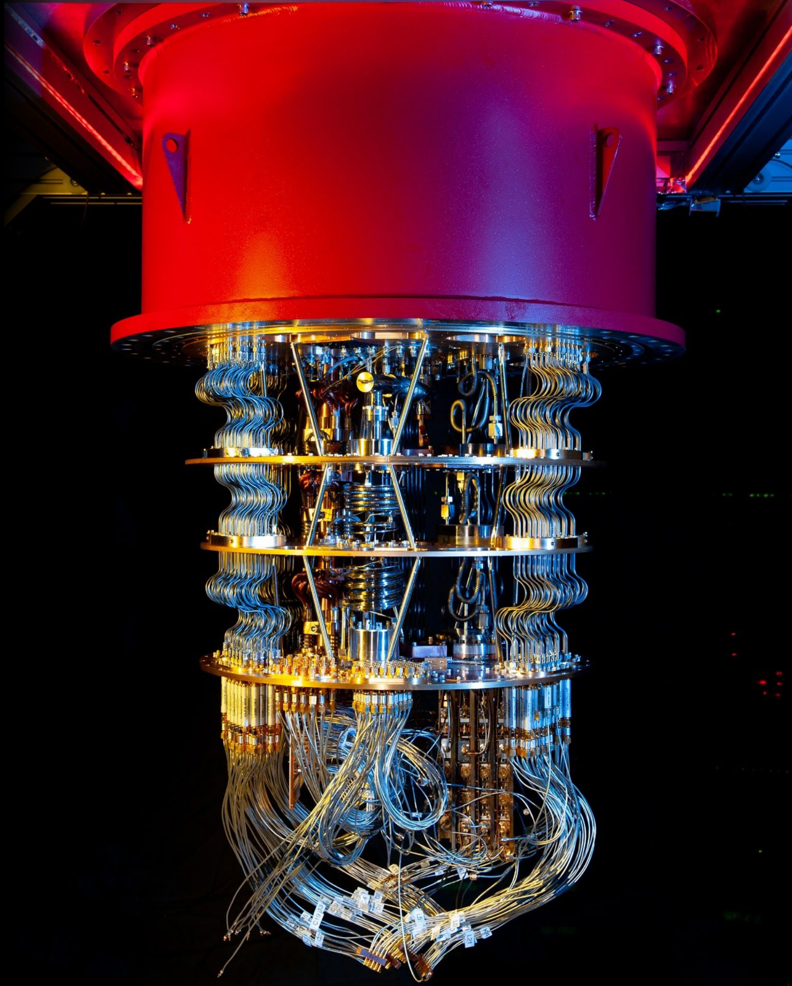
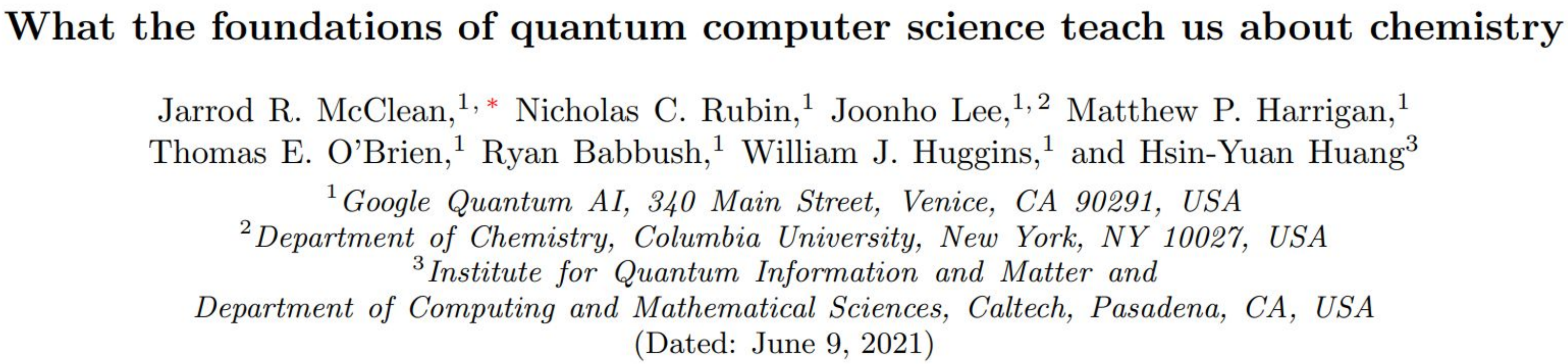
Google AI
Quantum



# What the foundations of quantum computer science teach us about chemistry

Jarrod McClean
@JarrodMcClean
Staff Research Scientist

# The context of this perspective



### What the foundations of quantum computer science teach us about chemistry

Jarrod R. McClean,[1,*] Nicholas C. Rubin,[1] Joonho Lee,[1,2] Matthew P. Harrigan,[1]
Thomas E. O'Brien,[1] Ryan Babbush,[1] William J. Huggins,[1] and Hsin-Yuan Huang[3]

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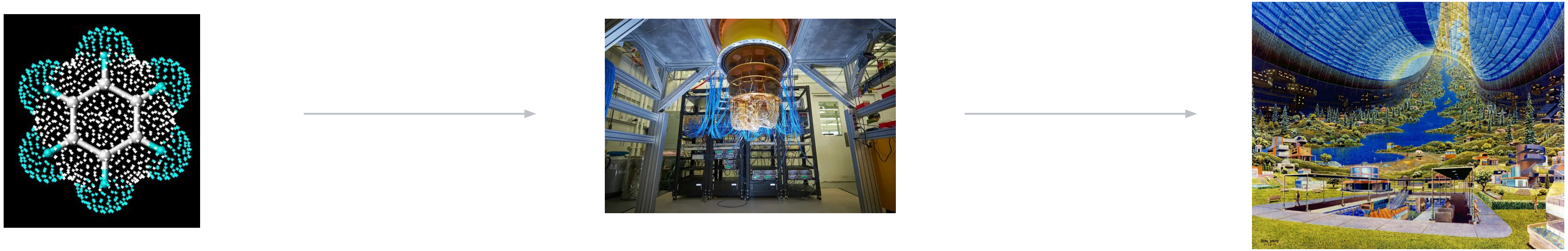
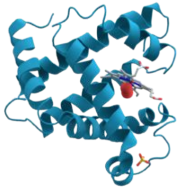
[2] *Department of Chemistry, Columbia University, New York, NY 10027, USA*
[3] *Institute for Quantum Information and Matter and*
*Department of Computing and Mathematical Sciences, Caltech, Pasadena, CA, USA*
(Dated: June 9, 2021)

