

# Quantum Computing for Science

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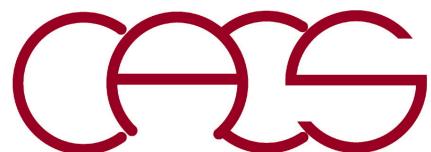
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and Quantitative & Computational Biology  
University of Southern California*

Email: [anakano@usc.edu](mailto:anakano@usc.edu)



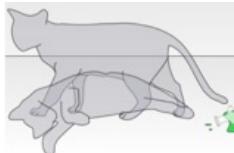
Supported by National Science Foundation,  
Award OAC-2118061



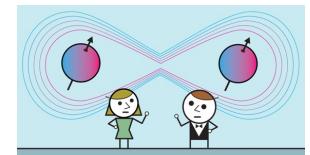
*CyberMAGICS Workshop  
June 30, 2023*



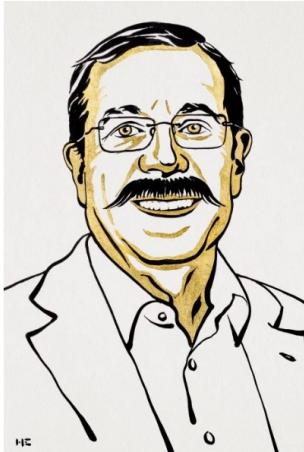
# What Is Quantum Computing?



Quantum computing utilizes quantum properties such as superposition & entanglement for computation



The Nobel Prize in Physics 2022 It's entanglement!



III. Niklas Elmehed © Nobel Prize Outreach

Alain Aspect

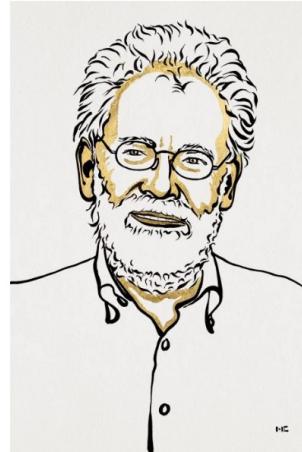
Prize share: 1/3



III. Niklas Elmehed © Nobel Prize Outreach

John F. Clauser

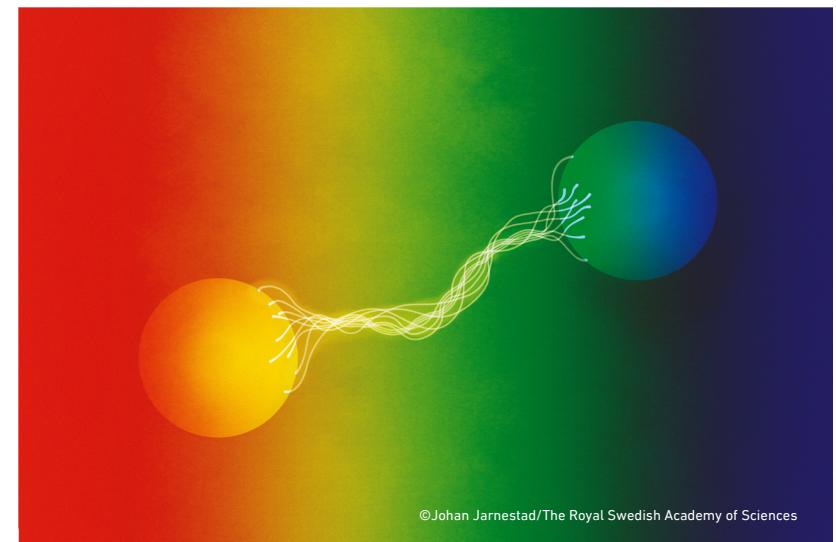
Prize share: 1/3



III. Niklas Elmehed © Nobel Prize Outreach

Anton Zeilinger

Prize share: 1/3



© Johan Jarnestad/The Royal Swedish Academy of Sciences

The Nobel Prize in Physics 2022 was awarded jointly to Alain Aspect, John F. Clauser and Anton Zeilinger "for experiments with entangled photons, establishing the violation of Bell inequalities and pioneering quantum information science"

