Quantum Computing for Science

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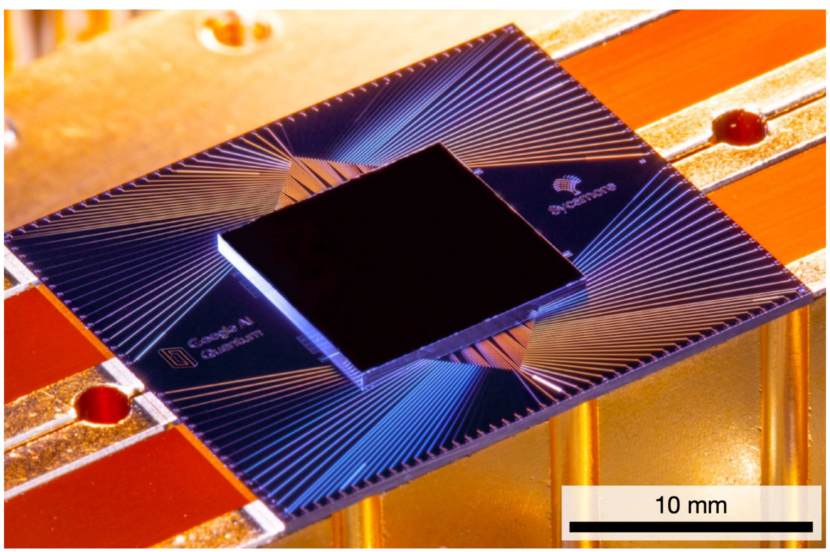
Changing Computing Landscape for Science

Postexascale Computing for Science

Compute Cambrian explosion

Quantum Computing for Science



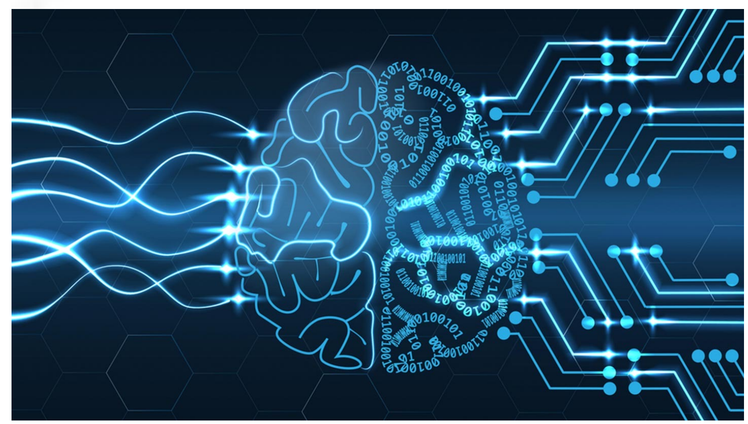
AI for Science

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)



Use all to advance science!

Quantum Computing (QC) for Science

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

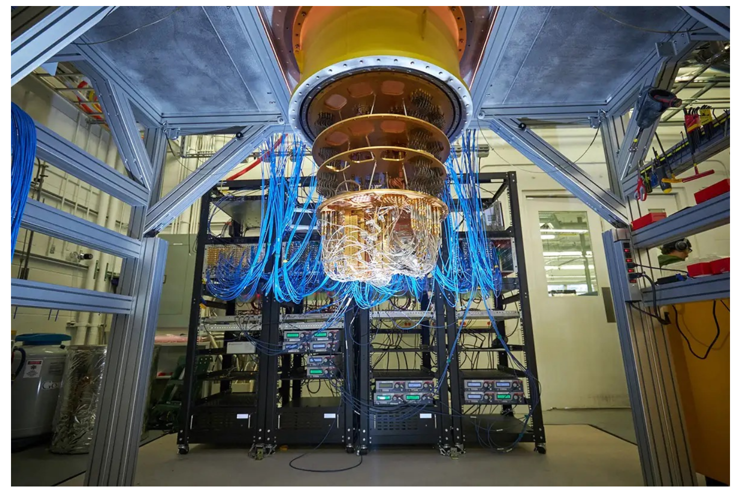
- **U.S. Congress (Dec. 21, ’18) signed National Quantum Initiative Act to ensure leadership in quantum computing & its applications**

