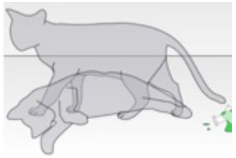
Quantum Computing for Science

Aiichiro Nakano

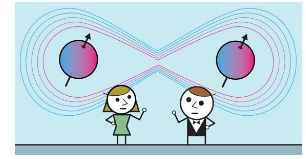
Collaboratory for Advanced Computing & Simulations
Departments of Computer Science, Physics & Astronomy,
and Quantitative & Computational Biology
University of Southern California

Email: anakano@usc.edu

What Is Quantum Computing?



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



The Nobel Prize in Physics 2022 **It's entanglement!**

Ill. Niklas Elmehed © Nobel Prize Outreach

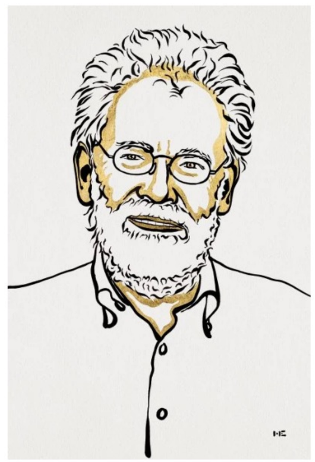
Alain Aspect

Prize share: 1/3

Ill. Niklas Elmehed © Nobel Prize Outreach

John F. Clauser

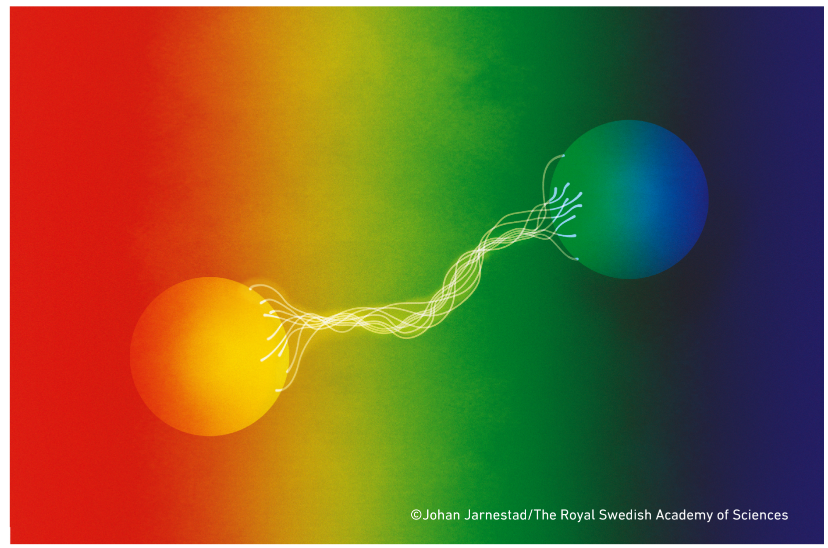
Prize share: 1/3



Ill. Niklas Elmehed © Nobel Prize Outreach

Anton Zeilinger

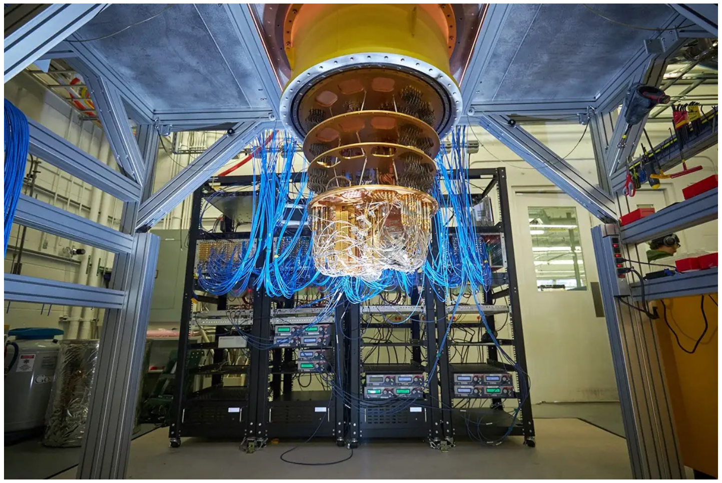
Prize share: 1/3

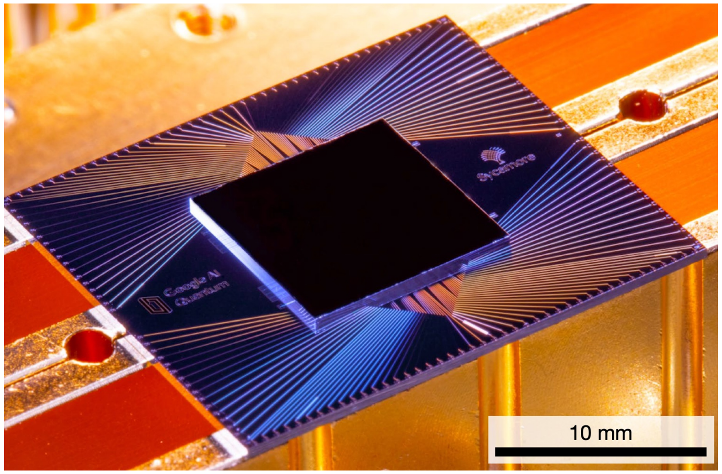