# Quantum Computing (QC) for Science

- U.S. Congress (Dec. 21, '18) signed National Quantum Initiative Act to ensure leadership in quantum computing & its applications

- Quantum supremacy demonstrated by Google

F. Arute, *Nature* **574**, 505 ('19)

- Quantum computing for science:  
*Universal simulator of quantum many-body systems*

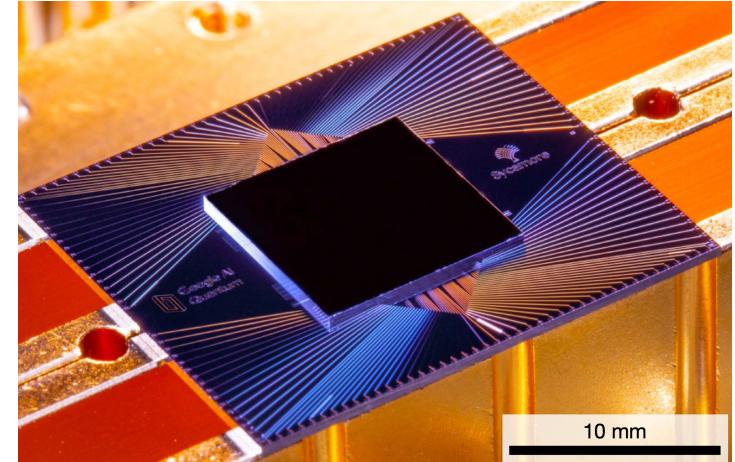
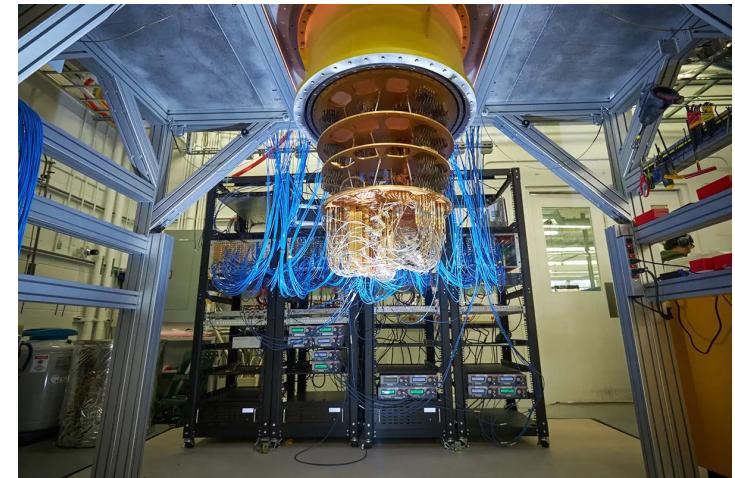
R. P. Feynman, *Int. J. Theo. Phys.* **21**, 467 ('82);  
S. Lloyd, *Science* **273**, 1073 ('96)

- Success in simulating *static* properties of quantum systems (*i.e.*, ground-state energy of small molecules)

A. Aspuru-Guzik *et al.*, *Science* **309**, 1704 ('05)

- Challenge: Simulate quantum many-body *dynamics* on current-to-near-future noisy intermediate-scale quantum (NISQ) computers

