

# Quantum Computing for Science

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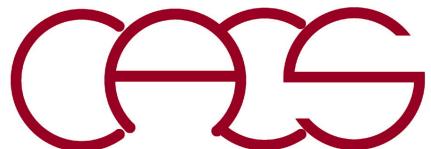
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Aiichiro Nakano

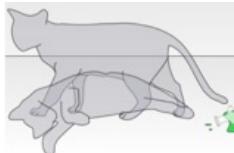
*Collaboratory for Advanced Computing & Simulations  
Departments of Computer Science, Physics & Astronomy,  
and Quantitative & Computational Biology  
University of Southern California*

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

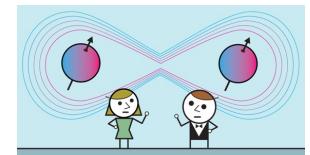
A fundamentally new way of computing — use it for science



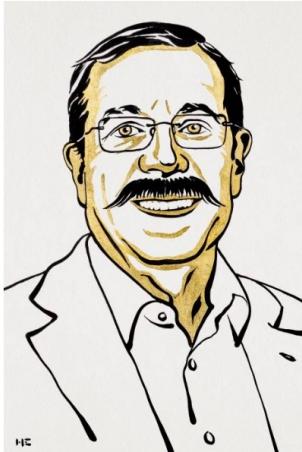
# What Is Quantum Computing?



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

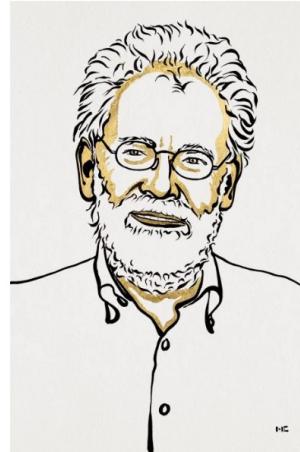
Prize share: 1/3



III. Niklas Elmehed © Nobel Prize Outreach

John F. Clauser

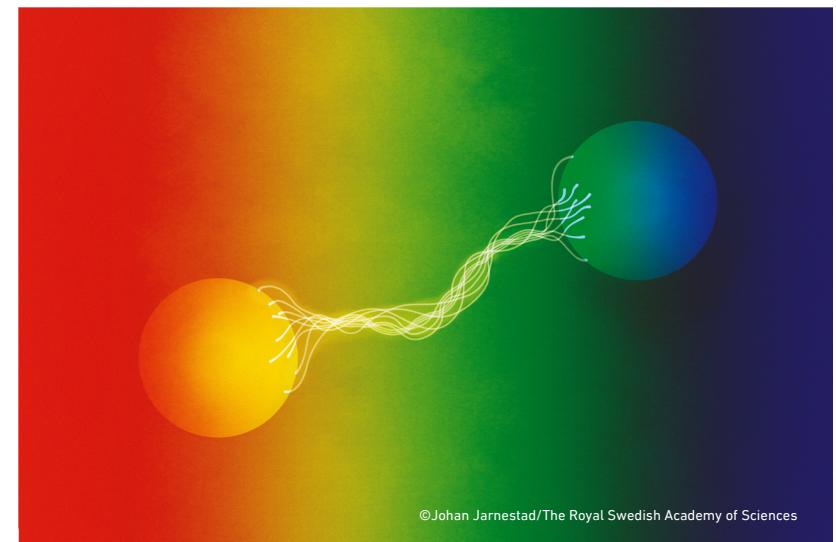
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III. Niklas Elmehed © Nobel Prize Outreach