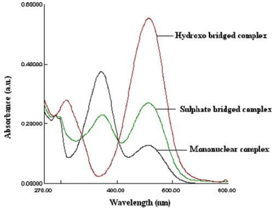


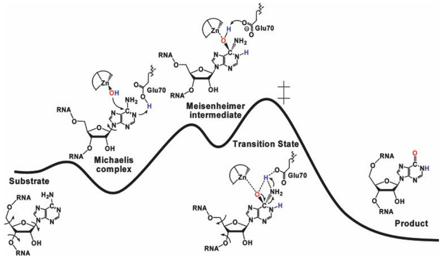
arXiv:2106.03997 [quant-ph]

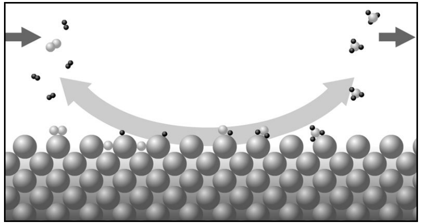
# Simulating Chemistry



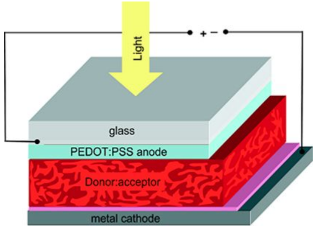
**Understanding**

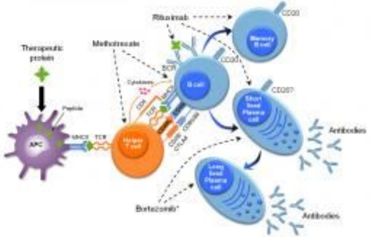






**Control**





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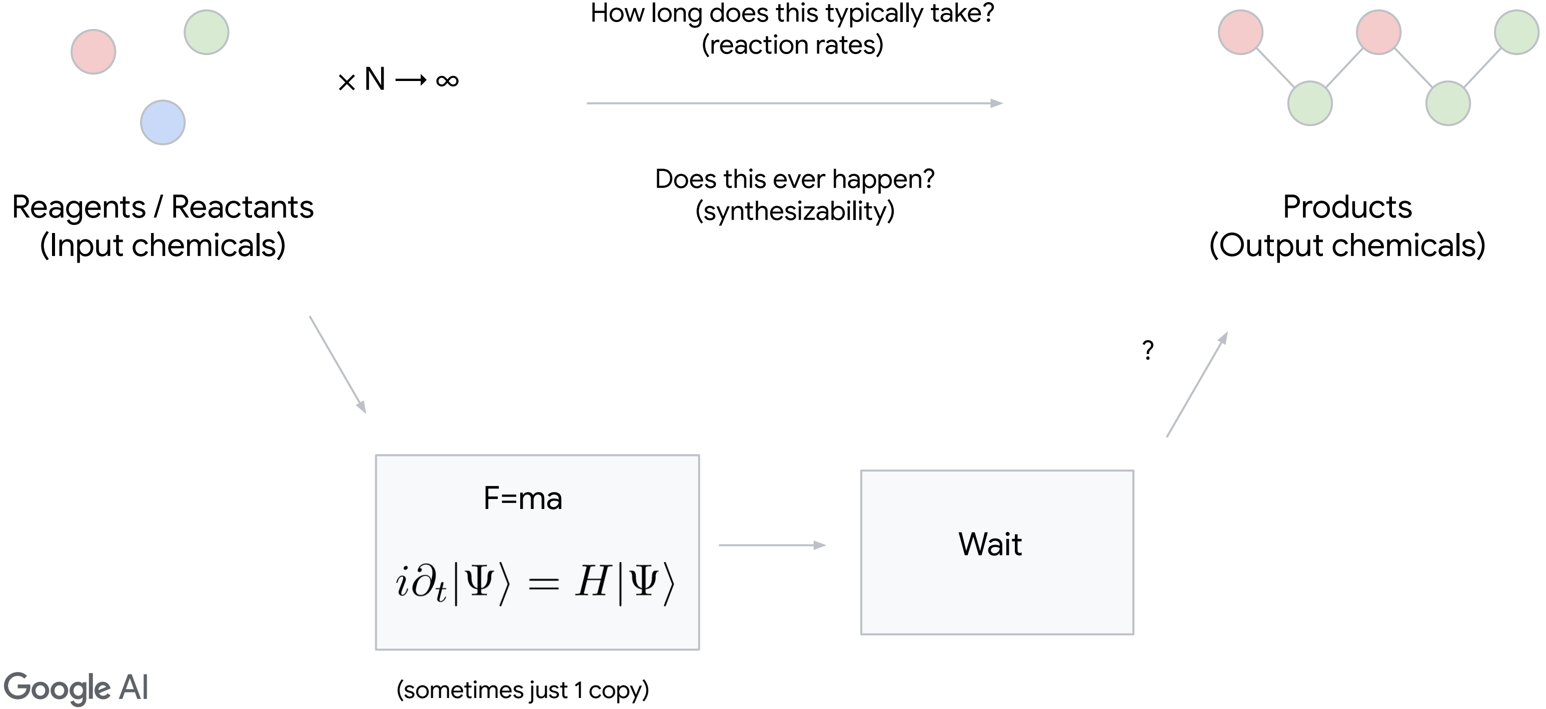
Quantum

# Simulating chemistry without theoretical chemistry



× N → ∞

How long does this typically take?
(reaction rates)

Does this ever happen?
(synthesizability)

Reagents / Reactants
(Input chemicals)

Products
(Output chemicals)

F=ma

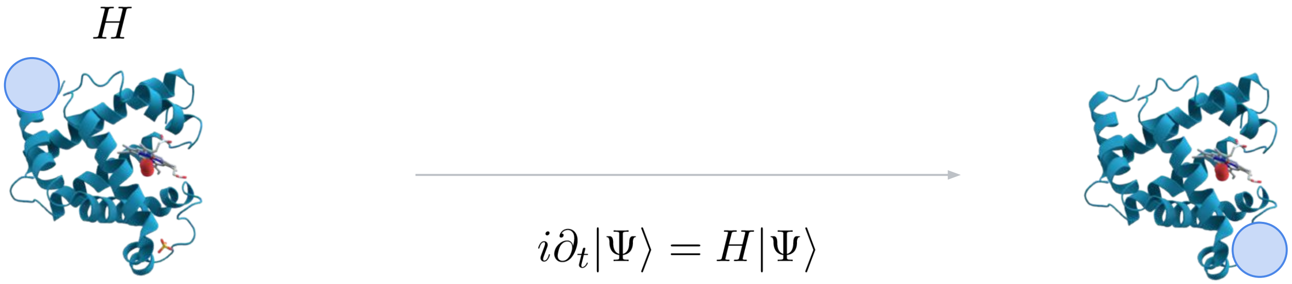
$$i\partial_t|\Psi\rangle = H|\Psi\rangle$$

(sometimes just 1 copy)

Wait

?

