Quantum Computing for Science
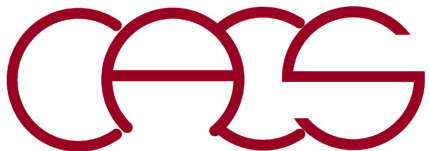
Aiichiro Nakano

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

Email: anakano@usc.edu

CyberMAGICS Workshop

July 1, 2022

Changing Computing Landscape for Science

Postexascale Computing for Science

AI for Science

Compute Cambrian explosion

Exa-quantum-AI nexus
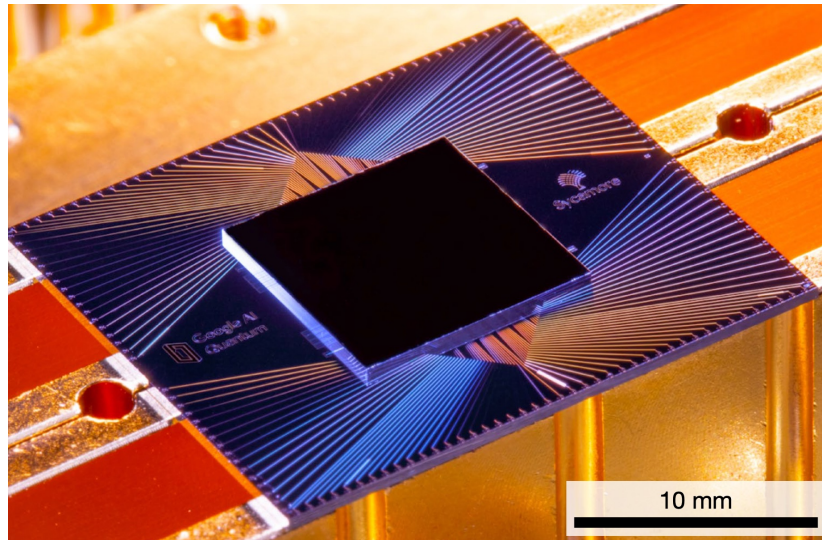
Quantum Computing for Science

DOE readies multibillion-dollar AI push

U.S. supercomputing leader is the latest big backer in a globally crowded field

By **Robert F. Service**, *in Washington, D.C.*

Science **366**, 559 (Nov. 1, '19)

10 mm

Use all to advance science!

Quantum Computing (QC) for Science

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

- **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

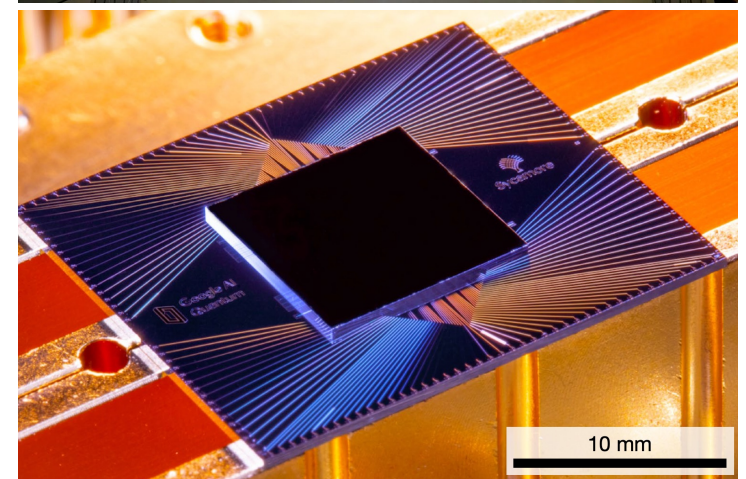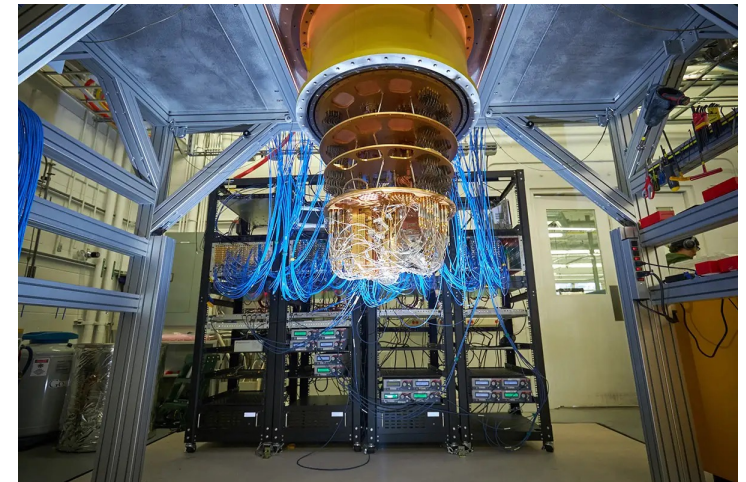 R. P. Feynman, *Int. J. Theo. Phys.* **21**, 467 ('82);
  S. Lloyd, *Science* **273**, 1073 ('96)