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*

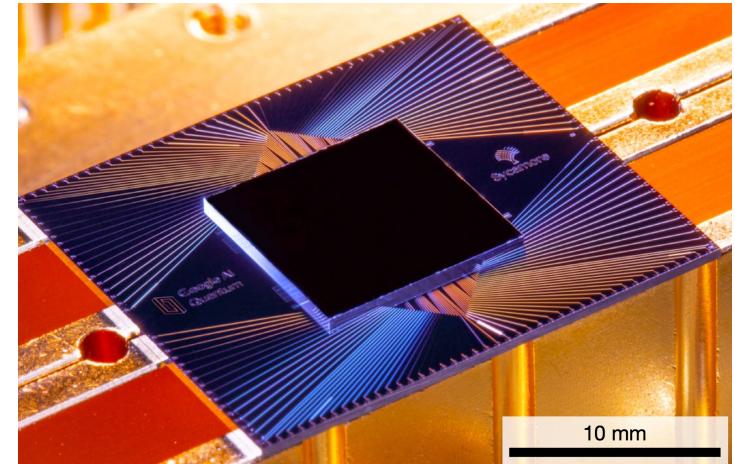
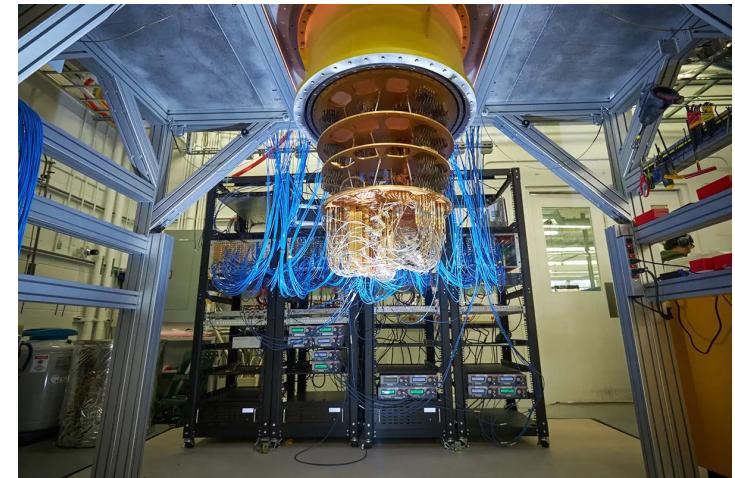
R. P. Feynman, *Int. J. Theo. Phys.* **21**, 467 ('82);  
S. Lloyd, *Science* **273**, 1073 ('96)

- 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

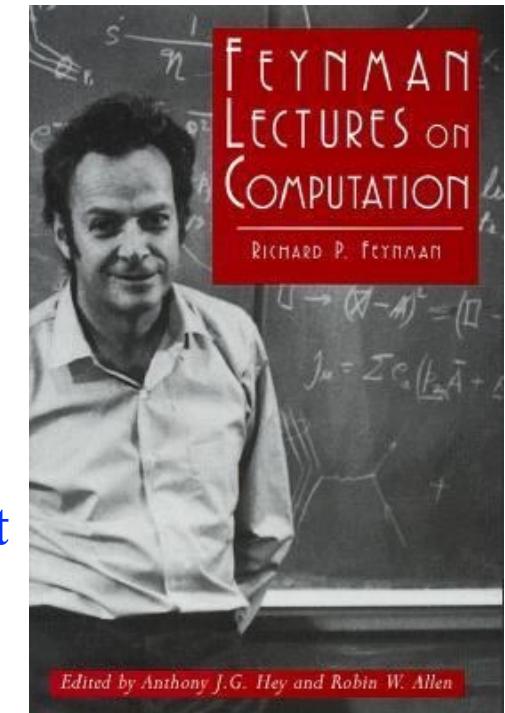
J. Preskill, *Quantum* **2**, 79 ('18)



