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# Photonic quantum simulators

Alán Aspuru-Guzik[1]* and Philip Walther[2]*

**Quantum simulators are controllable quantum systems that can be used to mimic other quantum systems. They have the potential to enable the tackling of problems that are intractable on conventional computers. The photonic quantum technology available today is reaching the stage where significant advantages arise for the simulation of interesting problems in quantum chemistry, quantum biology and solid-state physics. In addition, photonic quantum systems also offer the unique benefit of being mobile over free space and in waveguide structures, which opens new perspectives to the field by enabling the natural investigation of quantum transport phenomena. Here, we review recent progress in the field of photonic quantum simulation, which should break the ground towards the realization of versatile quantum simulators.**

About 2,000 years ago, the Greeks built orreries, mechanical devices constructed to simulate the classical dynamics of planetary motion. The construction of orreries was made possible by technological advances in mechanics and materials science. One of the present directions in quantum science is the development of modern quantum orreries (Box 1), that is, quantum-mechanical simulators of chemical and physical processes at the scale where quantum effects are crucial.

It was Richard Feynman who proposed the innovative idea for the efficient simulation of quantum systems: one could employ a controllable quantum system, he suggested, to reproduce the dynamics and the quantum state of the original system of study. Classical computers are unable to simulate quantum systems efficiently, because they need to enumerate quantum states one at a time. Quantum simulators allow us to bypass the exponential barriers imposed by entanglement and the superposition principle of quantum mechanics, which prevent classical computers from solving such problems efficiently. Thirty years after Feynman's original proposal[1], quantum simulators of physical systems are being successfully constructed using a variety of quantum architectures, such as atoms[2–6], trapped ions[7–13], nuclear magnetic resonance (NMR)[14,15] and superconducting circuits[16,17], as well as single photons[18–25], which are the focus of this Review. However, even though there are many recent exciting developments in various quantum architectures, such as ion-trap quantum computing[9,11], no physical implementation seems to have a definite edge in all aspects of the race at this point.

## Quantum simulation strategies

With respect to level of detail, there are two types of quantum simulators. For the first type, the goal is to simulate a collective property such as a quantum phase transition, and for this, global or coarse-grained control of the quantum particles is usually sufficient to observe these phenomena. The second class of simulators requires precise local control and addressability of individual particles to provide a platform for understanding mesoscopic and molecular systems.

Simulators can also further be classified into digital, when they use discrete quantum-gate operations, and analog (including adiabatic models), when they implement a surrogate Hamiltonian in an analog fashion[26]. Moreover, there is also the possibility of constructing hybrid systems combining quantum-gate models and analog quantum simulation techniques[23].

## Photonic quantum technology

Each quantum simulation platform has its strengths, and here we discuss the inherent advantages of photonic technology for precise single-particle quantum control and tunable measurement-induced interactions in realizing local photonic quantum simulators. One of the salient features of photons is that they do not interact easily. This results in a naturally decoherence-free system but also complicates the generation of entanglement. Photons can be easily manipulated and individually addressed with high precision by employing simple optical components that can be used at room temperature, which avoids the need for cryogenic operation, except for certain photon sources and detectors. These features also lead to the second advantage of photonic simulators: photons are easily moved either in free space or in waveguides, and are thus not restricted to interactions with nearest neighbours. The mobility of photons, ideally on a single chip, allows, in principle, almost arbitrary interconnections and facilitates the simulation of complex and non-local many-body interactions. Furthermore, photonic quantum simulators could potentially be scalable if we find a technology for the controlled generation of single and multiple photons. This is an area of intense research; an overview of the photonic 'quantum toolbox' is given in Box 2.

As shown in the examples below, photonic systems are a promising platform for simulating quantum phenomena of small-sized quantum systems. The mobility of photons enables even single-photon experiments to simulate quantum walks[21,22,24,25] and topological phases[27]. Recently, Lanyon *et al.*[20] simulated quantum aspects of the hydrogen molecule by using two entangled photons. In the experiment, one of entangled photons represented the wave function of a two-level system that encoded two spin orbitals, and the other was used to read out the molecular energy. Using two entangled photon pairs, Ma *et al.*[23] have simulated frustrated valence-bond states. The tunable interaction between the two entangled photon pairs made it possible to study the distribution of pairwise quantum correlations as a function of the competing spin–spin interactions.