# Quantum simulation and fast-forwarding



$$i\partial_t|\Psi\rangle = H|\Psi\rangle$$

Rapidly developing field - numerically exact evolutions in time sublinear in # basis functions*!

Exact classical competition is a hard exponential wall - entanglement truncation challenging

Even a quantum computer has limits - No Fast-Forwarding Theorem**

$$[\text{Simulation time}] > c \times [\text{Physical Time}]$$

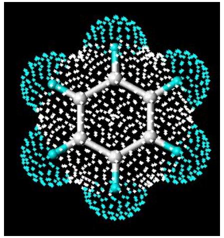
$$c \gg 1$$

Chemical reaction times ~ hours?

Google AI Quantum

* Babbush, Berry, McClean, Neven, *NPJ Quantum Information* Vol 5 No. 92 (2019)
** Berry, Ahokas, Cleve, Sanders, *Communications in Mathematical Physics* 270, 359 (2007)

# Electronic structure's favorite tagline



$$\mathcal{H} \left|\psi\right\rangle = E \left|\psi\right\rangle$$

"The underlying physical laws necessary for the mathematical theory of a large part of physics and **the whole of chemistry** are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble."

-Paul Dirac

# Why is this a useful perspective?

$$i\partial_t|\Psi\rangle = H|\Psi\rangle$$

$$\mathcal{H}\,|\psi\rangle = E\,|\psi\rangle$$

Dynamics - BQP

Stationary(often ground) States - QMA

Thermodynamics is predictive of longer time behavior

t ⟶ ∞ is predictive of t >> 1, I actually care about

Limited to physical time scales

+

Makes predictions on time scales much longer than physical

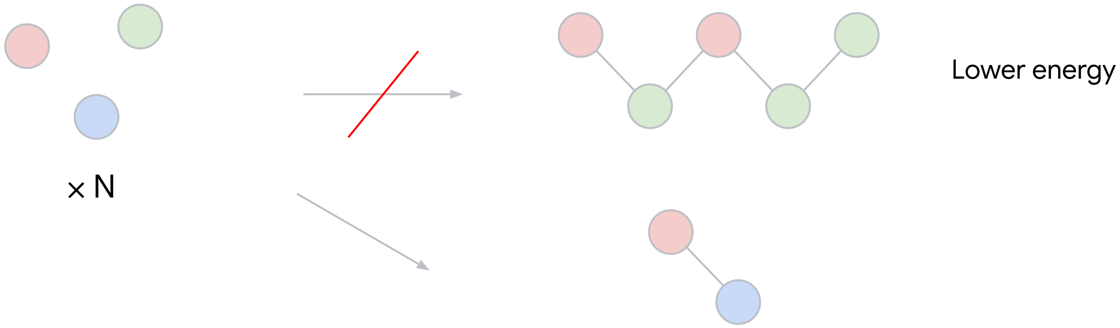
Thermo can't be better for all systems (physical systems special? e.g. overlap assumptions in QPE)
Worst cases are like state enumeration / diagonalization (is this a useful perspective?)

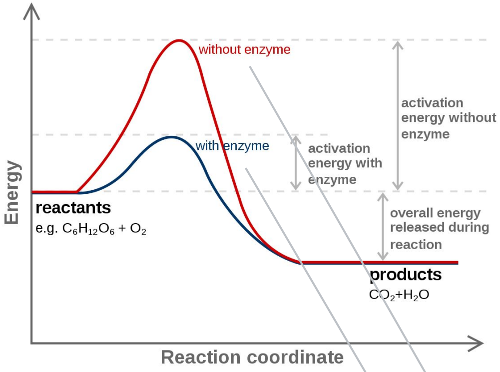
# Kinetics, Thermodynamics, and Nuclear Soups

$$\mathcal{H}\,|\psi\rangle = E\,|\psi\rangle$$

t ⟶ ∞ is predictive of t >> 1

Says nothing on its own about rates...



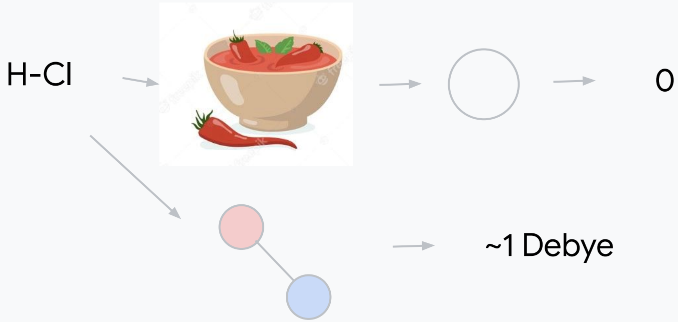


$$\mathcal{H}\,|\psi\rangle = E\,|\psi\rangle$$

+ Born-Oppenheimer (classical nuclei)

COM modes etc.

Keeping it real goes wrong - Dipole moment



Thermo of transition states
+ classical information

# The predictive power of (free) energies & reduced models

Can all physically interesting questions be answered by some reduced model?

**Recent***

- Does a system thermalize?
- Does a system have an electronic gap?
- Will molecule X ever form from constituents Y?

→ **Undecidable**

**Physical undecidability**** - as the system evolves in time, there are sudden, qualitative changes that cannot be predicted in any way except evolving forward in time and seeing if it happens, and no answer in finite time can indicate if it will never happen (for all systems).

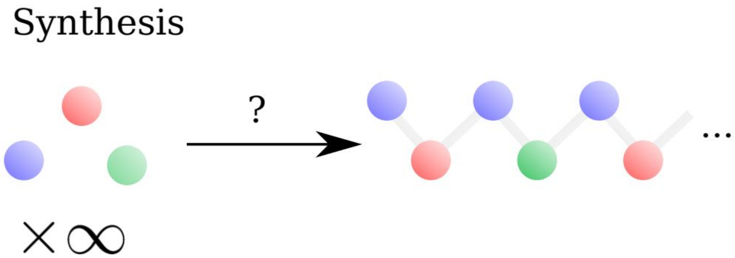
---

* Infinite systems specified by unit and translational invariance
Cubitt, Perez-Garcia, Wolf Nature Vol. 528, pg 207–211 (2015)
Shiraishi, Matsumoto arXiv:2012.13889 (2020)

** Unpredictability and undecidability in dynamical systems
Moore, *Phys. Rev. Lett.* 64, 2354 (1990)

# All models are wrong, but some are useful

-George Box



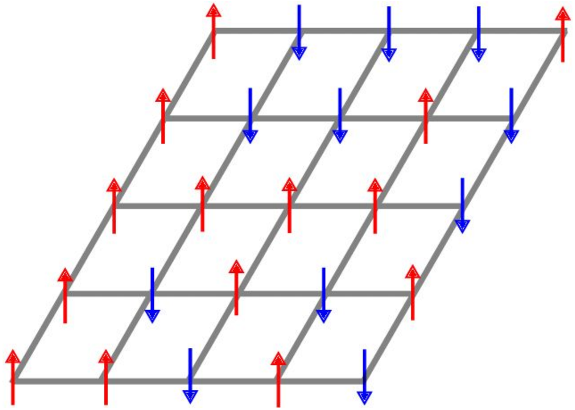
Universe suspected finite...

