on expectation values from short time propagation of Hamiltonians become more feasible. Smart partitioning of terms in the Hamiltonian allows to eliminate unnecessary measurements or join common measurements to reduce the overall sample complexity.[2] In order to reduce the sampling cost further, sample-based subspace diagonalization forgoes measurement of expectation values and only obtains sets of computational states from the quantum computation. However, qubit availability on current devices is not sufficient to treat realistic models of materials. Active space methods opt to select only the most relevant orbitals to perform the calculation, while keeping the others at the mean-field level.[3] Fragmentation techniques like quantum bootstrap embedding[4] are more sophisticated and try to split up the system in parts that can be treated separately and matched self-consistently at the boundaries. These effectively allow smaller quantum computers to treat larger systems.

Pauline Ollitrault

Dr Pauline Ollitrault is a quantum chemist specializing in quantum algorithms for molecular property predictions. Ollitrault received a PhD in chemistry from ETH Zurich and IBM Research Zurich, working on near-term quantum algorithms for chemistry. She continued as a researcher at IBM Research Zurich before joining QC Ware Corp. in Paris in 2022, where she focused on fault-tolerant quantum algorithms for chemistry. Since 2026 she has pursued entrepreneurial activities at the intersection of advanced electronic structure methods and machine learning.

As the technological capabilities increase, the separation between NISQ and FTQC becomes increasingly blurred. Research that spans both paradigms has the chance to stand the test of time and remain highly relevant. Trotter splittings for time evolution operators are a common building block of both near-term and long-term quantum algorithms. The level of truncation and grouping of the terms in the operators is most commonly decided by using a norm-based bound. Research in this collection shows that there is almost no correlation between the norm-based error bound and the true error and that perturbative estimates help make better decisions on the partitioning of terms.[5] Alternatively, one can introduce physically motivated approximations for the expectation value operator which significantly reduces the amount of terms.[6] A similar topic is the preparation of good initial states for ground state search. Translating a classical approximate ground state into an efficient quantum circuit[7] is a non-trivial primitive that will be necessary to perform efficient quantum simulation on large-scale systems. In this case as well, tree-based methods that partition the system in tractable pieces might prove useful.[8]

The goal of quantum computing in the chemical sciences is to scale up the simulated models beyond the classically attainable size or to obtain properties that are otherwise unavailable. Simulation of quantum dynamics is a promising candidate for an application that is provable on classical computers[9,10] but the current demonstrations remain small and need to be expanded to make a good case for practical use. This is where model systems like the Pariser–Parr–Pople (PPP) Hamiltonian can prove useful as a benchmarking system.[11] It encodes a minimal model for interactions governed by π-electrons that still has the hard physics while its reduced complexity requires less resources to implement on hardware. Also on the algorithmic side, more developments are needed. Classical computers are used in a wide array of processes while most quantum algorithms concentrate on either ground state search or electron dynamics. It is vital for the usefulness of quantum computing to expand this into areas like reaction rate determination, spectroscopy and ensemble properties, all while maintaining at least a scaling advantage over classical computers.[8] In that pursuit it will be vital to carefully deliberate which parts are executed classically and which parts are executed on a quantum computer.[12]

Quantum computing is an exciting area in research for chemistry, material science and biochemistry. The community still faces a tremendous task to fulfil its promise and to provide data that will help spur new previously unreachable applications. We hope that this collection provides some of the elements that will help bridge the gap that still remains.

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