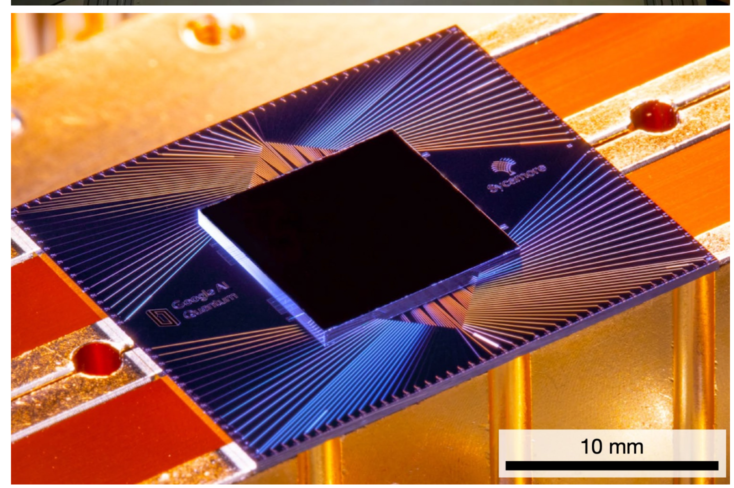
- **Quantum supremacy demonstrated by Google**
  F. Arute, *Nature* **574**, 505 (’19)

- **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)

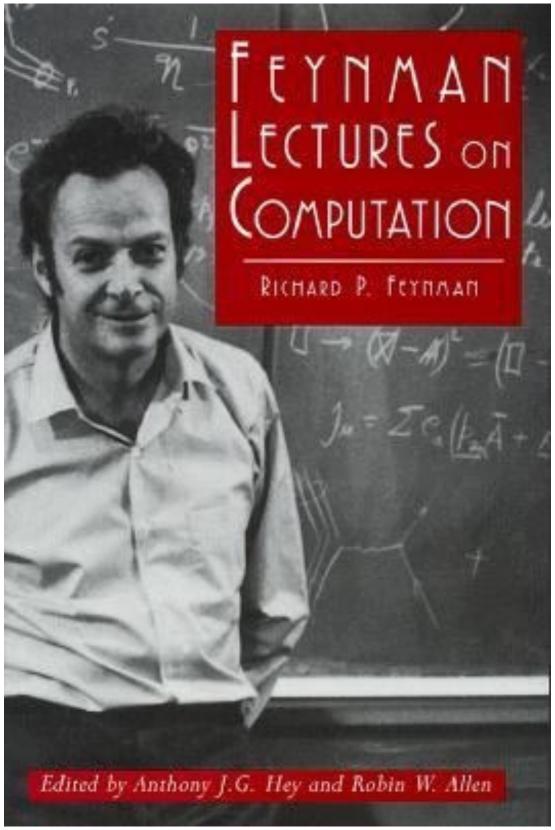




54-qubit Google Sycamore

An Excellent Reading

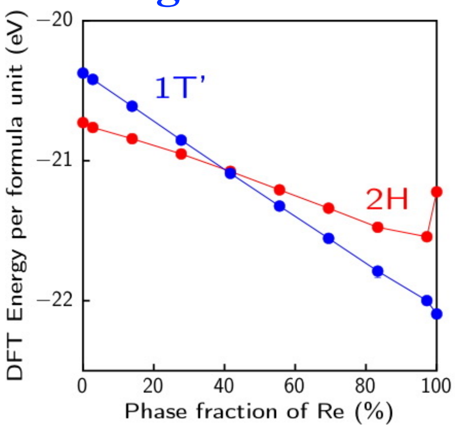
- **Second edition of *Feynman Lectures on Computation* will add a section on "Simulating quantum dynamics" by John Preskill**