Real systems have

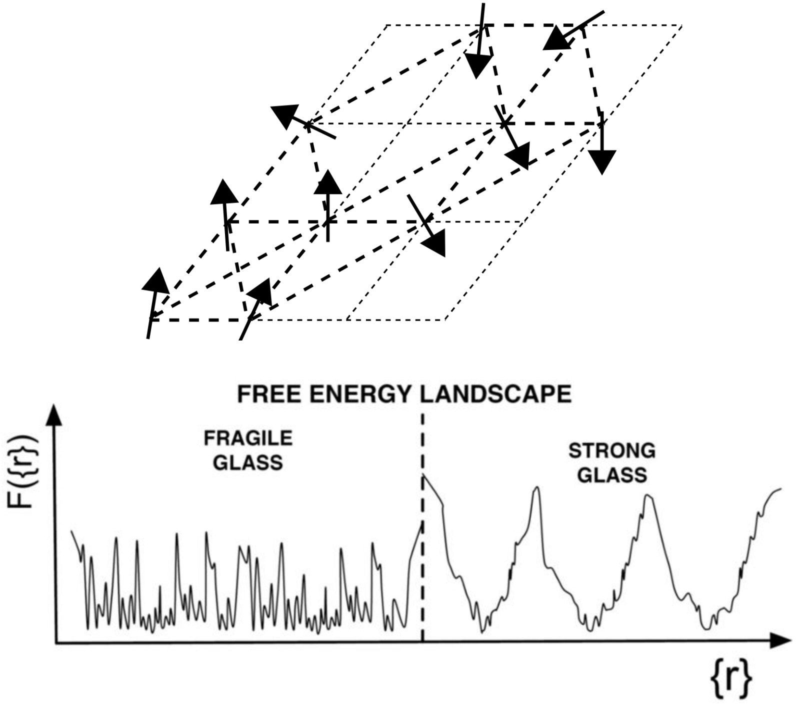
- Side reactions
- Kinetic transport (it's gone!)
- Autocatalytic chaos (Kauffman)

# Where have we seen hints of this in physics

Chemistry is often finite, but in physics we loooove taking N → ∞

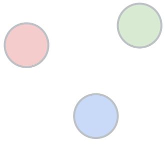


Spontaneous symmetry breaking

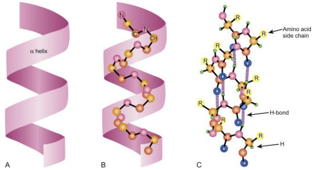


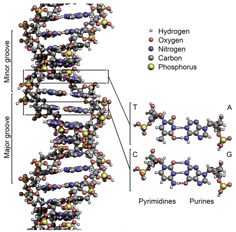
Gibbs measure

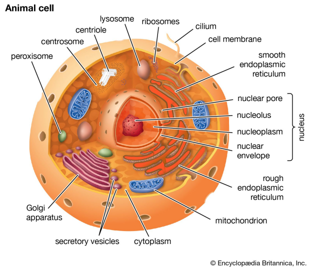
# Emergent life



$\times N \to \infty$







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**Physical undecidability**** - as the system evolves in time, there are sudden, qualitative changes that cannot be predicted in any way except evolving forward in time and seeing if it happens, and no answer in finite time can indicate if it will never happen (for all systems).

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**Undecidability** formally broken by **advice** in some cases

**Data** is a restricted form of **advice**

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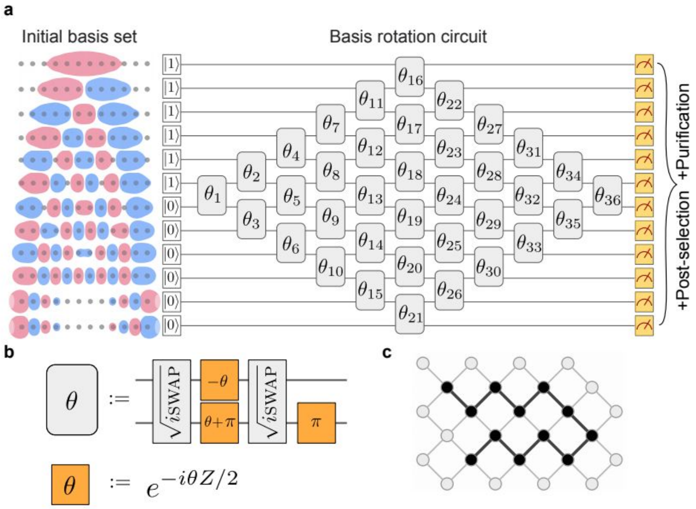
Cubitt, Perez-Garcia, Wolf Nature Vol. 528, pg 207–211 (2015)
Shiraishi, Matsumoto arXiv:2012.13889 (2020)

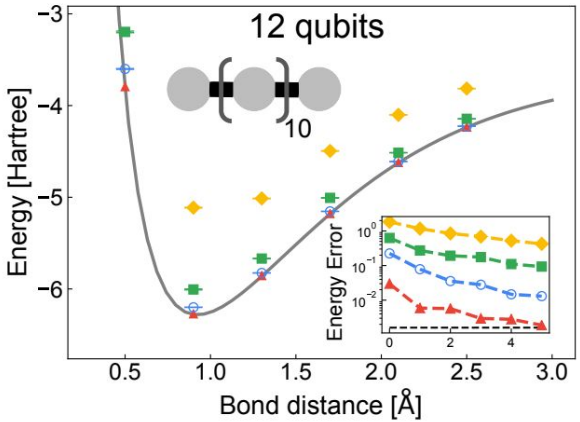
** Unpredictability and undecidability in dynamical systems
Moore, *Phys. Rev. Lett.* 64, 2354 (1990)