J. Preskill, *Quantum* **2**, 79 ('18)

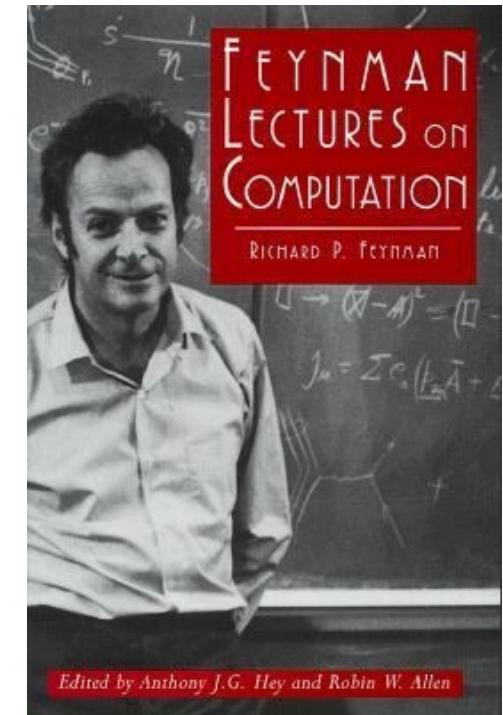


54-qubit Google Sycamore

# Quantum Dynamics Simulations

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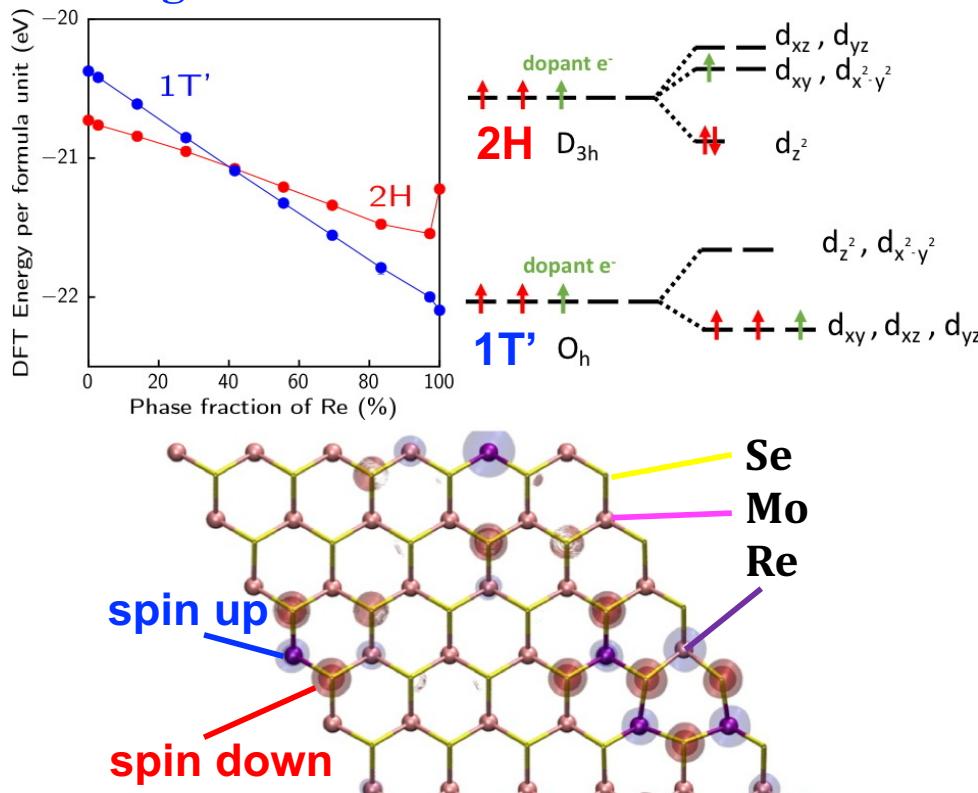
- An exciting scientific application of quantum computers is as a universal simulator of quantum many-body dynamics, as envisioned by Richard Feynman [*Int. J. Theor. Phys.* **21**, 467 ('82)]
- Seth Lloyd provided concrete algorithms and analysis [*Science* **273**, 1073 ('96)]
- Second edition of *Feynman Lectures on Computation* will add a section on “Simulating quantum dynamics” by John Preskill [*arXiv:2106.10522* ('21)]
- Simulated nontrivial quantum dynamics on publicly available IBM’s Q16 Melbourne & Rigetti’s Aspen NISQ computers, *i.e.*, ultrafast control of emergent magnetism by THz radiation in 2D material [*L. Bassman et al., Phys. Rev. B* **101**, 184305 ('20)]