54-qubit Google Sycamore

# Quantum Dynamics Simulations

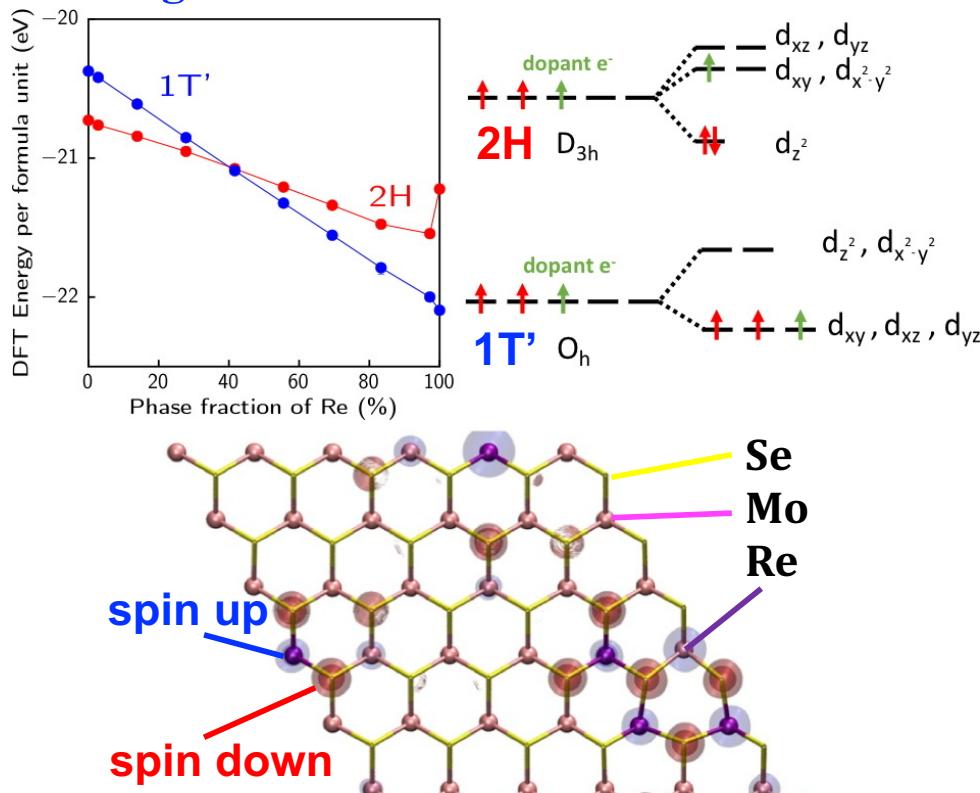
- An exciting scientific application of quantum computers is as a universal simulator of quantum many-body *dynamics*, as envisioned by Richard Feynman [*Int. J. Theor. Phys.* **21**, 467 ('82)]
- Seth Lloyd provided concrete algorithms and analysis [*Science* **273**, 1073 ('96)]
- Second edition of *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 & Rigetti 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)]
- Simulated topologically protected quantum dynamics on IBM Quantum [*M. Mercado et al., Phys. Rev. B* **110**, 075116 ('20)]