In the following sections, we will elaborate further on these examples and describe other recent and ongoing applications of quantum simulation using photons. The list is by no means exhaustive and is meant to be representative of the present state of the art.

## First application to quantum chemistry

Quantum chemistry and band structure calculations account for up to 30% of the computation time used at supercomputer centres[28].

[1]Department of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts 02138, USA, [2]Faculty of Physics, University of Vienna, Boltzmanngasse 5, Vienna A-1090, Austria. *e-mail: aspuru@chemistry.harvard.edu; philip.walther@univie.ac.at.

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**Box 1 | What is a quantum orrery?**

A quantum orrery or simulator is a quantum device capable of reproducing the behaviour of another quantum system. Although general purpose quantum computers can implement universal quantum simulation, a quantum orrery, like its classical counterpart, is designed to mimic the characteristics of a more complex system with fewer resources than a general purpose computational framework. Unlike quantum computers, quantum orreries are special purpose devices without the additional resource overhead of general purpose computation. Many types of simulator can be foreseen: simulators can either reproduce the time dynamics of a given system or they can be used to recreate quantum states of interest.

In a quantum simulation, a quantum system is mapped to a mathematical model that represents it. For example, a molecule can be mapped to the non-relativistic Schrödinger equation. This equation can be then executed by a quantum-software layer, which in turn is mapped to quantum hardware. The simulator is employed to measure the desired property (in this example, the molecular energy). Not all the desired properties are readily available in polynomial time: a full map of the wave function of the system would require a number of measurements that scales exponentially with the number of particles involved. Therefore, for a successful quantum-orrery experiment, the stages of preparation, simulation and measurement have to be designed such that they are carried out in a computationally efficient manner.

The most-employed techniques include density functional theory and tractable correlated-electronic-structure methods[29]. Although these methods can be used to predict novel materials[30], they are approximate in nature. Formally, the exact solution of the Schrödinger equation within a given numerical basis scales exponentially with the number of basis functions. This is known as the 'curse of dimensionality' and is one of the two fundamental reasons why quantum-chemistry problems are hard to simulate on a conventional computer. The second reason is that a classical computer might not be able to converge to the quantum state of all possible molecular input states. In computer science, one usually deals with the worst possible instance, which might correspond to a very strongly correlated molecule or material. For example, Schuch and Verstraete showed that finding an exact density functional for interacting electrons would be a Quantum-Merlin–Arthur-hard problem; that is, the task belongs to a class of problems thought too hard even for quantum computers[31,32]. Nevertheless, one of us has conjectured[33,34] that it will be easy to prepare typical instances of molecules on quantum computers.

In 2005, a quantum-chemistry algorithm was introduced[33] that scales linearly in the number of qubits and to fifth order in terms of the number of quantum gates[35]. This algorithm is based on a proposal by Abrams and Lloyd[36,37] and uses quantum phase estimation to obtain molecular eigenvalues. Such algorithms usually rely on time-slicing through the Trotter formula, which results in a large number of gates as a function of system size. The simplest possible quantum circuit for quantum chemistry on a quantum-information processor has already been implemented. The Hamiltonian of the hydrogen molecule in the smallest atom-centred chemistry basis is represented by a $6 \times 6$ matrix that has two $2 \times 2$ blocks and two $1 \times 1$ blocks. The $2 \times 2$ blocks can be diagonalized by carrying out an iterative phase-estimation algorithm[33]. Lanyon *et al.*[20] performed this experiment using two entangled photons, taking advantage of extra photonic degrees of freedom to implement an arbitrary controlled-unitary evolution[38] (Fig. 1). A few months later, the same experiment was also realized using an NMR quantum system[15]. Future experiments will require a scalable photonic architecture, as the number of required controlled-not (CNOT) operations—a two-qubit entangling gate defined for quantum computation—scales as the fifth power of the system size.