# Taking a chemical detour to the power of data



12 qubits
78 two-qubit gates
114 single qubit gates

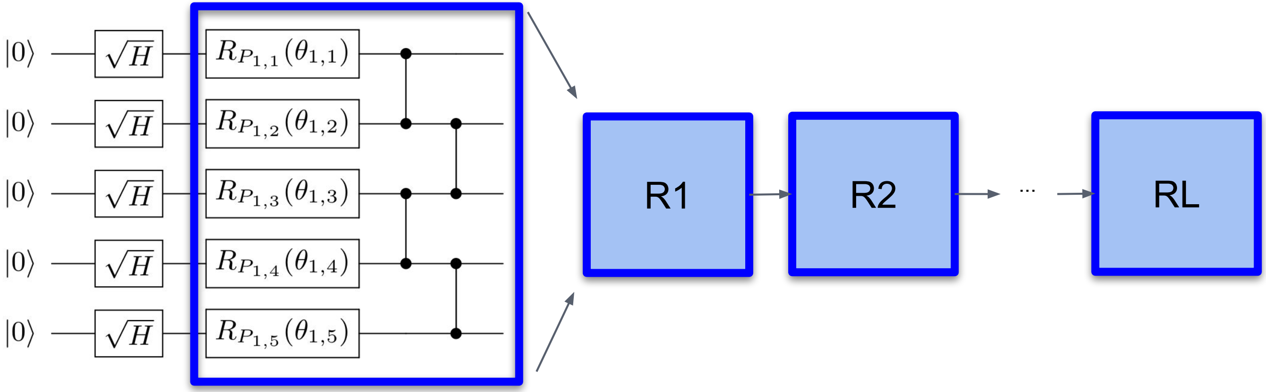
(Exponential space redundancy)

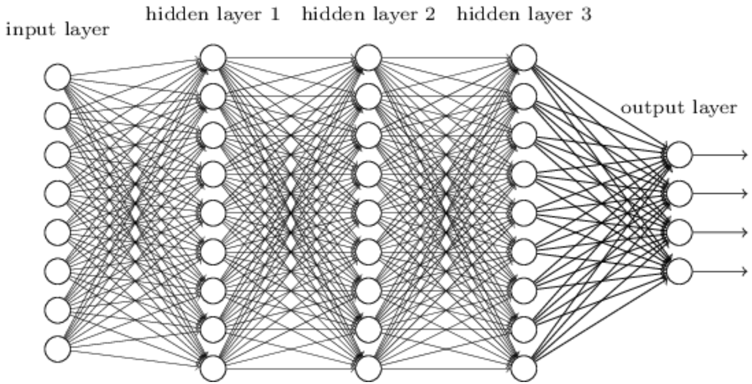


Google AI Quantum

“Hartree-Fock on a superconducting qubit quantum computer”, Google Quantum AI, **Science** 369 (6507), 1084-1089, (2020)

# Quantum circuits as “neural networks”(?)

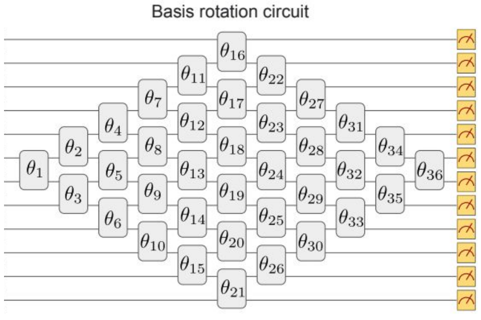


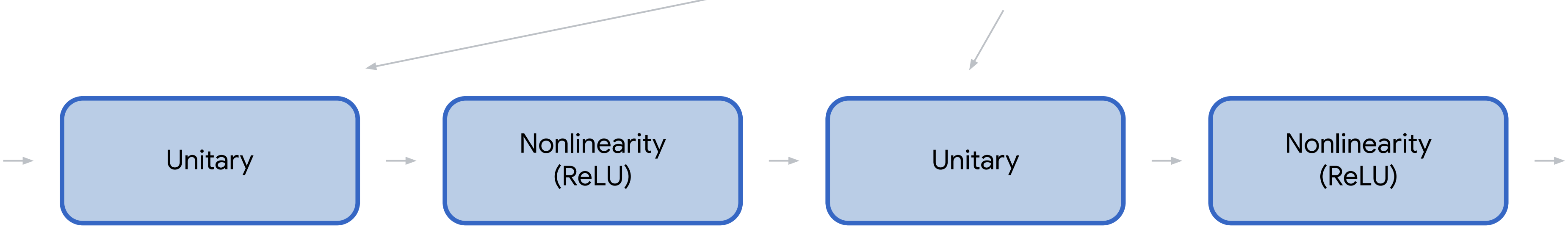


$$\min_{\vec{\theta}}\langle\Psi(\vec{\theta})|H|\Psi(\vec{\theta})\rangle$$

# An enticing connection with the classical community

Efficient unitary neural networks (EUNN)*





Unitary

Nonlinearity
(ReLU)

Unitary

Nonlinearity
(ReLU)

---

* Arjovsky, Shah, Bengio, *Proc. 33rd ICML, PMLR* 48:1120-1128 (2016)

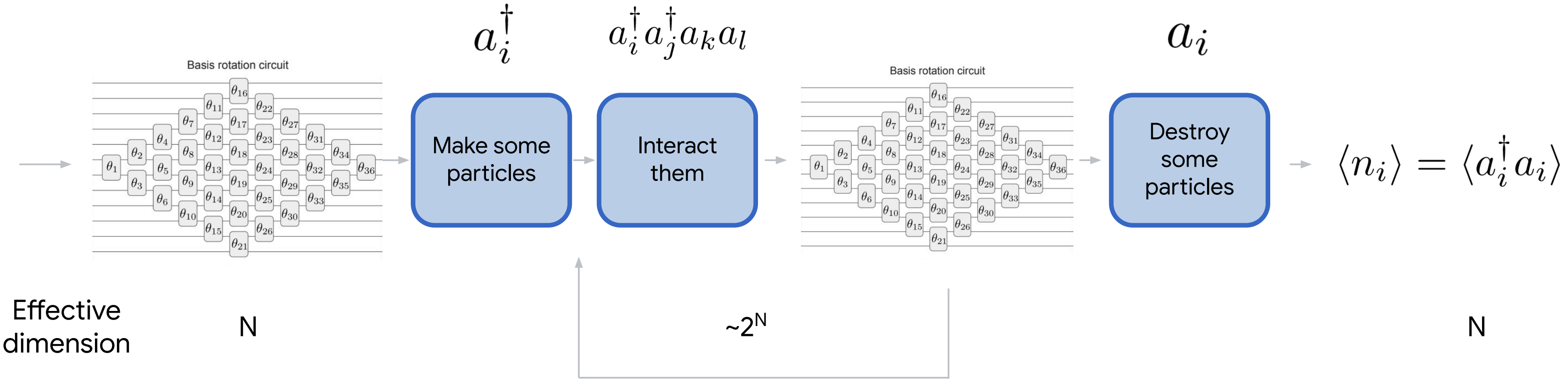
* Jing, Shen, Dubcek, Peurifoy, Skirlo, LeCun, Tegmark, Soljačić ; *Proc. 34th ICML, PMLR* 70:1733-1741, (2017)

# Boosting the power with quantum!

Classical case takes N inputs has N outputs

A natural choice $\langle n_i \rangle = \langle a_i^\dagger a_i \rangle$ with single particle initialized across N modes

Beef up the power with some new generators



$a_i^\dagger$ Make some particles

$a_i^\dagger a_j^\dagger a_k a_l$ Interact them

$a_i$ Destroy some particles

$\langle n_i \rangle = \langle a_i^\dagger a_i \rangle$

Effective dimension N ~$2^N$ N

Hard circuit!