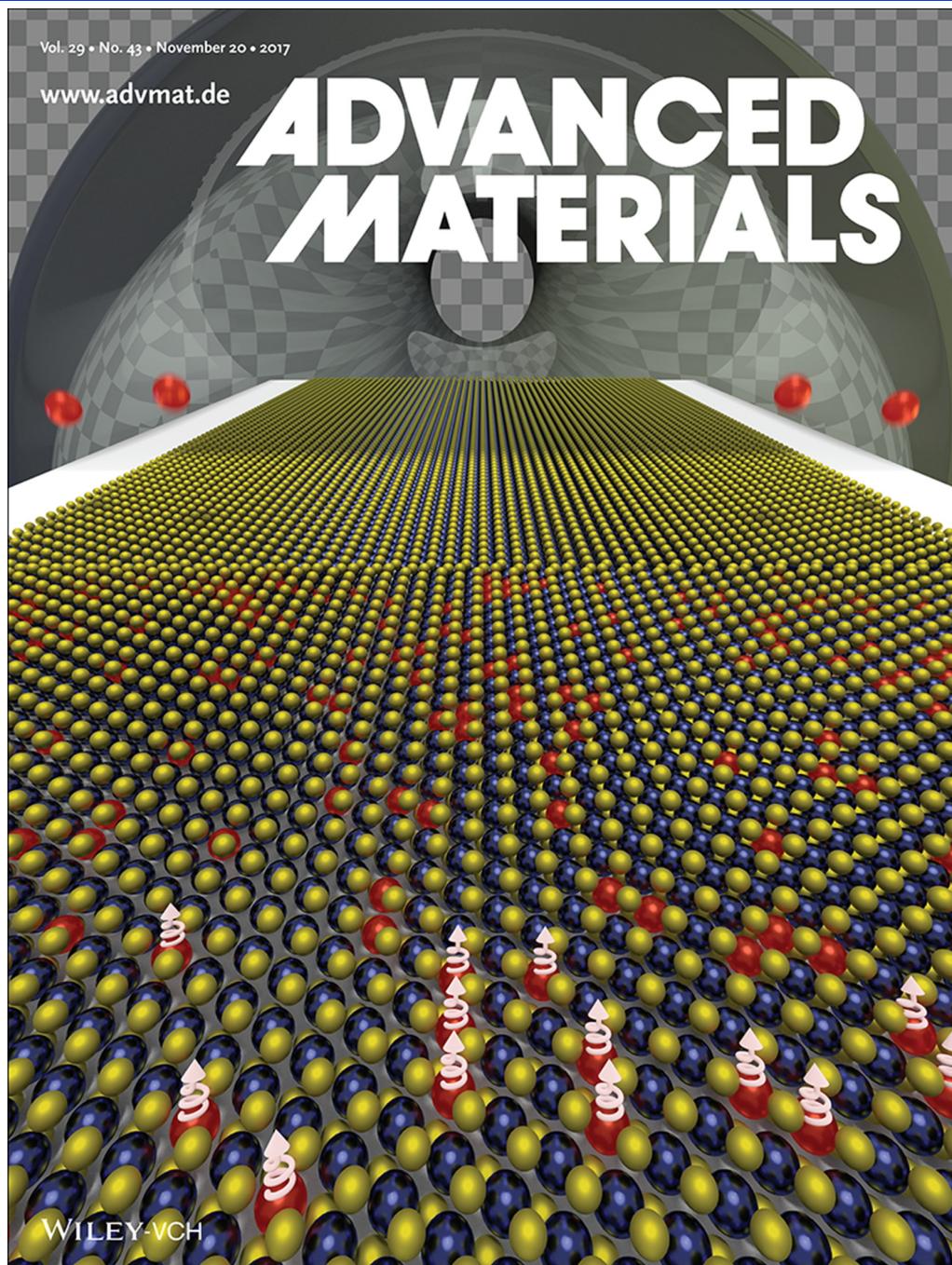
Do it yourself at <https://quantum-computing.ibm.com>

# 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



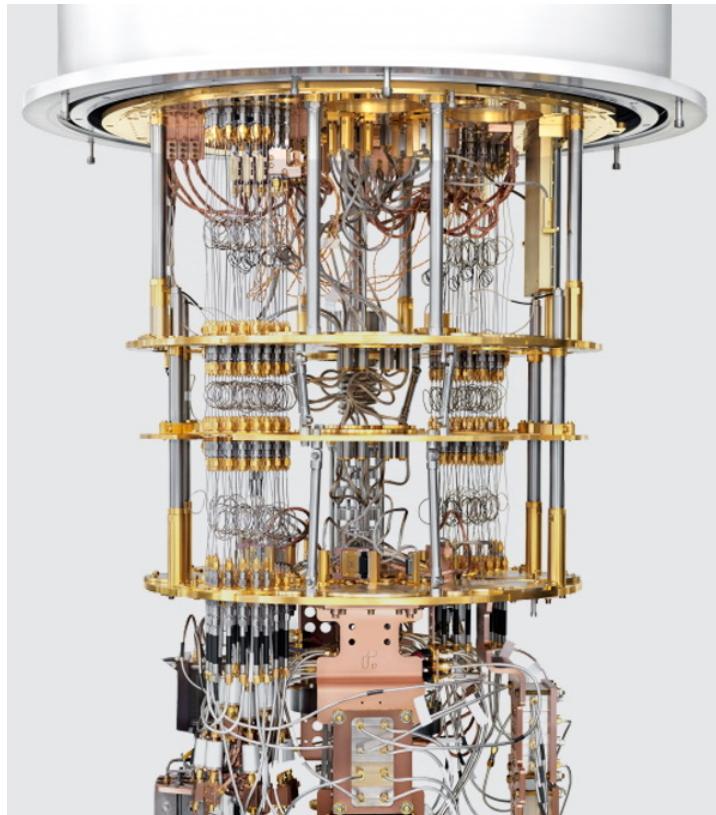
V. Kochat *et al.*, *Adv. Mater.* **29**, 1703754 ('17)