However, in the case of photonic quantum systems, arbitrary unitary matrices can also be implemented by interferometric beam-splitter arrays or so-called multiport arrays[39]. Recent advances in micro-optics using integrated waveguide structures have led to the demonstration of two-qubit circuits[40–42] and Shor's algorithm[43], the manipulation of the quantum state of light by phase shifters[44] or reconfigurable circuits[45] using planar devices[46]. In addition, laser-written waveguides not only allow the direct configuration of the circuit structure[47], but also open up promising perspectives regarding quantum-simulation experiments using three-dimensional structures[25,48] that are not restricted to a plane[24].

## Quantum walks and tight-binding Hamiltonians

The first experiments in integrated optics used classical laser light to demonstrate quantum-mechanical behaviour and features[49–53]. Only a few years ago, it was realized[54] that waveguide arrays could be employed to simulate quantum walks[55] and, if decoherence is involved, quantum stochastic walks[56] at the single-photon level. A walk is a distribution evolving over a given graph, following a defined equation of motion. Classical walks involve classical probability distributions following a classical transition matrix. Quantum walks, in contrast, involve a distribution of amplitudes following Schrödinger dynamics[57]. Finally, quantum stochastic walks involve density matrices following the dynamics of an open quantum system.

Walks can be formalized in both discrete time and continuous time. Although originally devised in the context of quantum computation, the concept of quantum walks can be used to simulate tight-binding Hamiltonians, either as closed systems or under the influence of decoherence. Quantum walks have been realized using bulk optics[21,27,58,59] and waveguides[22,25,44,48,54]. Single-particle quantum walks can also be carried out with coherent classical light[21], but truly novel effects happen when more than one photon is employed[24,25,48]. The use of loop-based architectures has enabled realizations of up to 28 steps in a discrete walk[58].

Similar methods can be used to study excitation transfer in biological systems. Recent experiments probing ultrafast dynamics in light-harvesting complexes have shown that long-lived quantum-coherent oscillations can be sustained in biological systems[60–65]. These long-lived oscillations are due to a convergence of timescales in the biological system that results in quantum oscillations lasting up to picoseconds at room temperature. Such open quantum systems—essentially electrons in a bath of phonons—are a possible target for quantum simulation. Making various connections to quantum information, the processes involved in the excitation transfer have been described as an environment-assisted quantum walk[63], as an environment-assisted quantum transport[64,65] or as a quantum stochastic walk[56]. In these different theoretical frameworks, the interplay of the photon bath and the natural environment is the key to the efficiency of the photosynthetic complex.

The first quantum-optics experiment along these lines simulated a quantum stochastic walk that interpolates between the quantum and the classical walk using a single photon[21]. Up to six steps of a discrete-time quantum walk were performed using this approach. A similar experiment was later implemented in an optical fibre-loop configuration[59]. Another approach that has been proposed recently suggests simulating the transition from coherent to incoherent transport, as well as environment-assisted quantum transport, using a set of coupled optical cavities traversed by a single photon[66].

**Box 2 | The photonic toolbox.**

Photonic quantum systems[78] are among the most mature and promising approaches for the realization of quantum computers and quantum simulators. Single photons are excellent carriers of quantum information, owing to their robustness and their mobility, which enables them to transmit information literally at the speed of light. Quantum bits, which represent any physical two-level quantum system, are often encoded in the polarization states of photons, as such states can be easily manipulated with high precision using birefringent phase retarders. In addition, photons also provide other degrees of freedom—such as path or angular momentum—for encoding quantum information.

The downside is that photons barely interact with each other, placing the main challenge on the engineering of photon–photon interactions. These are crucial for the realization of two-qubit-gate operations or the preparation of multi-photon entanglement using single photons as input states. In their seminal 2001 paper[79], Knill, Laflamme and Milburn have shown that effective nonlinearities can be introduced through the measurement process and that scalable photonic quantum computing is possible using only linear optical circuits, single-photon sources, and detectors[80]. The introduction of ancillary photons enables not only the heralding of successful gate operations[81–85] but also provides a basis for protocols in which probabilistic two-photon gates are teleported into a quantum circuit with high probability[86]. This has opened a path to building large-scale quantum simulators that, in contrast to many other physical platforms, do not face the technical challenges of low temperature and vacuum conditions.

