Abstracts

Alán Aspuru-Guzik

What to do with a near-term quantum computer?

In this talk, I will overview the field of algorithms for near-term intermediate-scale quantum computers. I will use examples of research from our group and others in the fields of molecular simulation as well as the idea of simulating quantum computers by other quantum computers.

Ryan Babbush

Prospects for simulating quantum chemistry on quantum computers

This talk will discuss the promise, and also the challenges, of using quantum computers to model the electronic structure of molecules and materials. We will focus on two distinct paradigms where quantum computers might have an impact: the noisy intermediate scale quantum (NISQ) devices of today, and the much larger devices of tomorrow which demonstrate full quantum error-correction (QEC). To give a feel for the prospects of quantum advantage for chemistry in the NISQ era, we will discuss several recent chemistry experiments performed using quantum hardware at Google. We will then survey the most efficient known algorithms for chemistry within QEC, and discuss estimates of the size and accuracy of the quantum computers that would be required to implement those algorithms for interesting problems.

Giulia Galli

Embedding theories for quantum simulations on hybrid classical-quantum architectures

We discuss a quantum embedding theory that we have recently developed[1] to study spin-defects and impurities in solids, which is scalable to large systems. We compare the theory (which we call quantum defect embedding [QDET]) with other embedding frameworks, pointing out differences and similarities and target applications. We also present calculations on classical and quantum computers of the electronic structure of qubits performed with QDET[2].

1 He Ma, Marco Govoni and Giulia Galli, npj, Comput. Mat., 6 (85), (2020); He Ma, Nan Sheng, Marco Govoni and Giulia Galli, J. Chem. Theory Comput., 17, 2116-2125 (2021); Nan Sheng, Christian Vorwerk, Marco Govoni and Giulia Galli 2022: https://arxiv.org/abs/2203.05493). **2** Benchen Huang, Marco Govoni and Giulia Galli, PRX-Quantum 3, 010339 (2022).

Christian Gogolin

Quantum computing research at Covestro

This talk will give an overview of recent on the application of (near) future quantum computers for the simulation of chemistry. Among other things it will cover constrictions of quantum number preserving VQE entangler circuits for ground and excited states, and methods for the efficient and robust computation of properties beyond energies, with a focus on derivative properties such as the nuclear gradient.

Munich Quantum Valley

Martin Head-Gordon

Nonorthogonal configuration interaction for strong electron correlations: General considerations and a nonorthogonal quantum eigensolver

Strong correlation is typically treated using a single set of molecular orbitals. However, the less common alternative of using multiple sets of orbitals, leading to non-orthogonal configuration interaction (NOCI) offers interesting advantages. For instance, each set of orbitals can describe a physically well-defined contributions to the wavefunction, such as ionic versus covalent determinants. This physical advantage also leads to some numerical advantages, in the form of fewer important determinants, and a more compact representation of the wavefunction. After discussing these considerations with examples, I will then address the question of how these advantages might be realized on a quantum device – leading to a proposal and preliminary results for a non-orthogonal quantum eigensolver[1].

1 "Say NO to Optimization: A Non-Orthogonal Quantum Eigensolver", Unpil Baek, Diptarka Hait, James Shee, Oskar Leimkuhler, William J. Huggins, Torin F. Stetina, Martin Head-Gordon, and K. Birgitta Whaley, submitted (May, 2022).

Michael Marthaler

Simulating open quantum systems with quantum computers

From electron transport to light-matter interaction, considering quantum mechanical systems including their environment can often be off substantial interest or even strictly necessary. When trying to solve problem involving open quantum system on conventional computers it is necessary to solve the master equation for the density matrix instead of the Schrödinger equation for the wave function. This squares the already exponentially large state of a quantum mechanical problem and makes it therefore even more challenging. Solving quantum mechanical problems is one of the most obvious use cases for quantum computers. But it is interesting to note that the current generation of NISQ computers are intrinsically open quantum systems. In this presentation we will discuss in how far it is possible to map interesting open quantum system to NISQ devices and include the fact that qubits are open quantum systems themselves as part of the mapping. Additional we discuss relatively common problems in ab-initio simulation which can in fact be mapped onto an open quantum system.

Kristel Michielsen

Emulation of quantum computation of molecular energies using VQE on high-performance computers

The variational quantum eigensolver (VQE) is a hybrid quantum-classical algorithm designed for current and near-term gate-based quantum computing devices. The quantum part of the algorithm involves the computation of the energy expectation value and the classical part involves a classical optimization algorithm.
We present and analyze large-scale simulation results of VQE to calculate the ground state energy of small molecules using the massively parallel Jülich Universal Quantum Computer Simulator (JUQCS), which is emulating the operation of an ideal pen-and-paper gate-based quantum computer on a digital (super)computer. We compare the runtime of the standard version of VQE for solving the ground state of molecules on the emulated ideal QC on a digital supercomputer and on a supposedly perfectly functioning real gate-based quantum computer.