Google AI Quantum

# Let our model have a little data as a treat

Some data $\{(x_i, y_i)\}_i$

$$|x_i\rangle = \sum_{k=1}^{p} x_i^k |k\rangle$$

$$y_i = f(x_i) = \langle x_i | U_{\mathrm{QNN}}^\dagger O U_{\mathrm{QNN}} | x_i \rangle$$

Arbitrary length quantum circuit

Hermitian operator

Direct simulation at least as hard as BQP, must be a powerful function of $x_i$ !

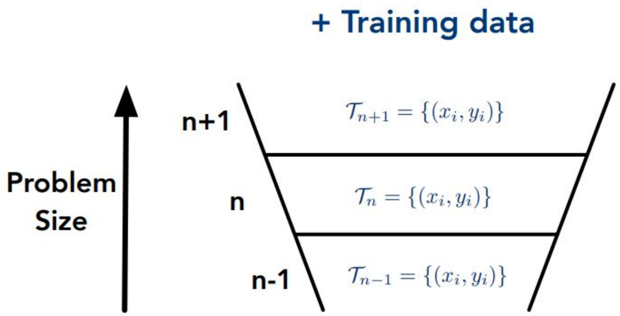
$$f(x_i) = \left( \sum_{k=1}^{p} x_i^{k*} \langle k| \right) U_{\mathrm{QNN}}^\dagger O U_{\mathrm{QNN}} \left( \sum_{l=1}^{p} x_i^l |l\rangle \right)$$
$$= \sum_{k=1}^{p} \sum_{l=1}^{p} B_{kl} x_i^{k*} x_i^l,$$

At most quadratic function on entries of $x_i$ with p$^2$ coefficients!

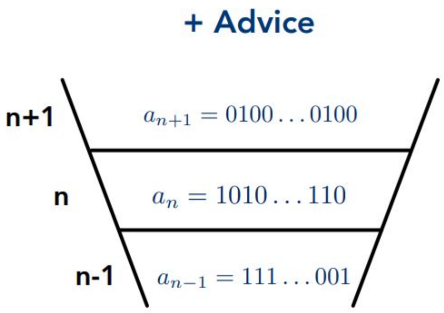
**No data** - hard quantum circuit
**With data** - Almost trivial learning task!

(More generally, need ~$\left(\frac{p^2}{\epsilon^2}\right)$ data pts)

# The power of data in quantum machine learning*

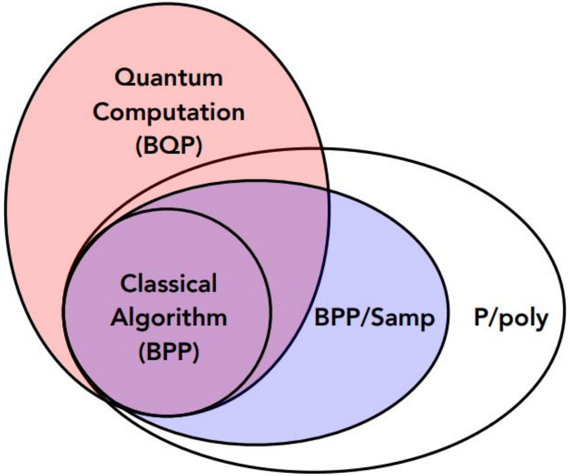


**Classical ML algorithm with data (BPP/samp)**



**P/poly**

$\mathrm{BPP} \subsetneq \mathrm{P/poly}$



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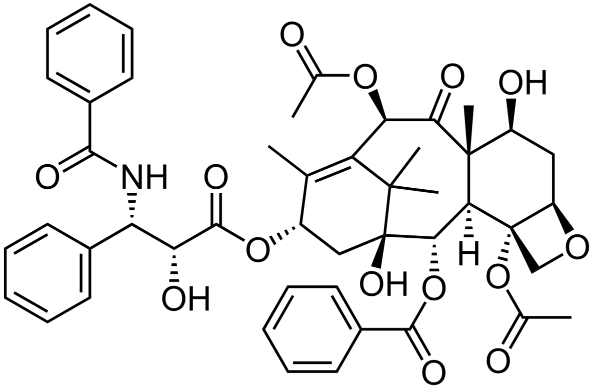
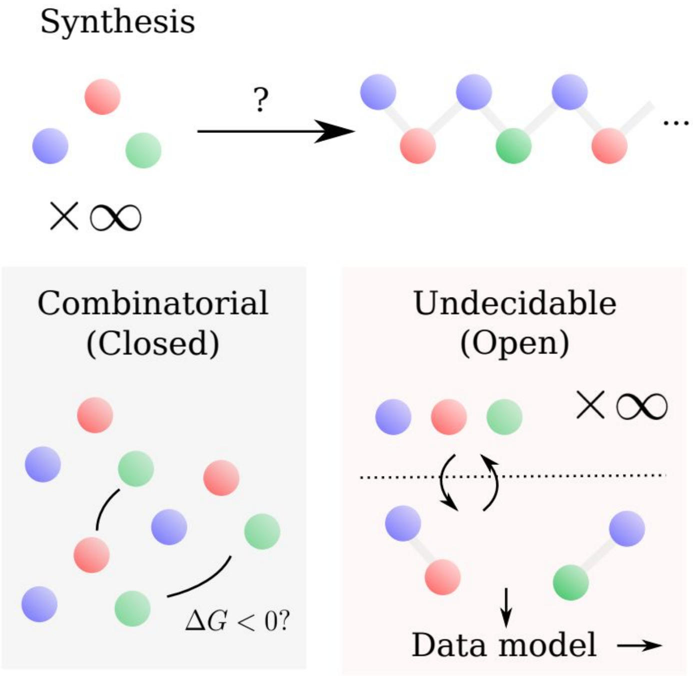
* Hsin-Yuan (Robert) Huang, Michael Broughton, Masoud Mohseni, Ryan Babbush, Sergio Boixo, Hartmut Neven, **Jarrod R. McClean** "Power of data in quantum machine learning" *Nature Communications* 12, No. 2631 (2021)