The controlled generation of single photons is at present the main challenge on the route to scaling up photonic quantum simulators. Today, multi-photon or quantum interference experiments with photons emitted from independent sources typically rely on the process of parametric down-conversion[87], where indistinguishable pairs of photons are generated by sending a strong laser pulse through a nonlinear crystal. This process, however, is spontaneous and thus creates photon pairs at random times, which restricts scalability, especially when dealing with the emission of multiple photon pairs and standard detectors without photon-number resolution. Other leading technologies in this effort are based on different physical systems, including single trapped atoms and atomic ensembles, quantum dots, or nitrogen-vacancy centres in diamond[78]. Once the technical challenges of low coupling efficiencies, the uncertainty in emission time and the distinguishability in frequency of the created photons are addressed, these systems will become promising candidates for controllable single-photon sources that can be integrated on chips. Similarly, significant effort is being put into developing high-efficiency superconducting detection units that can distinguish the number of detected photons[88–93,98], such that errors due to additional photons can be excluded to improve the quantum-state and quantum-gate fidelities. The ultimate vision of combining the heralded multi-photon sources[94,95], circuits and detection units on a single chip[25,40–42,44–48] (Fig. B2), seems to be a tremendously challenging, long-term goal—but it is certainly not out of reach.

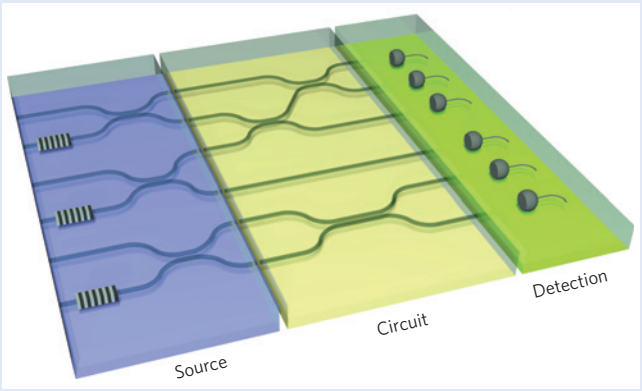


**Figure B2 | Schematic of an integrated photonic quantum simulator.** Advances in micro-optics and waveguide technologies have opened up promising perspectives for the integration of single-photon sources, tunable circuits and high-efficiency detection units on a single chip.

The measurement of interference effects on classical states of light propagating through lattices of evanescently coupled waveguides[67] preceded a recent experiment[48] that showcased quantum correlations between two photons in three-dimensional directly-written waveguide arrays. Such experiments could be a precursor to the simulation of photosynthetic complexes, where the delocalization over different bacteriochlorophyll molecules is a key feature to describe the correct energy-transfer dynamics.

## Applications to condensed-matter physics

In addition to the exquisite level of quantum control, photonic quantum simulators offer the possibility of using quantum interference effects at beam splitters, which can lead to interesting forms of photon entanglement that correspond to ground states of correlated chemical or solid-state systems[68]. Ma *et al.*[23] have shown that frustration in Heisenberg-interacting spin systems can be investigated using such a photonic quantum simulator. The pairing of quantum correlations of spin systems is an important mechanism in chemical (or valence) bonds, where pairs of electrons from different atoms share an anti-correlated spin state. Valence-bond states are of particular interest because it was conjectured that a transition from a localized valence-bond configuration to the superposition of different valence-bond states might explain the phenomenon of high-temperature superconductivity in cuprates[69].