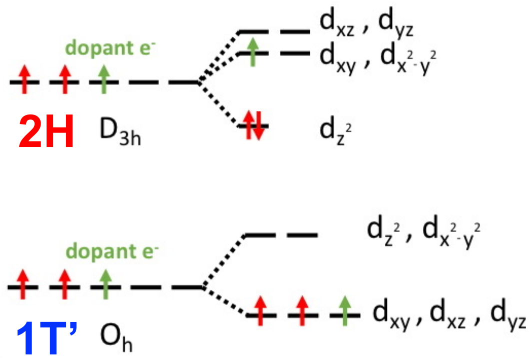


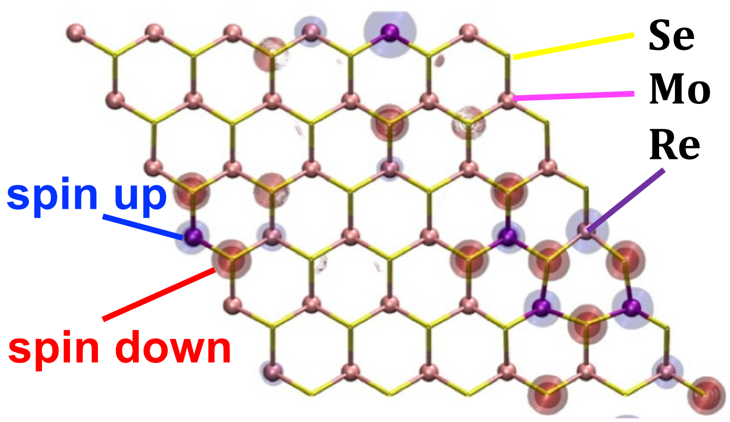
Preskill, *arXiv*:2106.10522 ('21)

Application: Emergent Magnetism

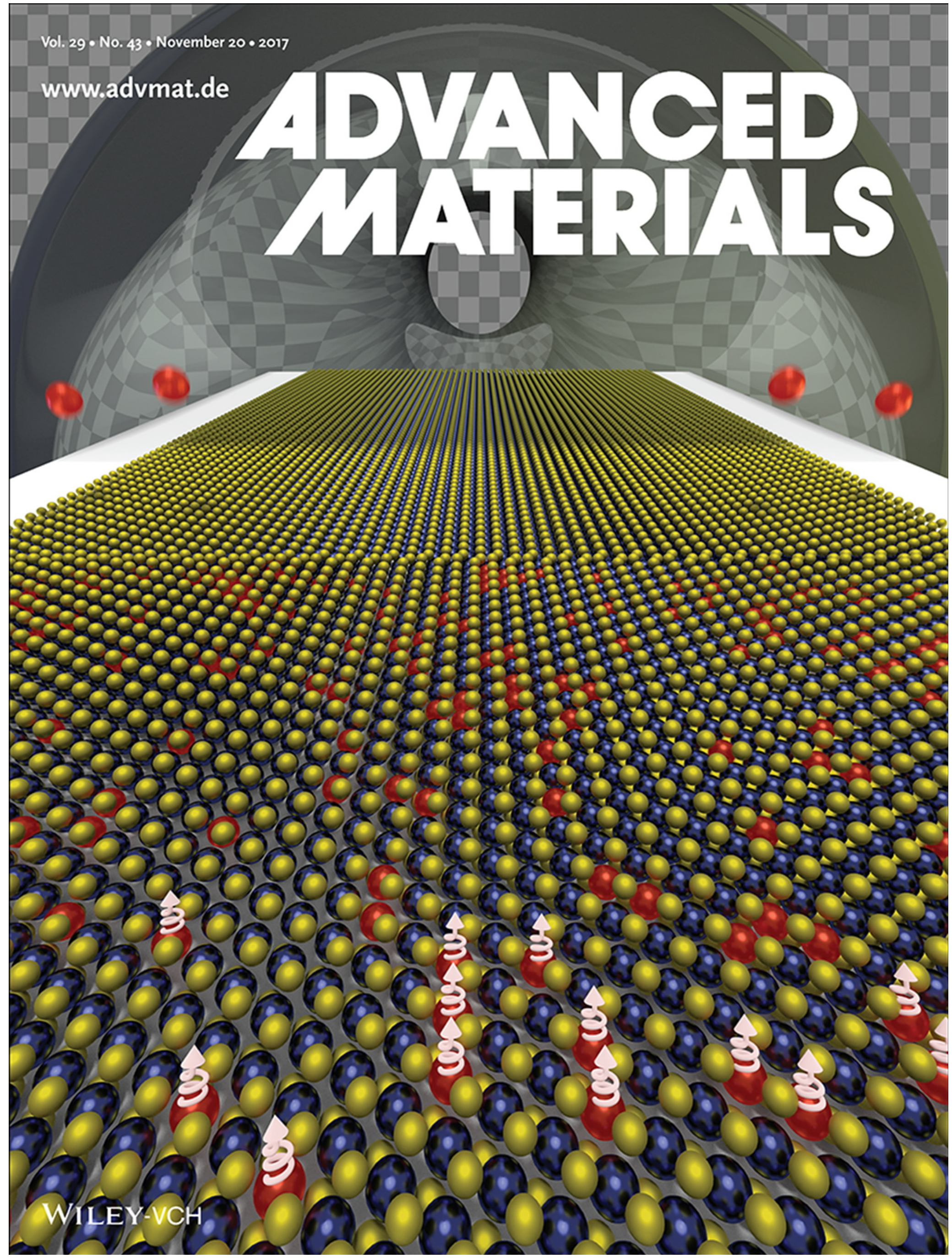
- Experiment at Rice shows 2H-to-1T' phase transformation by alloying $MoSe_2$ with Re
- QMD simulations at USC elucidate its electronic origin
- Simulation & experiment show novel magnetism centered at Re atoms