# Taking another look at chemical synthesis

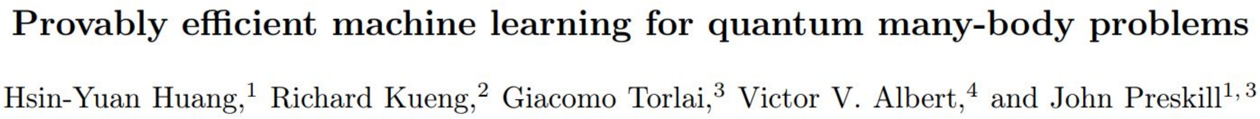
Natural product synthesis



Huge open question - synthesizability
(Screening can't help you if you can't make it)



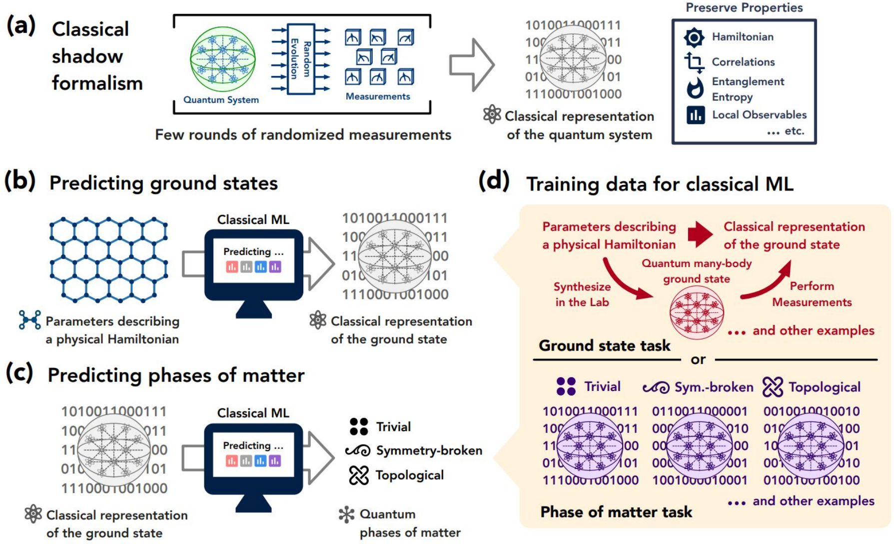
# Learning gets another leg up



Provably efficient machine learning for quantum many-body problems

Hsin-Yuan Huang,[1] Richard Kueng,[2] Giacomo Torlai,[3] Victor V. Albert,[4] and John Preskill[1,3]

arXiv:2106.12627 (2021)



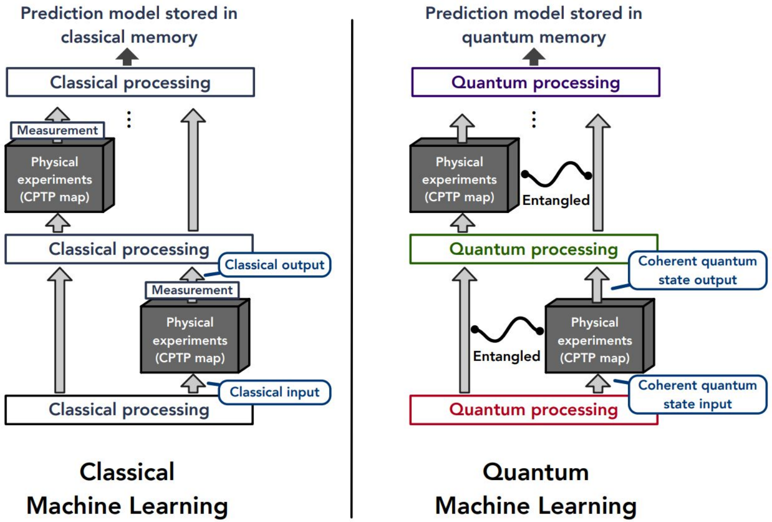
Chemistry is a little more discrete in properties, do these results naturally apply there?

Is the fate of quantum computers in chemistry to provide training data for classical models?

# So what’s left for a quantum computer?

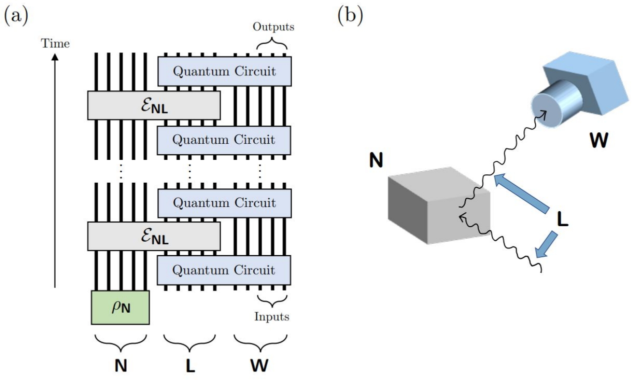
**Information-theoretic bounds on quantum advantage in machine learning**

Hsin-Yuan Huang,[1,2] Richard Kueng,[3] and John Preskill[1,2,4,5]



**Quantum Algorithmic Measurement**

Dorit Aharonov[1,a], Jordan Cotler[2,3,b], Xiao-Liang Qi[3,c]



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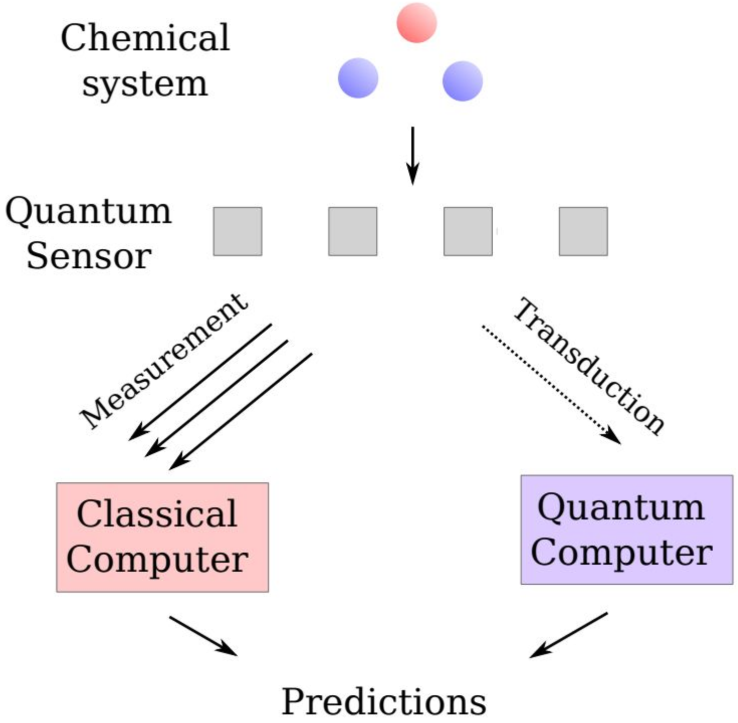
# Imagining a future with (multi-qubit) quantum data