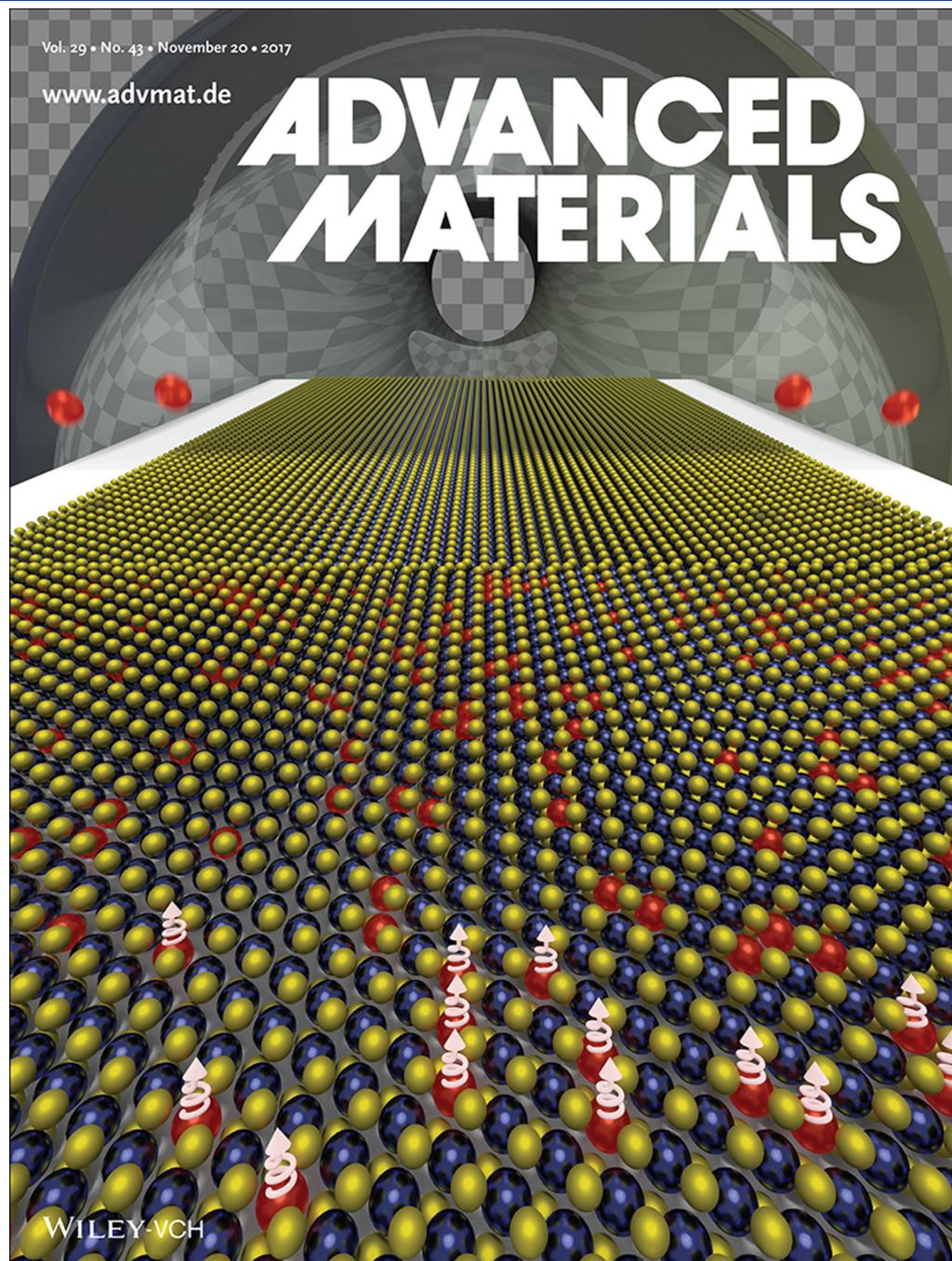
Do it yourself at <https://quantum-computing.ibm.com>