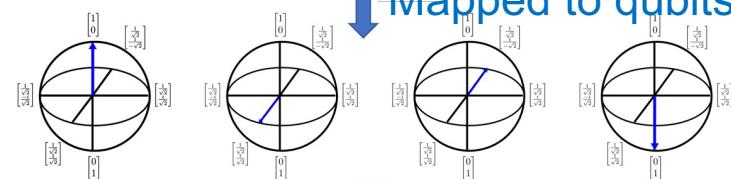
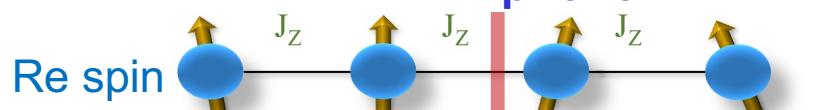
# Quantum Computing of Magnetism

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

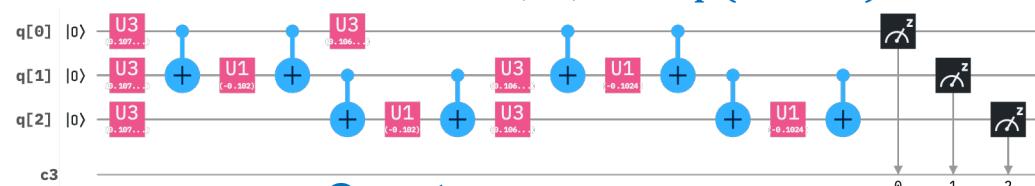
L. Bassman *et al.*, Phys. Rev. 101, 184305 ('20)