The quantum correlation of valence-bond states can be simulated using a pair of photons that is maximally entangled in the polarization degree of freedom, in a way that the two photons are always orthogonally polarized. The experiment of Ma *et al.*[23] used two entangled photon pairs in a singlet state to simulate the spin of a Heisenberg-interacting spin tetramer, where the singlet state corresponds to the anti-ferromagnetic coupling of two spin-1/2 particles, equivalent to a valence-bond state. Then an analog quantum simulation was performed by superimposing photons from each pair at a beam splitter with a tunable splitting ratio, followed by a measurement of the photons at the output ports (Fig. 2a). Depending on the interaction strength, the transition from a local to a resonant valence-bond ground state was observed. The addressability of individual photons provided insight into the pairwise quantum correlations; it was observed that the energy distribution is restricted by the role of quantum monogamy[70,71]. Such quantum simulation experiments will also be of interest for quantum-chemistry phenomena with small numbers of particles and might in the near future allow the simulation of aromatic systems such as benzene (Fig. 2b). Several challenges remain for the simulation of more complex systems, in particular the realization of two-qubit and multi-qubit interactions with high fidelity, the generation of systems with more qubits, and the development of efficient methods for simulating other classes of complex Hamiltonians using optical elements.

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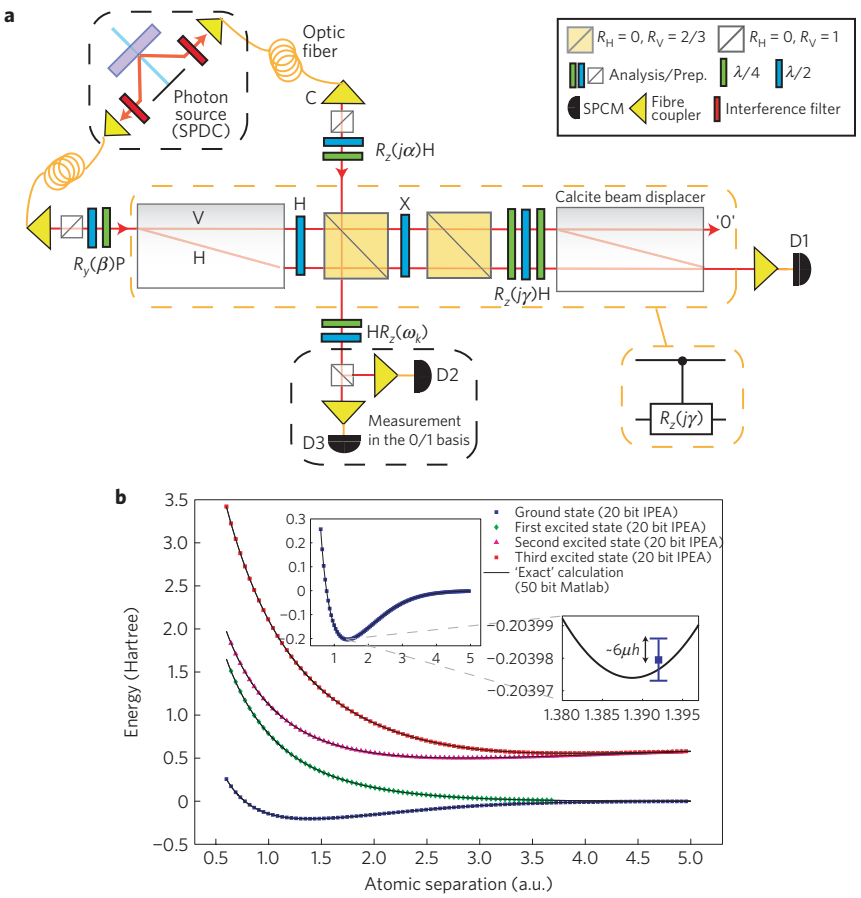