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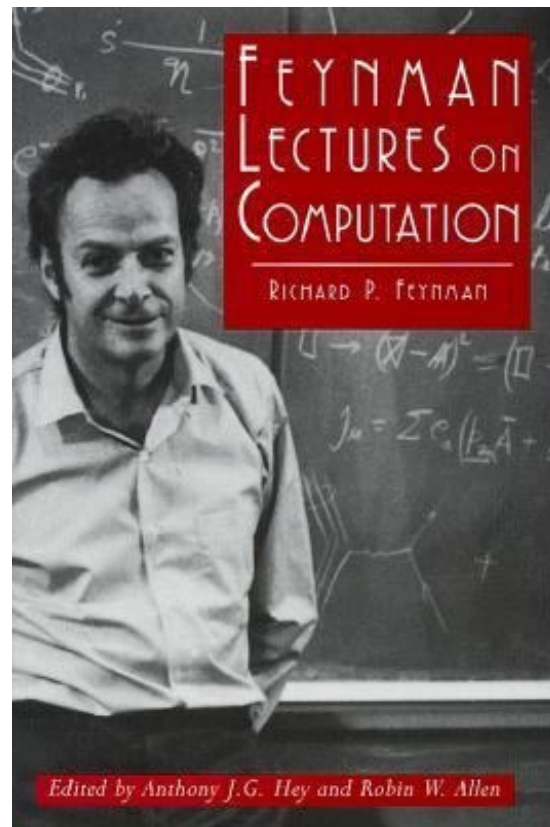
  J. Preskill, *Quantum* **2**, 79 ('18)

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54-qubit Google Sycamore

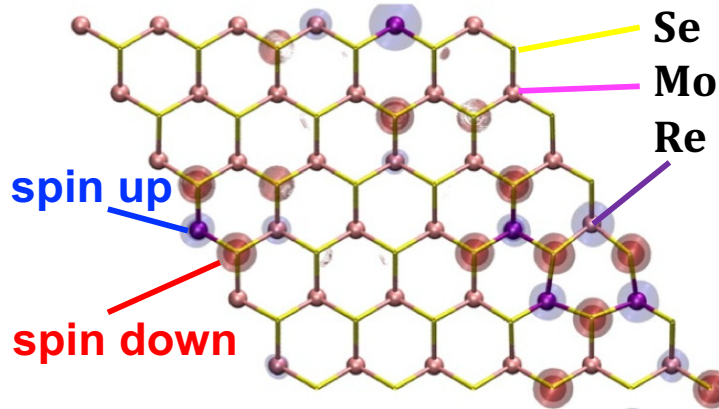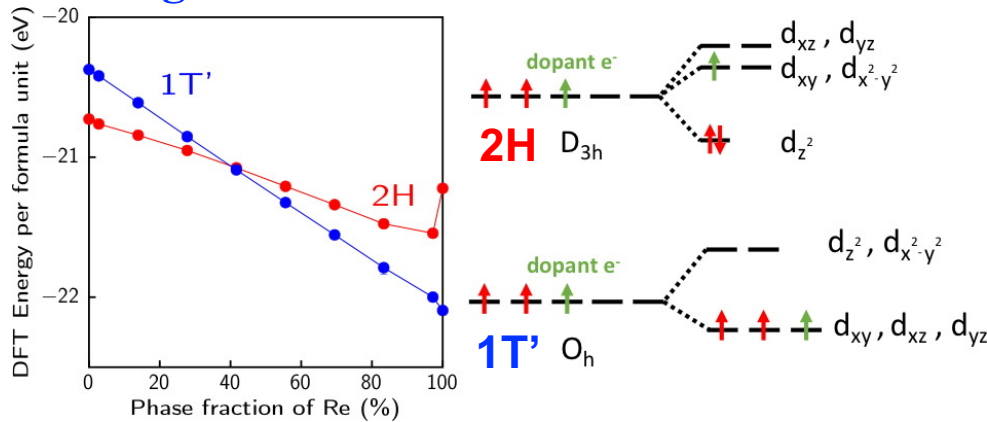# An Excellent Reading