Munich Quantum Valley

Mario Motta

Tackling the electronic structure problem on near-term quantum devices: algorithmic improvements and error mitigation techniques

The electronic structure (ES) problem is an important application for a quantum computer, and recent years have witnessed the emergence of the first quantum algorithms for ES simulations[1]. Notwithstanding this progress, due to the immaturity of contemporary quantum computation platforms, so far quantum ES simulations have only provided conceptually interesting results. Progress in increasing the relevancy of quantum ES simulations requires the concerted development of algorithms tailored for contemporary quantum devices, and error mitigation techniques. This contribution will describe examples of both methodologies.

A challenge in quantum ES simulations is the high cost of performing Trotter steps of time evolution and measuring the Hamiltonian. The complexity of such operations can be reduced using two-step low-rank factorizations of the Hamiltonian, accompanied by truncation of small terms[2]. As an application, we will examine the combination[3] of low-rank factorizations with quantum filter diagonalization (QFD). The combination of low-rank factorizations and QDF requires reasonably short circuit depths and modest measurement cost, and can provide accurate predictions for low-lying eigenvalues, when circuit reduction and post-selection error mitigation strategies are deployed.

Another challenge in quantum ES simulations is the presence of dynamical electronic correlation. As an example of a strategy to treat dynamical electronic correlation on contemporary quantum devices, we will examine the integration of quantum ES algorithms in the workflow of N-electron valence perturbation theory (NEVPT2)[4]. As an application, we will examine the relative stability of OH- and OH. The quantum elevation of NEVPT2 correctly predicts OH- to be more stable than OH, if basis sets with diffuse orbitals are employed.

1 B. Bauer et al, Chem. Rev. 120, 12685–12717 (2020); **2** M. Motta et al, npj Quantum Inf. 7, 83 (2021); **3** J. Cohn, M. Motta and R. Parrish, PRX Quantum 2, 040352 (2021); **4** A. Tammaro, D. E. Galli, J. Rice and M. Motta, arXiv:2202.13002 (2022)

Markus Reiher

Prospects of Quantum Computing in Chemistry

Although some problems in the molecular sciences, which is governed by the dynamics of electrons and atomic nuclei, can be adequately addressed by classical mechanics, many demand an explicit quantum mechanical description. In such quantum problems, the representation of wave functions grows exponentially with system size and therefore should naturally benefit from quantum computation on a number of logical qubits, which scales only linearly with system size. In this talk, I will elaborate on the potential benefits of quantum computing for molecular systems.

Munich Quantum Valley

Ivano Tavernelli

Quantum computing applications in quantum chemistry

The original idea that a quantum machine can potentially solve many-body quantum mechanical problems more efficiently than classical computers is due to R. Feynman who proposed the use of quantum co mputers to investigate the fundamental properties of nature at the quantum scale. In particular, the solution of problems in electronic structure, many-body physics, and high energy physics (just to mention a few) is a challenging computational task for classical computers as the number of needed resources increases exponentially with the number of degrees of freedom. Thanks to the recent development of quantum technologies, we have now the possibility to address these classes of problems with the help of quantum computers. To achieve this goal, several quantum algorithms able to best exploit the potential quantum speedup of state-of-the-art, noisy, quantum hardware have been proposed[1,2].
In this talk, I will discuss applications of quantum computing for the solution of problems in many-body physics and quantum chemistry, focusing on those aspects that are relevant to achieve quantum advantage with near-term quantum computers. In particular, I will present recent results on applications in electronic structure calculations[3] and quantum dynamics[4-6].

1 N. Moll, et al., 'Quantum optimization using variational algorithms on near-term quantum devices', Quantum Sci. Technol., 3, 030503 (2018). **2** A. Kandala et al., 'Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets', Nature, 549, 242 (2017). **3** P. Baroutsos, et al., 'Quantum algorithms for electronic structure calculations: Particle-hole Hamiltonian and optimized wave-function expansions', Phys. Rev. A, 98, 022322 (2018); P. Ollitrault et al., 'Quantum equation of motion for computing molecular excitation energies on a noisy quantum processor', Phys. Rev. Res., 2, 043140 (2020). **4** P.J. Ollitrault, et al., 'Nonadiabatic molecular quantum dynamics with quantum computers', Phys. Rev. Lett., 125, 260511 (2020). **5** P.J. Ollitrault, et al., 'Molecular Quantum Dynamics: A Quantum Computing Perspective', Acc. Chem. Res., 54, 4229 (2021). **6** P.J. Ollitrault, et al., 'Quantum algorithms for grid-based variational time evolution', arXiv:2203.02521 (2022).

Matthias Troyer

Towards a Quantum Future for Quantum Chemistry

Still in early development, quantum computing is already overturning our contemporary notions of computational methods and devices. Using new concepts of computing based in quantum physics, quantum computers will be able to solve certain problems that are completely intractable on any imaginable classical computer, such as accurate simulations of molecules and materials. While this potential is real, quantum computers are best viewed as special purpose accelerators for specific problem classes, and I will present guidelines for the most promising applications, which include computational chemistry. Diving deeper into these applications I will discuss that disruptive quantum breakthroughs in computational chemistry requires conceptual and classical algorithmic advances in addition to the development of large-scale quantum computers.