The Nobel Prize in Physics 2022 was awarded jointly to Alain Aspect, John F. Clauser and Anton Zeilinger "for experiments with entangled photons, establishing the violation of Bell inequalities and pioneering quantum information science"

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

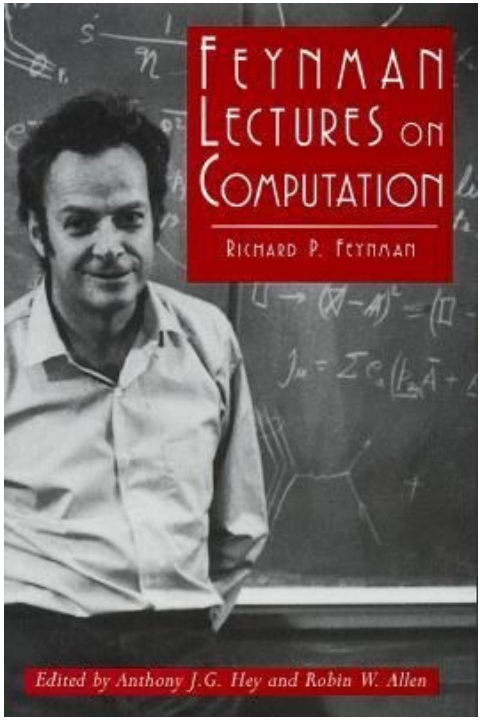
- **An exciting scientific application of quantum computers is as a universal simulator of quantum many-body *dynamics*, as envisioned by Richard Feynman** [*Int. J. Theor. Phys*. **21**, 467 ('82)]

- **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)]

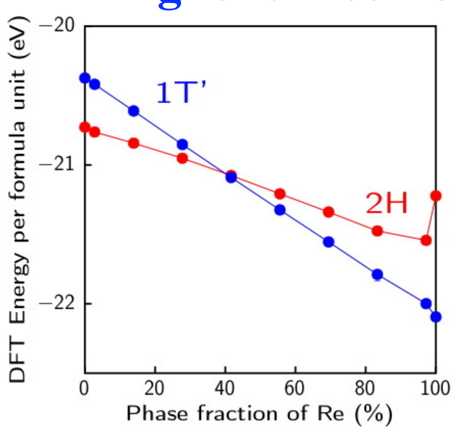
- **Simulated topologically protected quantum dynamics on IBM Quantum** [M. Mercado *et al.*, *Phys. Rev. B* **110**, 075116 ('20)]

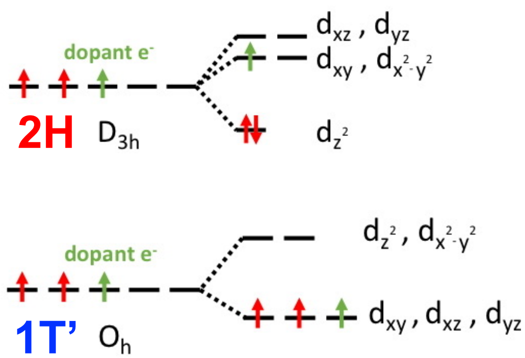


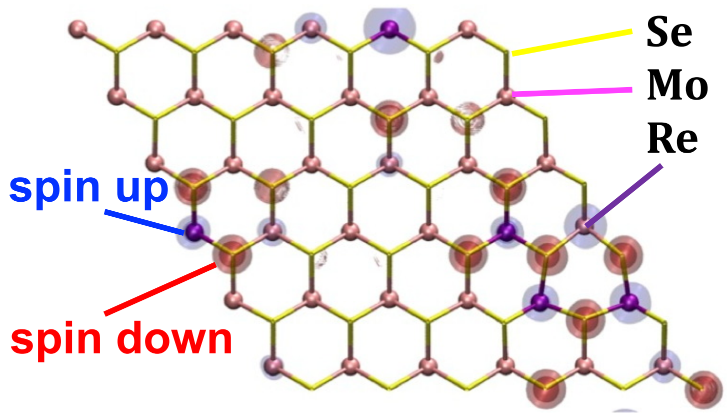
Do it yourself at https://quantum-computing.ibm.com