**Figure 1 | First quantum chemistry experiment on a quantum information processor. a**, Quantum optics experiment for simulating the energy of the hydrogen molecule in the minimal basis set. A pair of entangled photons generated via the spontaneous parametric down-conversion (SPDC) process implements an iterative phase-estimation scheme where one of the photons represents two $2 \times 2$ blocks of the $6 \times 6$ full configuration interaction matrix of $H_2$ in the minimal quantum chemistry basis set[20]. The photons are coupled into free space optical modes C (control) and R (register) and manipulated by using half-wave plates ($\lambda/2$) and quarter-wave plates ($\lambda/4$) to implement single-qubit rotations around the Bloch axes, $R_y$ and $R_z$, as well as Hadamard (H) and Pauli X gate (X) operations. Coincident detection events between single photon counting modules (SPCMs) D1 and D3 (D2 and D3) herald a successful run of the circuit. Panel reproduced from ref. 20. **b**, Plot of the molecular energies of the different electronic states as a function of interatomic distance obtained with the device to 20 bits of precision using an iterative phase-estimation procedure (IPEA) and a majority-voting scheme as a simple error correction protocol.

An area of recent interest in quantum physics is the study of quantum phases with particular topological properties that could yield topologically protected states. As these states might be useful for quantum-information processing, condensed-matter systems such as topological insulators have been intensively studied theoretically and experimentally. The direct observation of topological states is a challenging experimental problem. One approach to the problem is to build an orrery where the effect can be observed. Recently[27], an optical set-up similar to that employed for the simulation of quantum walks[21] was modified to achieve a one-dimensional topologically protected pair of states, using a Hamiltonian describing a periodically driven system. This enabled the direct experimental observation of topologically protected bound states using a discrete-time quantum walk (Fig. 3).

## Particle statistics and elementary interactions

In quantum physics, there exist two fundamental particle classes: bosons, which obey Bose–Einstein statistics, and fermions, which satisfy Fermi–Dirac statistics. Whereas bosonic particles can occupy the same quantum state and therefore can bunch, fermionic particles must follow the Pauli exclusion principle and thus anti-bunch. These non-classical particle statistics can be simulated with photons that interact with multiport beam-splitter structures in bulk[72,73] or integrated[42,45] optics. Photon bunching is observed when superimposing indistinguishable single photons at beam splitters[74]. However, when polarized photons are used as input, boson-like bunching or fermion-like anti-bunching can be generated, depending on whether the photons share a symmetric (triplet) or an anti-symmetric (singlet) state. The ability to observe non-bosonic statistics with photons was originally used in experiments in the context of quantum-information processing[75,76], but recent demonstrations of two-photon interference in integrated waveguides used the phenomenon to simulate quantum interference of fermions and bosons, as well as that of so-called anyons[24,25], which generalize the concept of exchange statistics in two dimensions.

In general, the flexibility of photons makes such systems promising for studying a variety of different quantum-physical properties. For example, a theoretical work by Semião and Paternostro[77] suggests using photons to obtain insights into particle physics. These authors propose using a combination of CNOT gates and multiports[39] to emulate the nucleonic spin states that result from the combination of their quark components. Obviously, such quantum simulation experiments would cover basic quark models,

**Box 3 | Towards outperforming classical computers**

A question commonly posed to researchers in quantum information science is when a quantum computer or quantum simulator is expected to outperform a classical computer. Classical computers have had a head start of many years. The first classical simulations were performed in the MANIAC computer at Los Alamos National Laboratories in the 1940s. The first photonic quantum simulations are just being realized this decade, almost 70 years later. The computational power of present-day supercomputers has enabled approximate calculations, such as the full molecular-dynamics simulation of a protein[96]. Such achievements cannot be directly compared with the results of few-qubit experiments carried out nowadays. The promise of quantum simulation is to provide exact simulations that scale polynomially in quantum resources. This would be crucial to benchmark present approximate methods. For simulations in quantum chemistry, beyond approximately 150 quantum bits, a quantum simulator would beat the best algorithms on a classical computer. Quantum simulators could have a lower crossover threshold for strongly correlated systems, as these are intractable using classical computers (Fig. B3).