- **Second edition of *Feynman Lectures on Computation* will add a section on "Simulating quantum dynamics" by John Preskill**
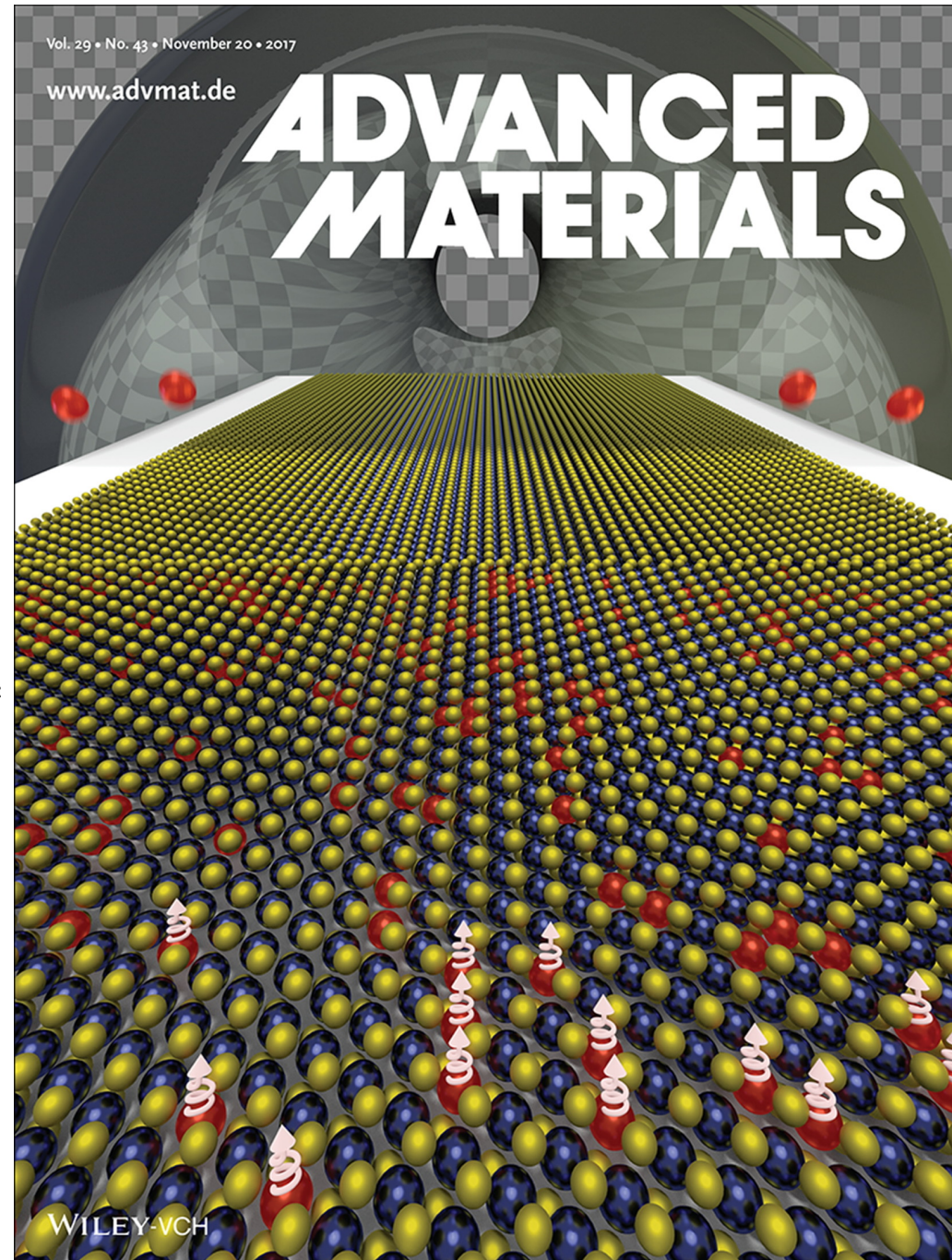