Application: Emergent Magnetism

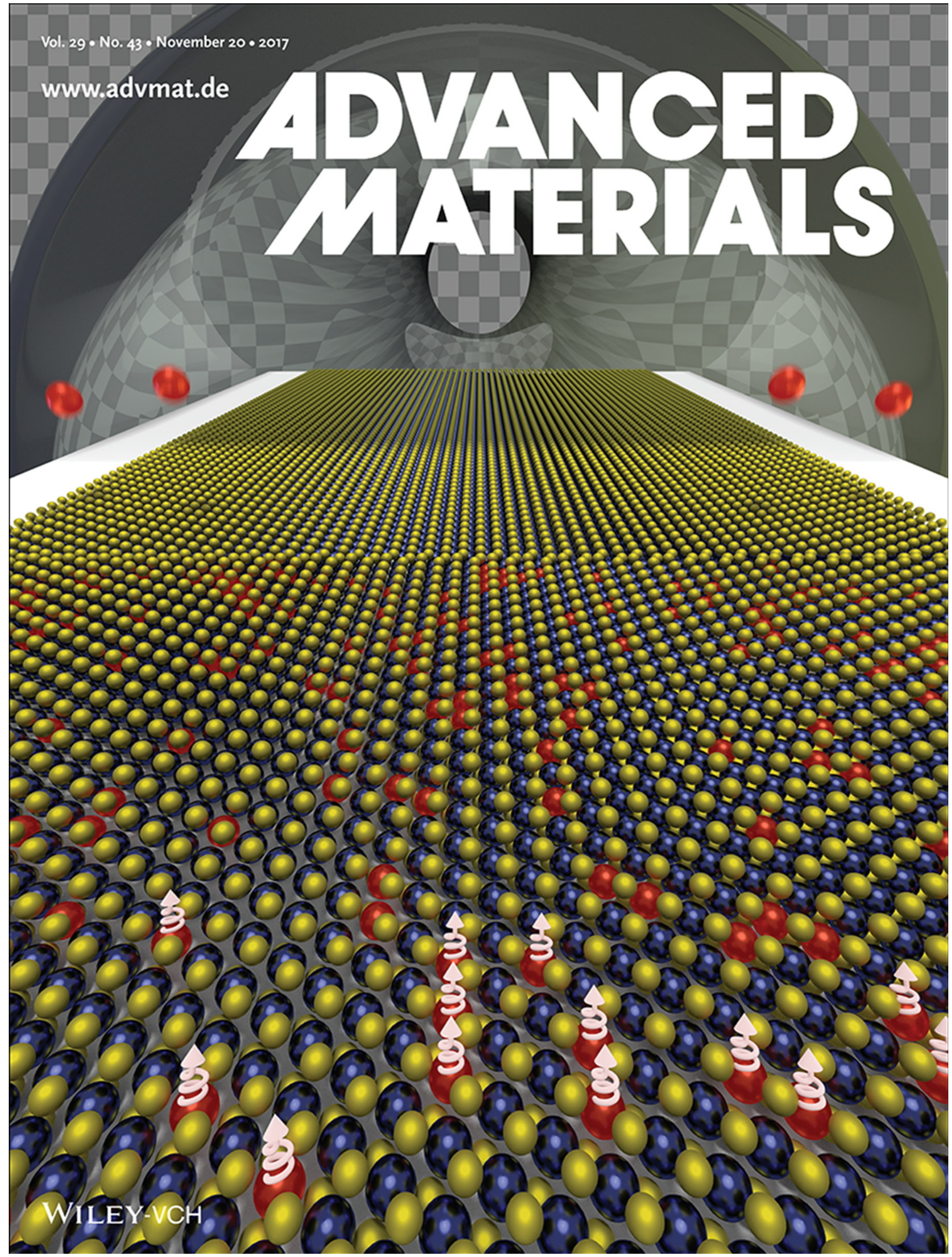
- Experiment at Rice shows 2H-to-1T' phase transformation by alloying $MoSe_2$ with Re
- QMD simulations at USC elucidate its electronic origin
- Simulation & experiment show novel magnetism centered at Re atoms