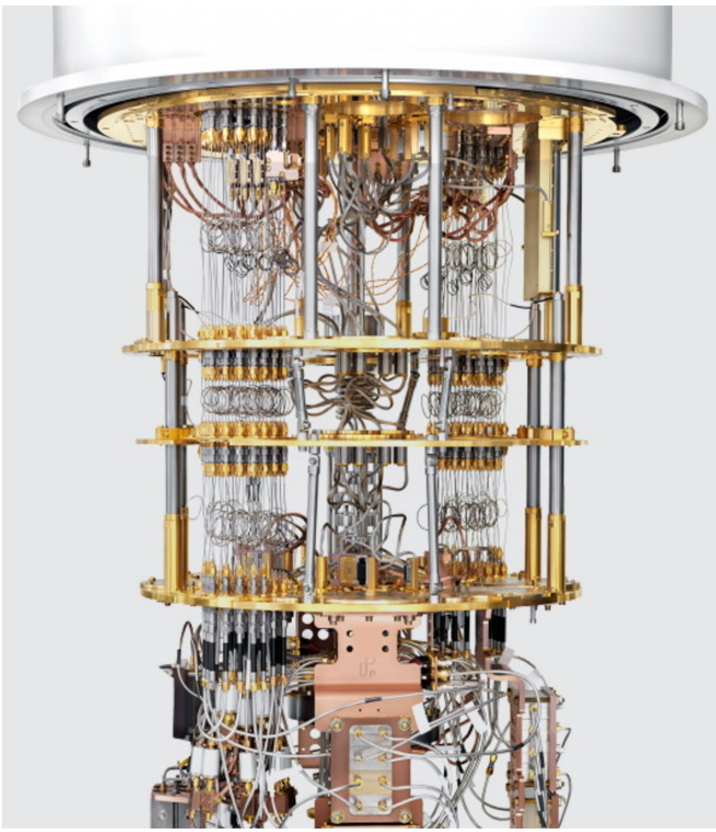
V. Kochat *et al.*, *Adv. Mater*. **29**, 1703754 ('17)



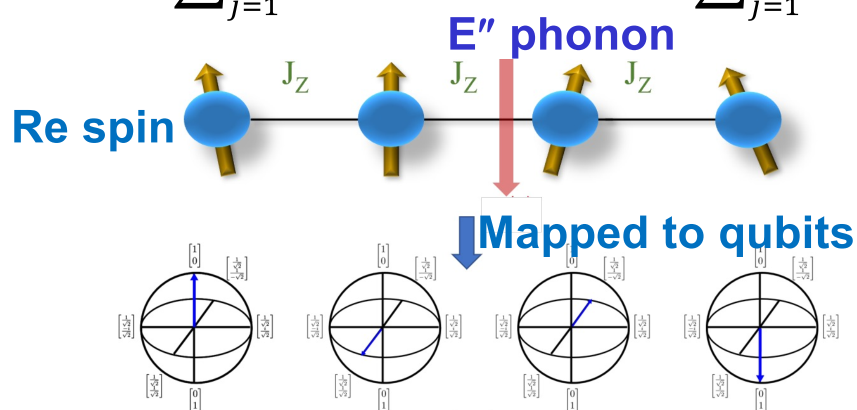
Quantum Computing of Magnetism

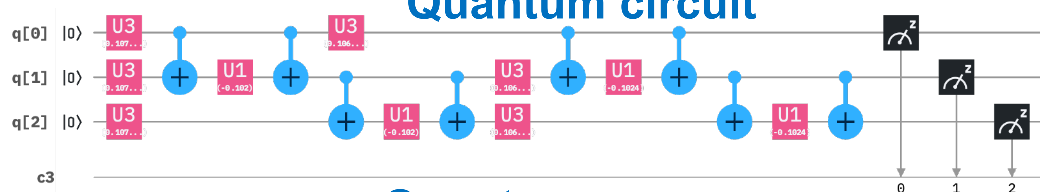
- **Simulated quantum many-body dynamics on IBM's Q16 Melbourne & Rigetti's Aspen quantum processors**