Preskill, *arXiv*:2106.10522 ('21)

Application: Emergent Magnetism

- **Experiment at Rice shows 2H-to-1T' phase transformation by alloying $MoSe_2$ with Re**

- **QMD simulations at USC elucidate its electronic origin**

- **Simulation & experiment show novel magnetism centered at Re atoms**

2H D_{3h}

d_{xz}, d_{yz}
d_{xy}, $d_{x^2-y^2}$
d_{z^2}
dopant e⁻

1T' O_h

d_{z^2}, $d_{x^2-y^2}$
d_{xy}, d_{xz}, d_{yz}
dopant e⁻

Se
Mo
Re

spin up
spin down

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

Vol. 29 · No. 43 · November 20 · 2017
www.advmat.de

ADVANCED MATERIALS

WILEY-VCH

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)

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

E″ phonon

Re spin J_Z J_Z J_Z

Mapped to qubits

Quantum circuit

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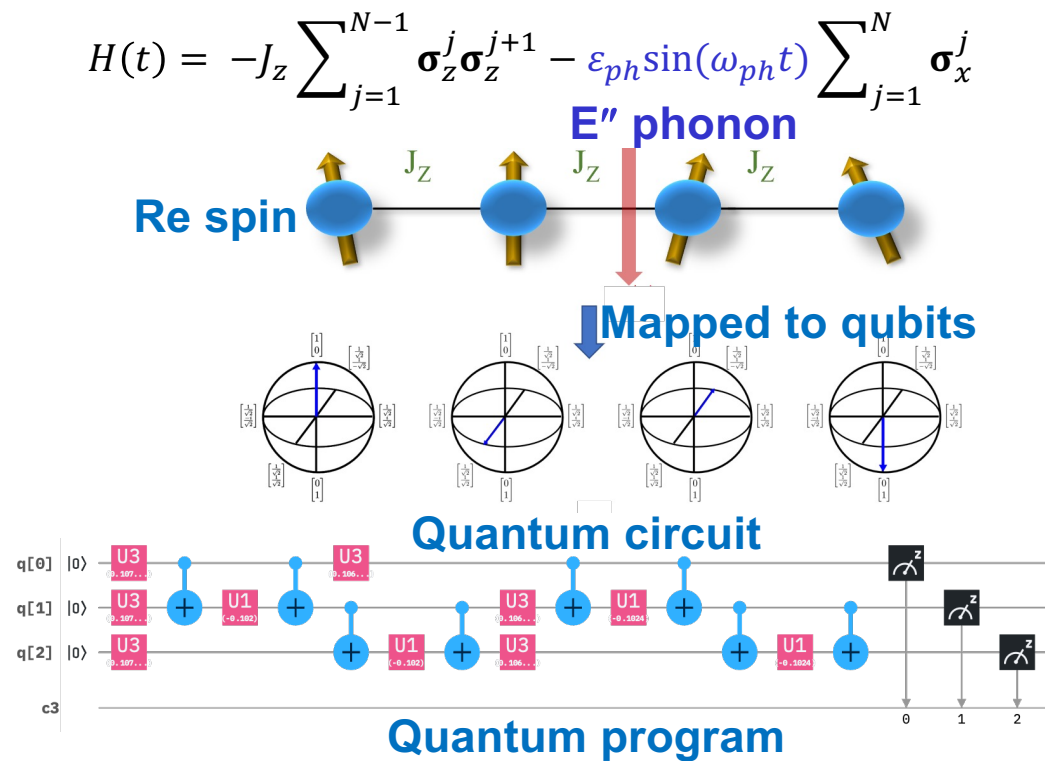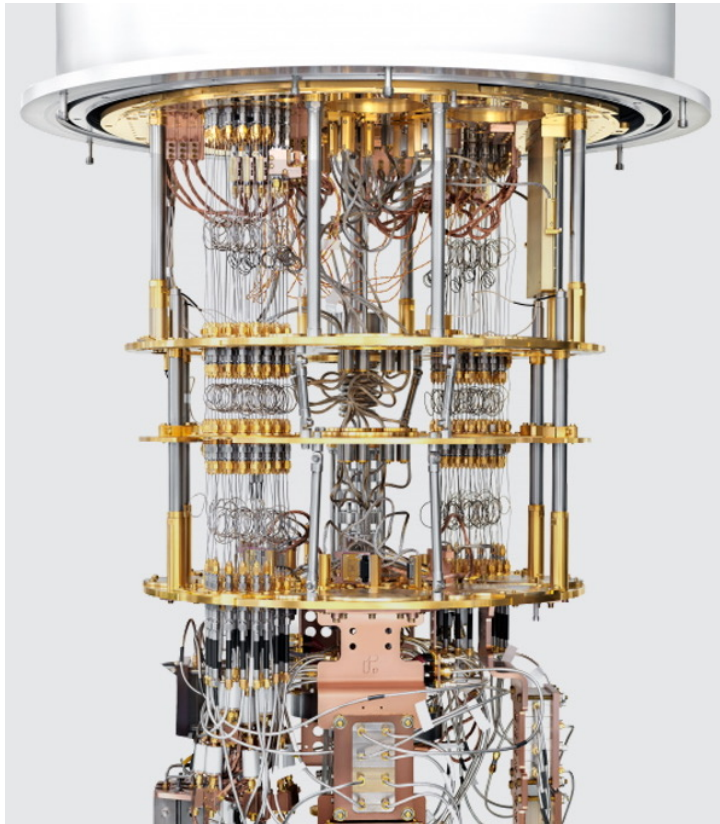
```