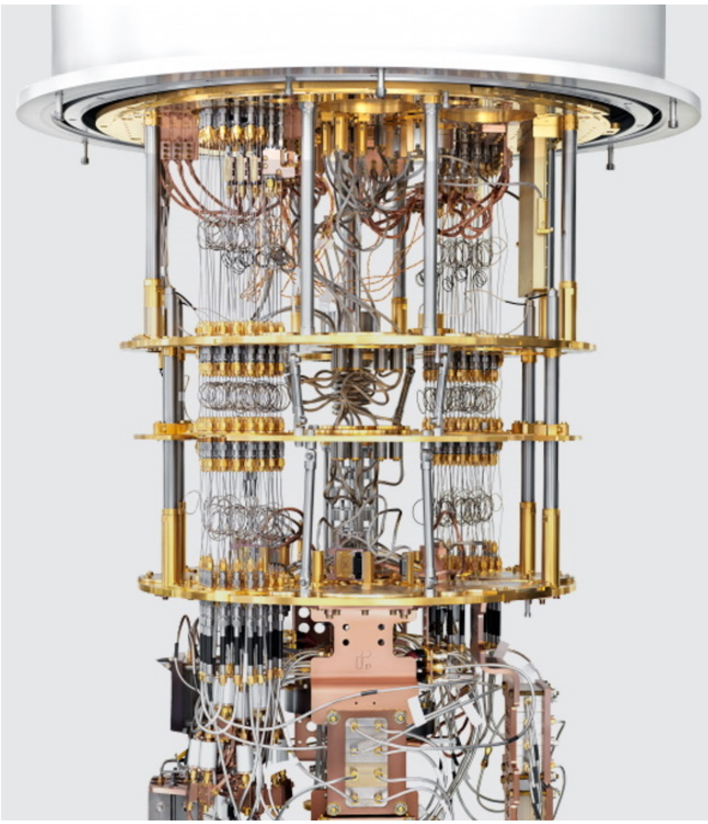
V. Kochat *et al.*, *Adv. Mater*. **29**, 1703754 ('17)



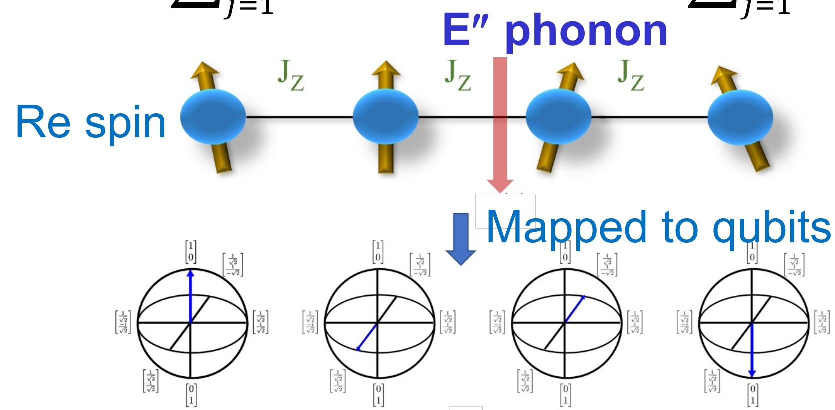
Quantum Computing of Magnetism

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

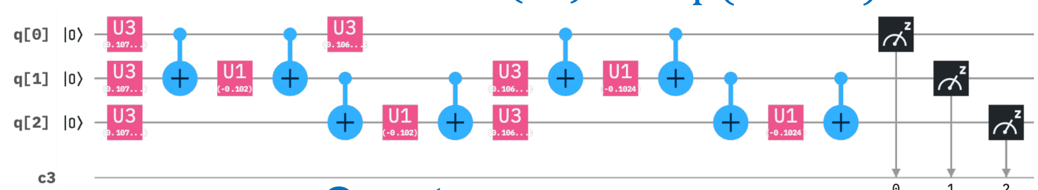
L. Bassman *et al.*, *Phys. Rev.* **101**, 184305 ('20)



$$H(t) = -J_z \sum_{j=1}^{N-1} \boldsymbol{\sigma}_z^j \boldsymbol{\sigma}_z^{j+1} - \varepsilon_{ph} \sin(\omega_{ph} t) \sum_{j=1}^{N} \boldsymbol{\sigma}_x^j$$