# Application: Emergent Magnetism

- Experiment at Rice shows 2H-to-1T' phase transformation by alloying MoSe<sub>2</sub> with Re
- QMD simulations at USC elucidate its electronic origin
- Simulation & experiment show novel magnetism centered at Re atoms



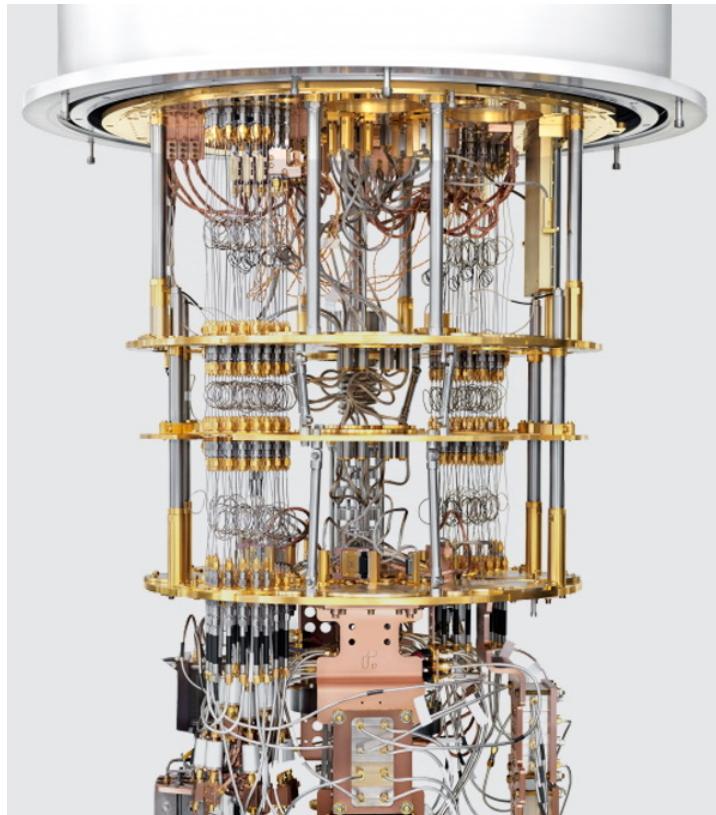
V. Kochat *et al.*, *Adv. Mater.* **29**, 1703754 ('17)



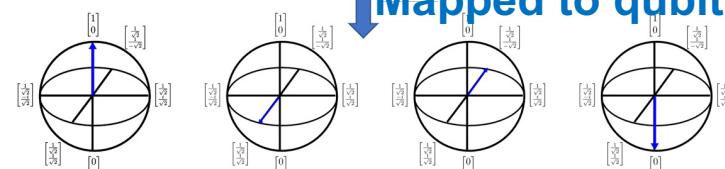
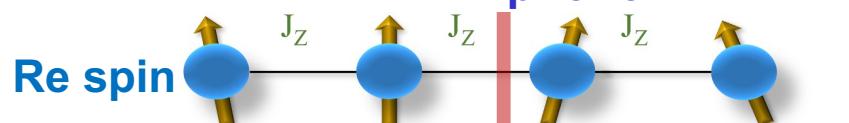
# Quantum Computing of Magnetism

- Simulated quantum many-body dynamics on IBM's Q16 Melbourne & Rigetti's Aspen quantum processors