32   ····#define·the·two·non-commuting·terms·that·comprise·the·Hamiltonian¬
33   ····Hz·=·PauliTerm("Z",·0,·epsilon_0)¬
34   ····Hy·=·PauliTerm("Y",·0,·epsilon_ph*np.sin(w_ph*t))¬
35   ····#exponentiate·the·terms·of·the·Hamiltonian·for·use·in·Trotter·approx¬
36   ····exp_Hz·=·exponential_map(Hz)(delta_t/(2.0*hbar))¬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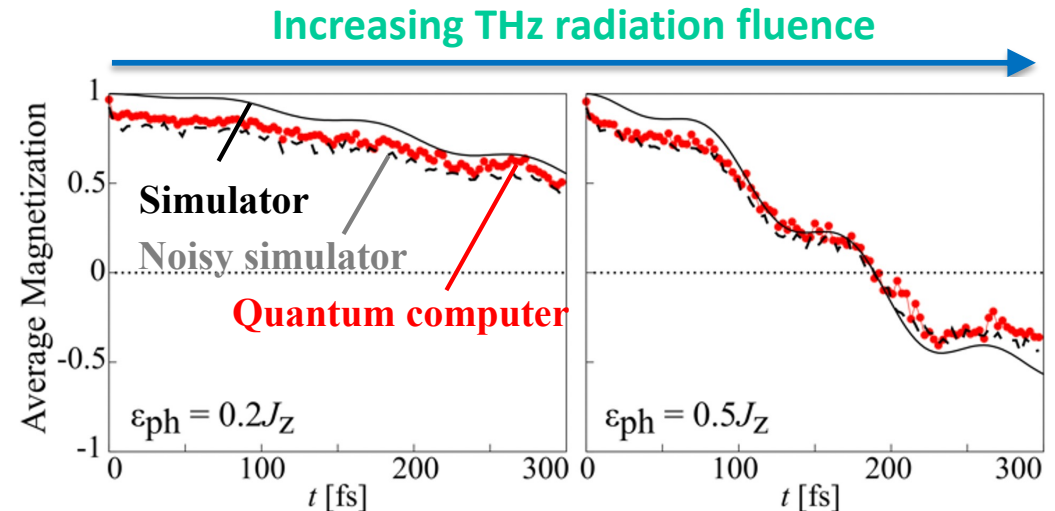
Quantum Dynamics on NISQ Computers

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

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

Increasing THz radiation fluence

Simulator
Noisy simulator
Quantum computer

$\varepsilon_{ph} = 0.2 J_z$

$\varepsilon_{ph} = 0.5 J_z$

Average Magnetization

t [fs]

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

Vendor compiler

54 gates

26 gates

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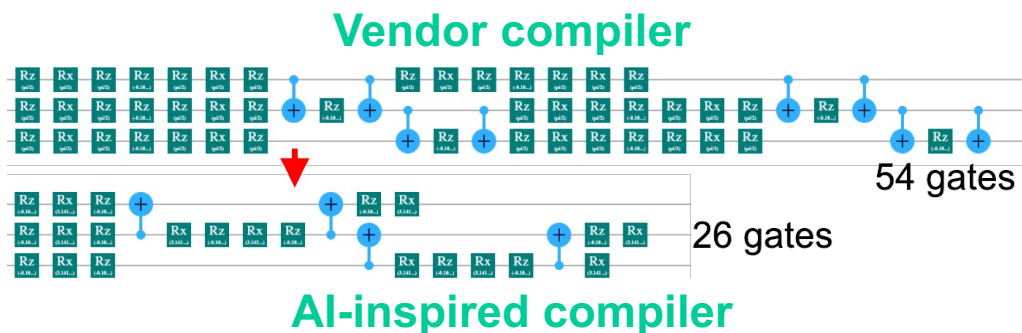
L. Bassman *et al.*,
Quantum Sci. Tech. **6**, 014007 ('21)