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



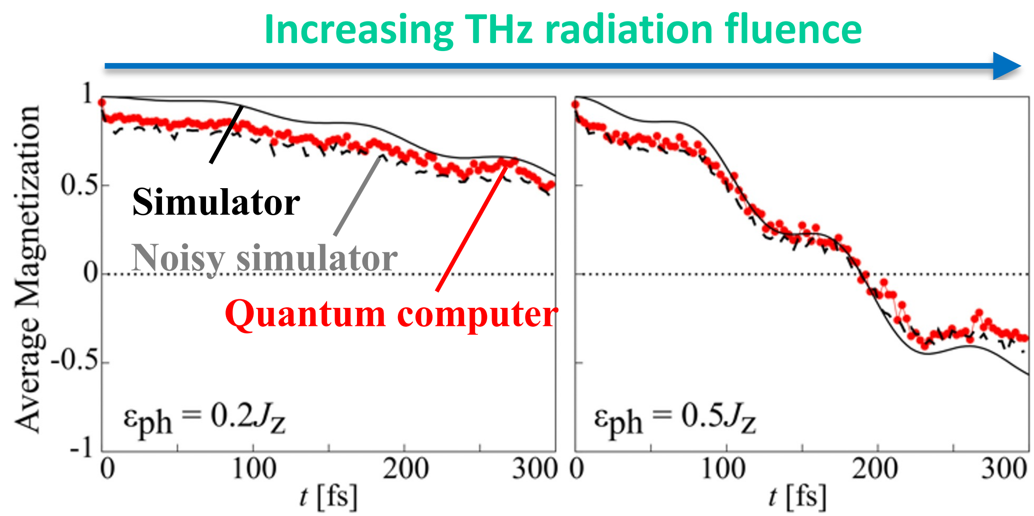
Quantum program

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

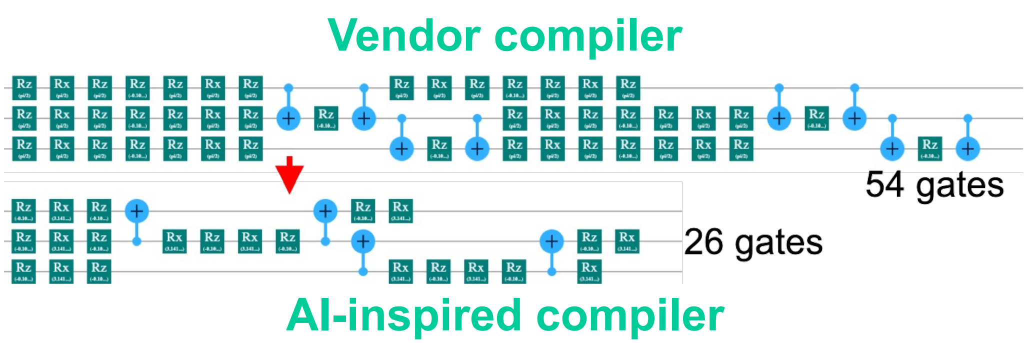
Quantum Dynamics on NISQ Computers

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

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

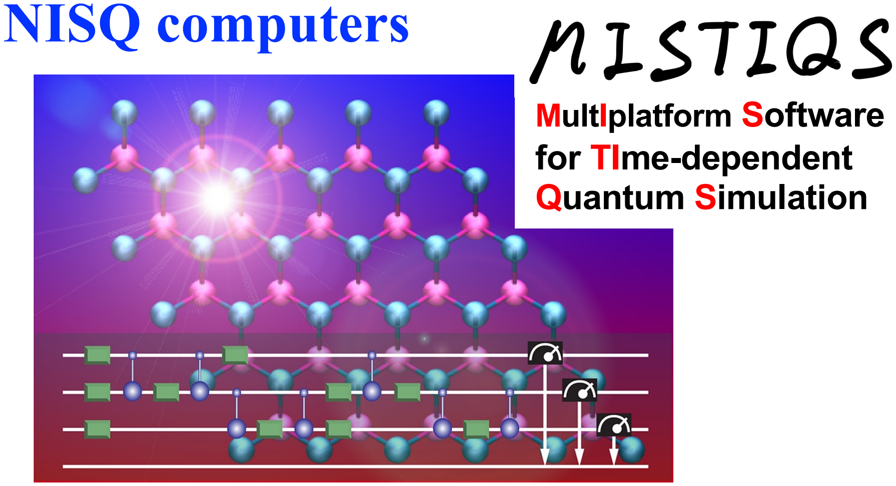


- **AI-inspired quantum compiler reduced the circuit size by 30% to mitigate environmental noise**



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

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**

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