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



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





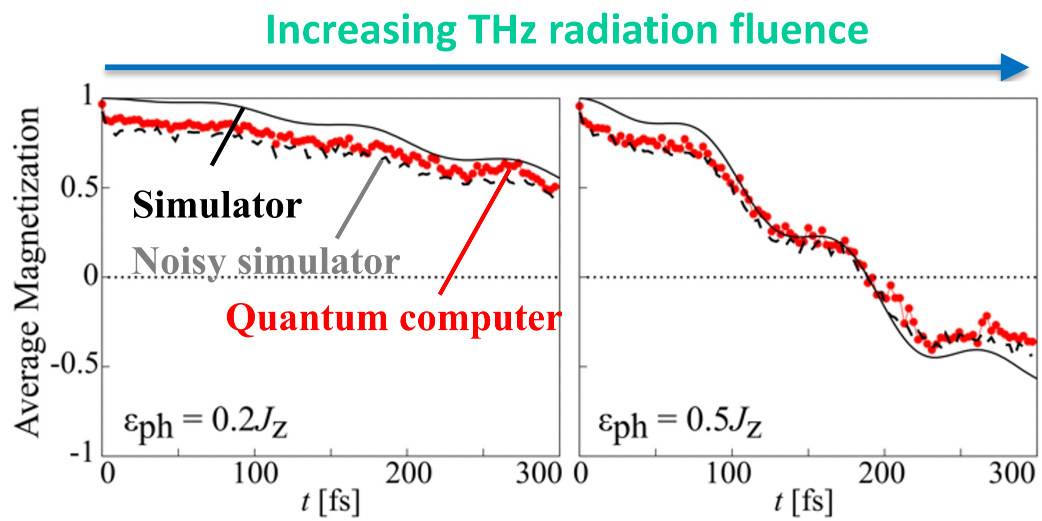
Quantum program

```
    #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)
```

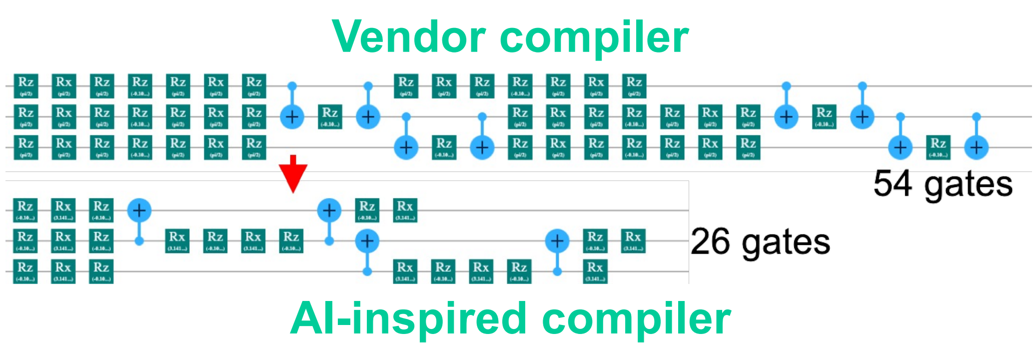
Quantum Dynamics on NISQ Computers

- **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**

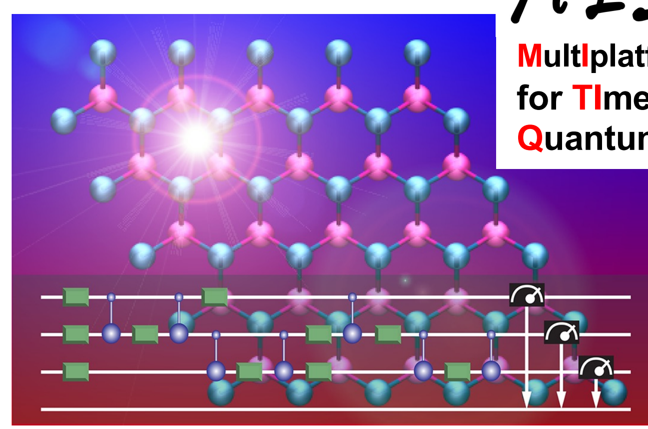


L. Bassman *et al.*,
Quantum Sci. Tech. **6**, 014007 ('21)

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

MISTIQS

Mult**I**platform **S**oftware for **TI**me-dependent **Q**uantum **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

- **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