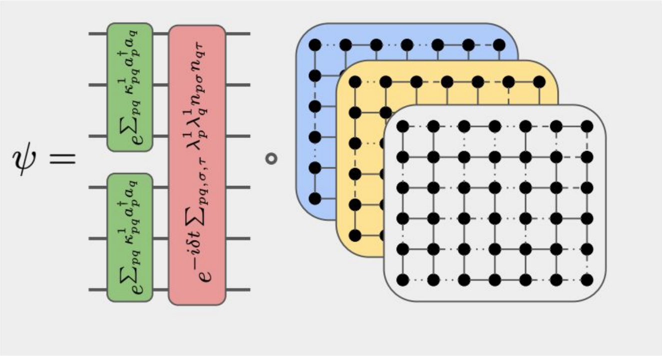


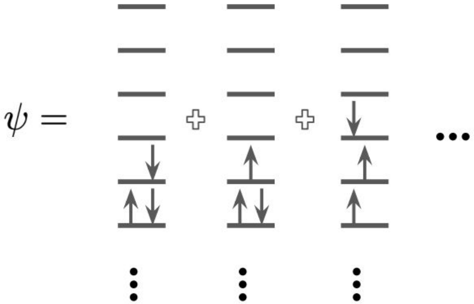
Flips the narrative on quantum sensing, but where do you get good multi-qubit data about a molecule?

NMR is popular, but close to DQC1

Spatially resolved diamond sensors, zero field?

# Some untapped technology in quantum computing





Clifford states can express some entanglement structures efficiently, easy to rotate orbitals after (at least as good as HF)

Relation to graph states makes for interesting connection to chemical bonds.

Any relationship between stabilizer states and quasi-degeneracy in metal catalyst clusters?

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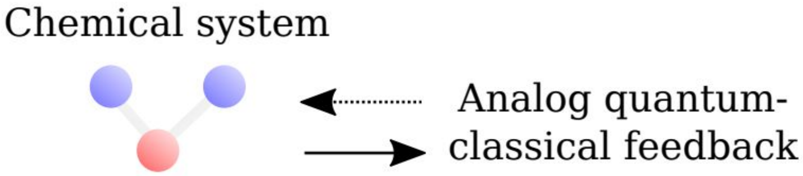
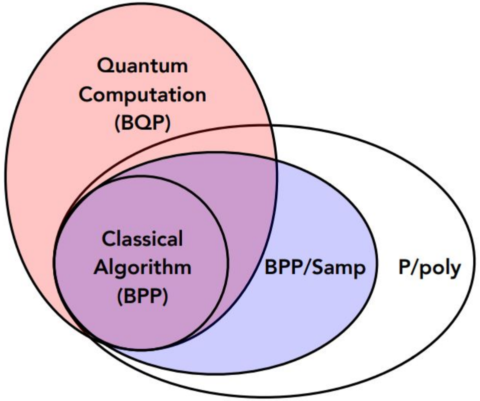
# Some untapped technology in quantum computing



Chemical system

Analog quantum-classical feedback

# Taking another computational look at chemistry



Many problems in design, synthesis, and biology “feel” like undecidable chemistry problems - what can we say about the way data from nature helps us?

Data from quantum computers can lift classical machine learning above its direct simulation competition - what can quantum simulation data do for chemistry?

Is the fate of quantum computers largely to provide data to classical machine learning algorithms?

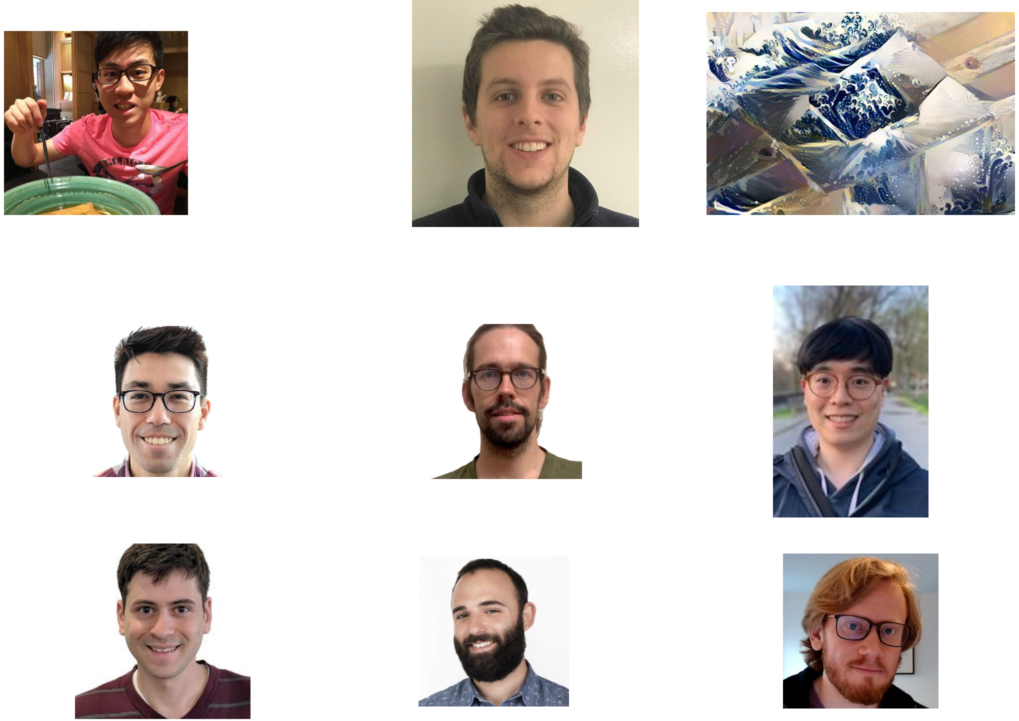
Perhaps not, but how can chemistry utilize this for practical purposes?

Are there some more untapped tools from quantum computing that can help chemistry before a full QC?

Google AI Quantum

**McClean**, Rubin, Lee, Harrigan, O'Brien, Babbush, Huggins, Huang
“What the foundations of quantum computer science teach us about chemistry” arXiv:2106.03997 (2021)

# Acknowledgements



Quantum AI

Google AI
Quantum

**McClean**, Rubin, Lee, Harrigan, O'Brien, Babbush, Huggins, Huang
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