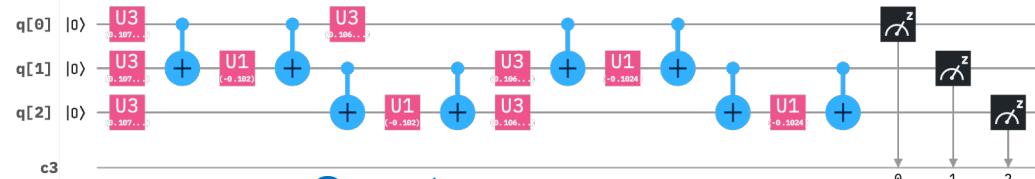
L. Bassman *et al.*, Phys. Rev. 101, 184305 ('20)



$$H(t) = -J_z \sum_{j=1}^{N-1} \sigma_z^j \sigma_z^{j+1} - \varepsilon_{ph} \sin(\omega_{ph} t) \sum_{j=1}^N \sigma_x^j$$



Quantum circuit:  $U(\Delta t) = \exp(-iH\Delta t)$



Quantum program

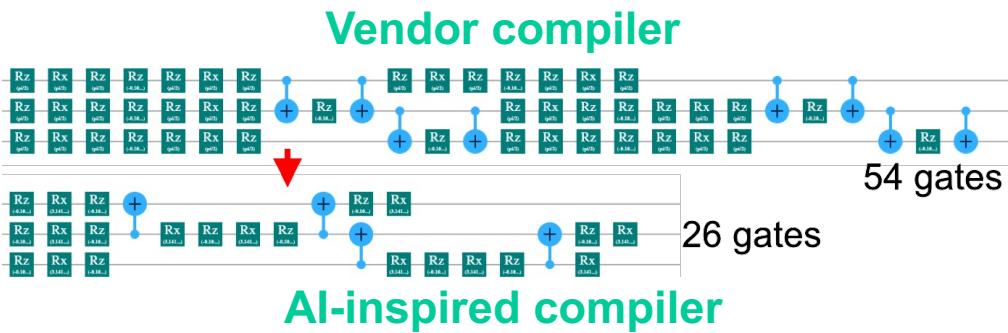
```
32  ....#define the two non-commuting terms that comprise the Hamiltonian-
33  ....Hz = PauliTerm("Z", 0, epsilon_0)-
34  ....Hy = PauliTerm("Y", 0, epsilon_ph*np.sin(w_ph*t))-#
35  ....#exponentiate the terms of the Hamiltonian for use in Trotter approx-
36  ....exp_Hz = exponential_map(Hz)(delta_t/(2.0*hbar))-#
37  ....exp_Hy = exponential_map(Hy)(delta_t/hbar)-
```

# Quantum Dynamics on NISQ Computers

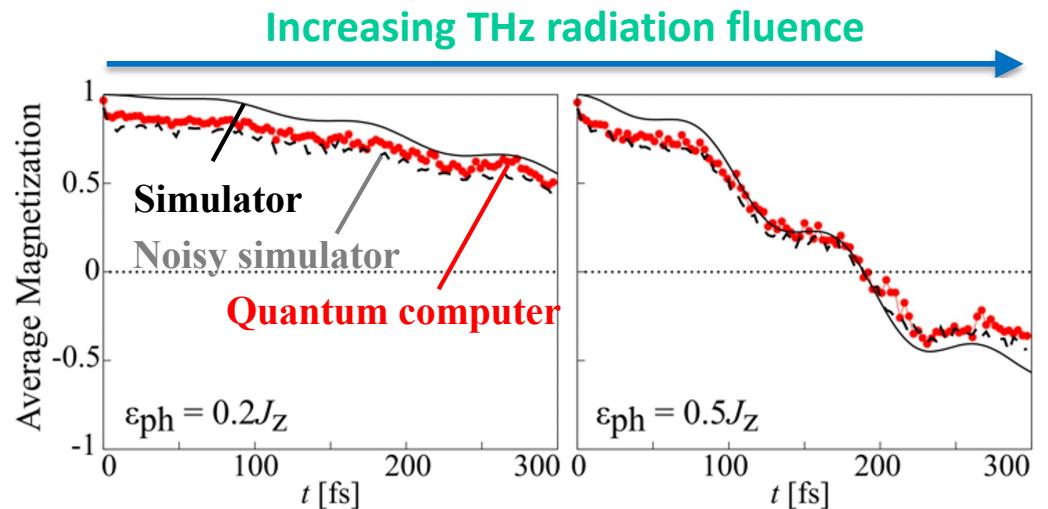
- Quantum-dynamics simulations on NISQ computers show dynamic suppression of magnetization by THz radiation