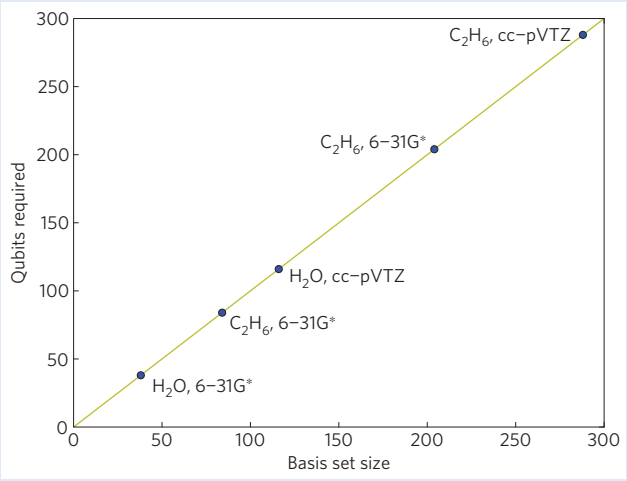


**Figure B3 | Number of quantum bits required for molecular electronic structure calculations.** Several molecules in their ground-state electronic configuration are shown, using different quantum chemistry basis sets[34,97]. A full configuration interaction (FCI) on 75 basis functions is at present intractable for classical computers. A quantum simulator with approximately 150 logical quantum bits would be able to outperform quantum computers at tasks such as the simulation of chemical reaction dynamics and molecular electronic structure. The 6−31G* basis is a double-zeta (exponent) set that includes polarization functions. It is one of the most-employed basis sets in quantum chemistry. The correlation consistent, polarized valence triple zeta (cc-pVTZ) is a triple-exponent basis set that includes polarization that is commonly employed for quantum-chemistry calculations using correlated methods.

but not provide the full quantum-chromodynamical picture. But, in analogy to orreries, such experiments might provide insights into the phenomenological properties of nucleonic states. More generally, the fact that state-of-the art technology should enable the mimicking of such interactions of three or more bodies underlines the potential value of photonic networks for future simulation experiments of the fundamental phenomena that exist in subatomic particles.

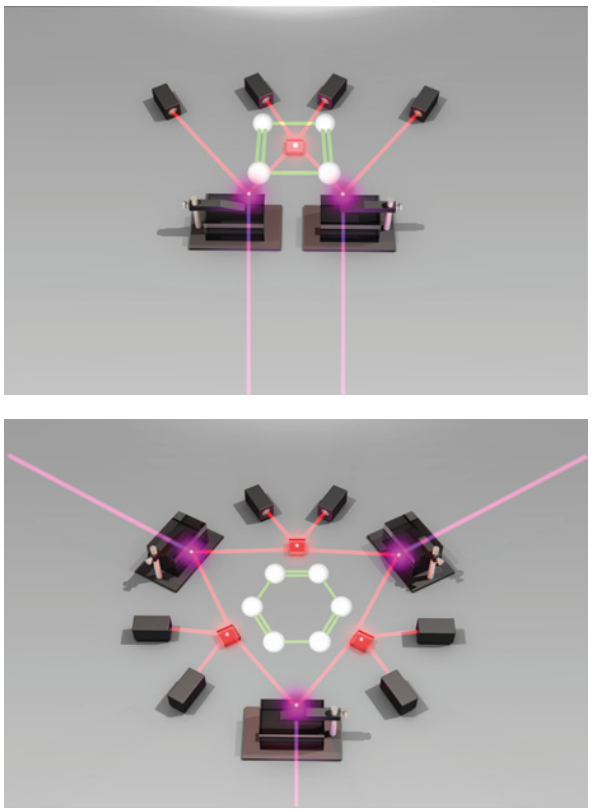


**Figure 2 | Schematic of the photonic quantum simulation of delocalized chemical bonds. a**, Two entangled photon pairs are generated through the process of parametric down-conversion. Superimposing one single photon from each pair at a tunable beam splitter results in quantum interference, such that the measured four-photon coincidences correspond to the ground state, for example of a Heisenberg-interacting spin tetramer. Dependent on the reflectivity of the beam splitter, frustration in valence-bond states or so-called spin-liquid states can be investigated[23]. **b**, Future experiments using more entangled photon pairs may allow the study of the ground-state properties of molecular ground states, such as the delocalized bonds in benzene.