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

MISTIQS

Mult**I**platform **S**oftware
for **TI**me-dependent
Quantum **S**imulation
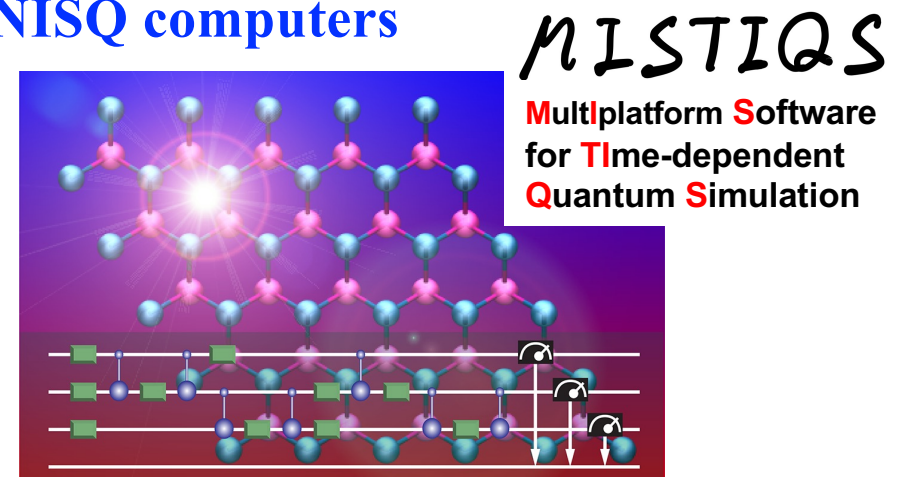
C. Powers *et al.*, *SoftwareX* **14**, 100696 ('21)
https://github.com/USCCACS/MISTIQS

Where to Go from Here

Extensive tutorial on quantum computing

- **You will be ready for** [Learn quantum computation using Qiskit](#)

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 ([Li, *PRX* '20](#));** *cf.* **variational quantum eigensolver (VQE) & quantum approximate optimization algorithm (QAOA) in Qiskit tutorial**

- **Error-tolerant quantum computing: Quantum error correction & mitigation ([LaRose, *arXiv* '21](#))**

Next: Hands on at IBM Quantum

- **Quantum computing basics: Qubits and quantum gates**

- **Advanced: Quantum computation of transverse-field Ising model**

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