L. Bassman *et al.*,  
*Phys. Rev. B* **101**, 184305 ('20)

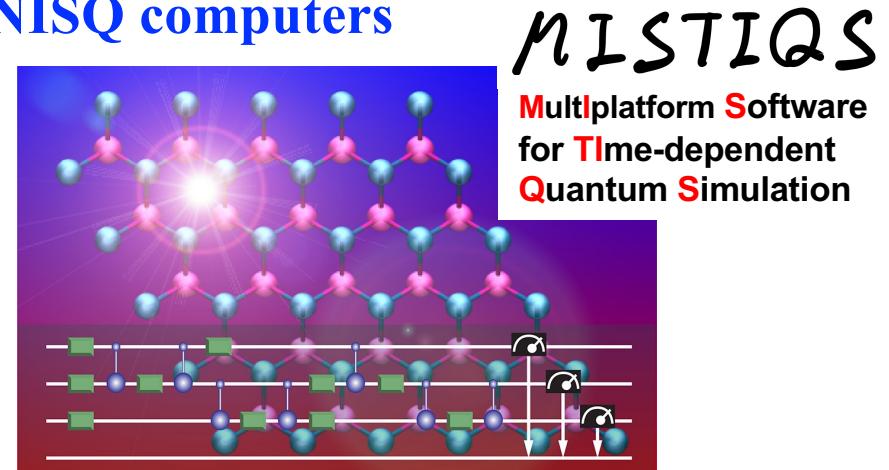
- AI-inspired quantum compiler reduced the circuit size by 30% to mitigate environmental noise



L. Bassman *et al.*,  
*Quantum Sci. Tech.* **6**, 014007 ('21)



- Full-stack, cross-platform software for quantum dynamics simulations on NISQ computers



C. Powers *et al.*, *SoftwareX* **14**, 100696 ('21)  
<https://github.com/USCCACS/MISTIQS>

# Where to Go from Here

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Extensive tutorial on quantum computing

- You will be ready for [Qiskit textbook](#)

## Learning Opportunities at USC

- New MS degree in Quantum Information Science ([MSQIS](#)) started in 2021
- Phys 513: Application of Quantum Computing (co-taught with Prof. Rosa Di Felice) — quantum simulations on quantum circuits & adiabatic quantum annealer ([syllabus](#))

## Research Topics

- Hybrid quantum-classical computing: Accelerate computation on a classical computer using exponentially faster but inaccurate quantum processing units; *cf.* variational quantum eigensolver (VQE) & quantum approximate optimization algorithm (QAOA) in Qiskit tutorial
- Error-tolerant quantum computing: Quantum error correction & mitigation

# Next: Hands on at IBM Quantum

- Quantum computing basics: Qubits and quantum gates
- Advanced: Quantum computation of transverse-field Ising model

Download from <https://cybermagics.netlify.app/workshop-resources.html>

Do it yourself at <https://quantum-computing.ibm.com>

The screenshot shows the IBM Quantum web interface. At the top, there's a dark header bar with the IBM logo and the text "IBM Quantum". Below it is a light-colored main area. On the left, there's a sidebar with a "Recent notifications" section and a "Welcome, Aiichiro Nakano" message. The main content area has two main sections: "Graphically build circuits with IBM Quantum Composer" (with a "Launch Composer" button) and "Develop quantum experiments in IBM Quantum Lab" (with a "Launch Lab" button). To the right, there's a "Jump back in:" list with several items like "BCS-GroundState.ipynb", "HeisenbergDynamics.ipynb", "VariationalFermiHubbard.ipynb", and "Untitled5.ipynb". There's also an "API token" input field containing "\*\*\*\*\*" and a "View account details" link.