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NTU Q

EVENTS

QISKIT HACKATHON TAIWAN 2023

Aug 8-10th at Taipei

This activity open to all who interest in quantum computing! Registration will open on Jun 15th.

Check more info on NTU Q Web

IBM QUANTUM SPRING CHALLENGE

May 17 at 8:00 PM (local) — May 25 at 4:00 AM (local)

Every year, IBM Quantum releases a public challenge as part of the ongoing global education efforts. The Spring Challenge is free to participate in. This year's Challenge focuses on Dynamic Circuits, a technology that makes it easier to run more advanced quantum algorithms.

Check on Web

HIGHLIGHTING NEWS

VERY-LARGE-SCALE INTEGRATED QUANTUM GRAPH PHOTONICS

A new concept of quantum hardware has been showed on nature photonics. A quantum photonic device base on graph theory.

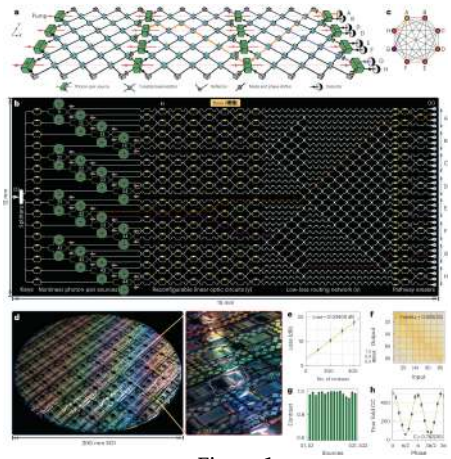

Figure 1

The device is constructed of a synthetic lattice of nonlinear photon-pair waveguide sources and linear optical waveguide circuits(Figure 1a, b). And is realized by very-large-scale integration (VLSI) of silicon quantum photonics(Figure 1d).

The graphs are physically defined by the connectivity of sources and by the pathway of circuits. Reconfiguring the quantum device can make different topologies of complex-weighted graphs. Different task implements are associated with the perfect matching property of graphs.

READMORE

DRUG DESIGN ON QUANTUM COMPUTERS

Quantum computers are expected to offer a clear advantage in finding the ground state energy of a molecular Hamiltonian (i.e. solving the electronic structure problem) for strongly correlated systems.The ground state energy is computed with a combination of state preparation and quantum phase estimation (QPE).

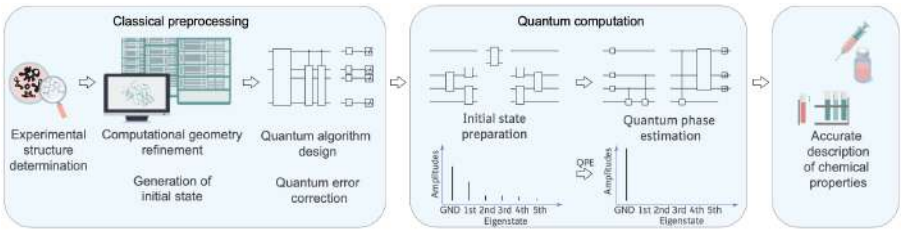

Figure 2

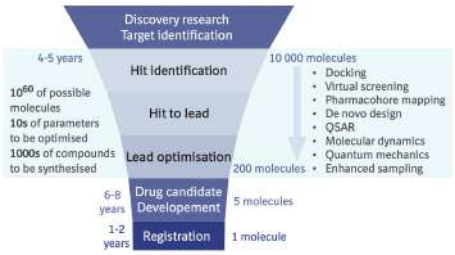

Figure 3

Figure 2 give an example of how these calculations can be performed on quantum computers for a chemical system. The cost of estimating the correct ground state energy depends directly on the overlap of the initial state with the ground state.

Steps and methods for drug design are summarized in Figure 3. Two major areas where computational chemistry can support drug design have been identified:

(1) the prediction of pharmacokinetic properties (how the compound is absorbed, distributed, the prediction of pharmacokinetic properties (how the compound is absorbed, distributed, metabolized and excreted from the body), commonly realized by machine learning models trained on data from the pharmaceutical companies.

(2) the calculation of the binding strength or binding affinity of a compound to the target, which is one of the most important properties of a drug candidate. It directly corresponds to the required local drug concentration at the target. However, state-of-the-art methods based on molecular dynamics simulations with classical force fields do not perform reliably. In contrast to force fields, density functional theory (DFT) or coupled cluster (CC), which are methods based on quantum mechanics, lead to much better descriptions of molecular interactions but at a much higher computational cost.

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