## Perspective and outlook

One of the main goals for future experiments will be to outperform existing conventional supercomputers in tasks involving the simulation of quantum systems. Although the resource requirements are less demanding in the case of quantum simulators as opposed to general-purpose quantum computation, at present the required number of input states and the measurement-based processing push such benchmark experiments out of reach. However, it was recently shown that the simulation of bosonic particle statistics might be the first application in which photons will outperform classical devices. The work by Aaronson and Arkhipov[32] suggests that rudimentary photonic networks built entirely out of linear-optical elements cannot be efficiently simulated by classical computers. The coincidence probability for photons exiting a multiport linear-optical circuit is related to the permanent of a matrix associated with the quantum circuit. Recent progress has been made towards addressing this challenge[42]. This has two immediate consequences: first, the bosonic nature of photons themselves is already hard to simulate on conventional computers, which means that particle symmetry alone leads to a fundamental complexity that goes beyond that with which classical computers are expected to be able to cope. Second, the first benchmark quantum-simulation experiment might be built purely from passive linear-optical elements, without a requirement

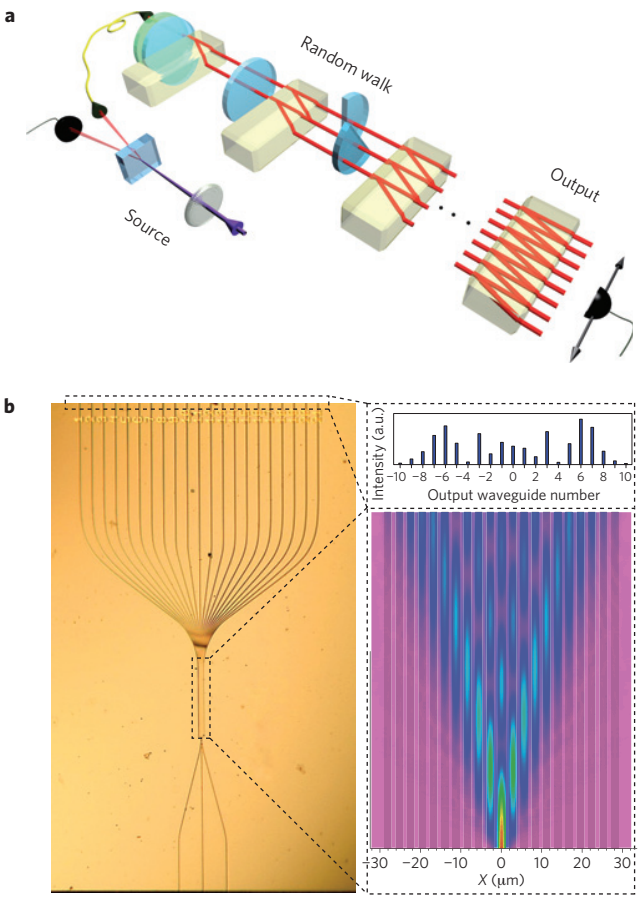


**Figure 3 | Photonic quantum circuits for the simulation of quantum and quantum stochastic walks. a**, The bulk-optics set-up employed to simulate a quantum-stochastic-walk transition between a pure quantum walk and a classical walk[21]. **b**, Continuously coupled waveguide arrays were also used to realize correlated-photon quantum walks[22]. The optical micrograph of a 21-waveguide array shows the three input waveguides on the bottom, bending into the 700-μm-long coupling region, and exiting at the top towards the output ports, where the signal is detected. The output pattern (upper inset) and a simulation of the intensity of laser light propagating in the array (lower inset) are also shown. Panel reproduced with permission from ref. 22, © 2010 AAAS.

for additional ancilla photons to introduce measurement-based interactions. Sending identical photons through an optical network without any kind of adaptive measurements might thus lead to the first simulation of complex phenomena that are classically intractable under plausible assumptions.

If progress on future quantum orreries based on the many available quantum technologies is steady, we expect that grand computational challenges such as the accurate simulation of molecules and materials will become accessible (Box 3). En route to realizing this long-term goal, photonic quantum simulators should provide a useful test bed for the realization of Feynman's dream.

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## Additional information

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