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



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



Quantum program

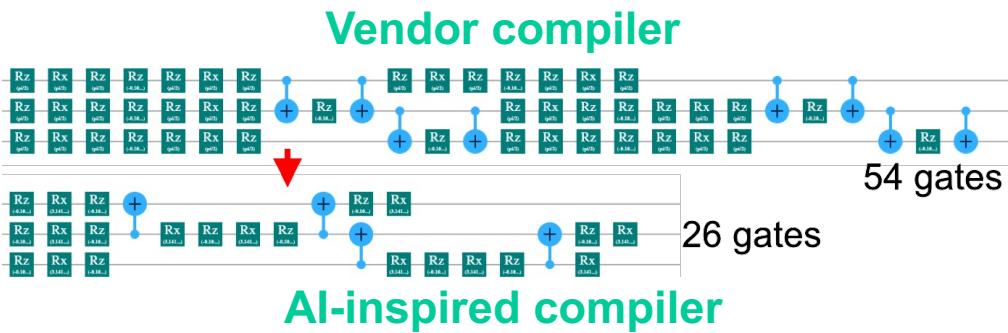
```
32  ....#define the two non-commuting terms that comprise the Hamiltonian-
33  ....Hz = PauliTerm("Z", 0, epsilon_0)-
34  ....Hy = PauliTerm("Y", 0, epsilon_ph*np.sin(w_ph*t))-#
35  ....#exponentiate the terms of the Hamiltonian for use in Trotter approx-
36  ....exp_Hz = exponential_map(Hz)(delta_t/(2.0*hbar))-#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

# Quantum Dynamics on NISQ Computers

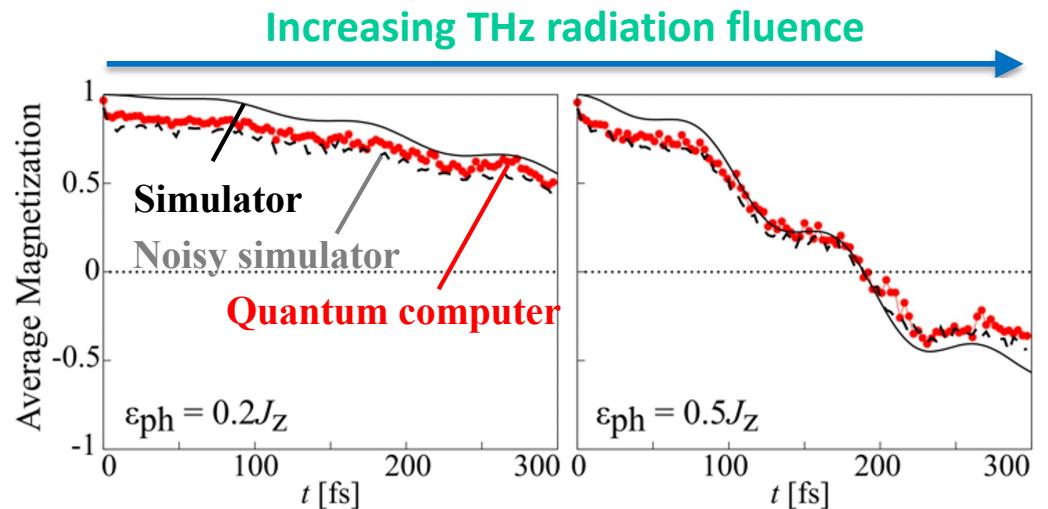
- Quantum-dynamics simulations on NISQ computers show dynamic suppression of magnetization by THz radiation

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

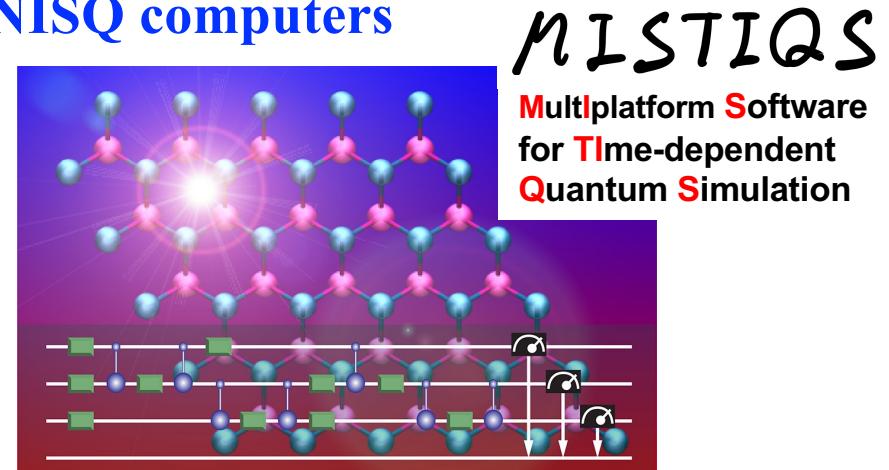
- AI-inspired quantum compiler reduced the circuit size by 30% to mitigate environmental noise



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



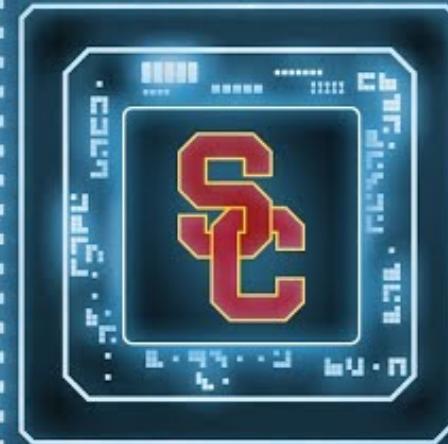
- Full-stack, cross-platform software for quantum dynamics simulations on NISQ computers



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

# Why quantum computing at USC?

## USC Frontiers of Computing



**USC launches \$1B-plus initiative for computing including advanced computation, quantum computing, AI and ethics**

<https://computing.usc.edu>

# 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
- **Quantum-centric supercomputing:** Do it with post-exaflop/s supercomputers
- **Error-tolerant quantum computing:** Quantum error correction & mitigation

# Next: Hands on at IBM Quantum

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

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

