

# Chemistry Meets Quantum Computing: A New Era of Simulation and Study

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SmallTalks [about Nanoscience]

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Chemistry and Chemical Engineering,  
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Gothenburg, June 1, 2023



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# Outline

- **Part I:** Motivation – take-home messages
  - Computational chemistry
  - The case for quantum computing
- **Part II:** Motivation: Quantum chemistry
  - Reducing hardware requirements with the **transcorrelated** method
  - Applications: Reducing the number of qubits for chemistry
  - Conclusions and outlook

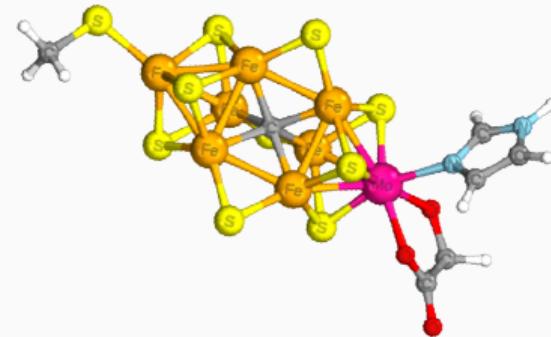
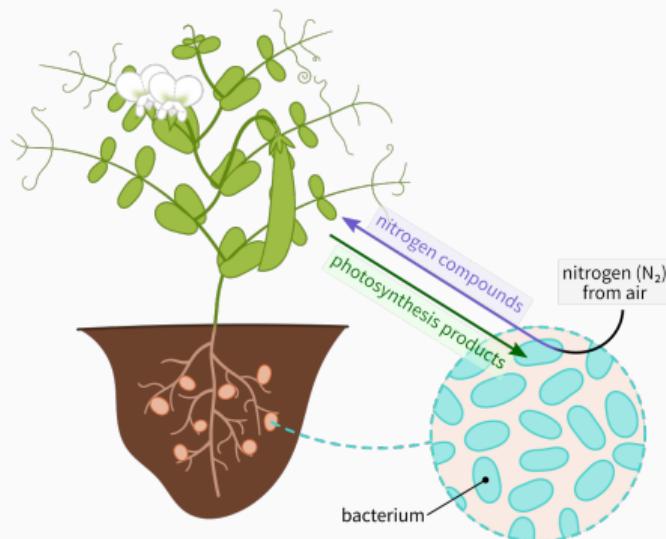
## Learning goals:

- What is **computational chemistry**?
- Why is it worthwhile?
- Why do we need computers for chemistry?
- Why and how could **quantum computing** help?

Why is it worthwhile?  
Surprisingly small molecules responsible for fascinating  
physical and chemical effects

# Nitrogen fixation

Conversion of molecular nitrogen,  $\text{N}_2$ , to ammonia,  $\text{NH}_3$ ,  $\rightarrow$  important for fertilizers  
Haber-Bosch process: **1-2% of global energy consumption**, huge  $\text{CO}_2$  emission

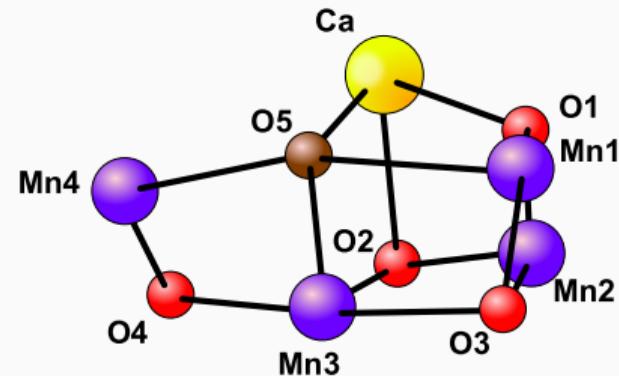
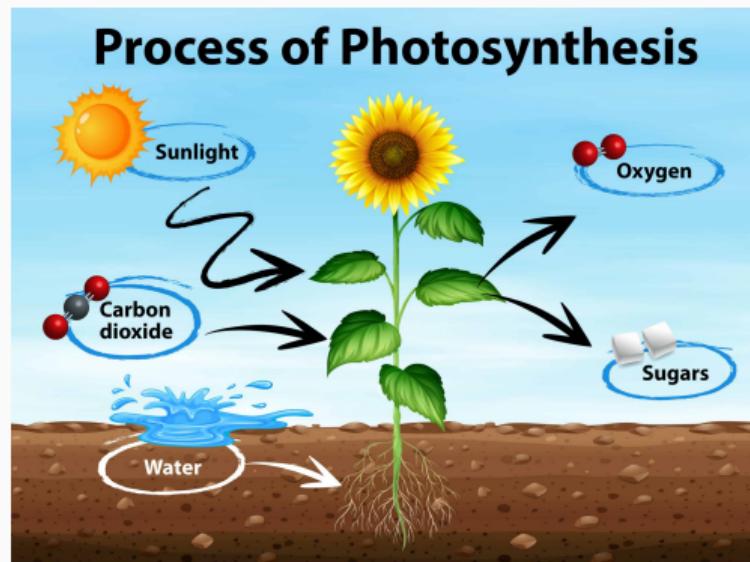


Iron-sulfur clusters

Artificial nitrogen fixation for cheaper and cleaner ammonia production for fertilizers

# Photosynthesis

Conversion of solar energy into chemical energy



Manganese-Calcium-Oxygen Clusters

Artificial photosynthesis for carbon capture and hydrogen and oxygen for fuel cells

# Scientific method

- We want a **theoretical understanding** of these phenomena and explain the physical and chemical behavior of these systems
- We want to derive a mathematical description/model
- We want to test the validity of these models and compare with experiments
- We want to predict properties of new materials based on our models

✓ Mathematical description possible! Schrödinger equation

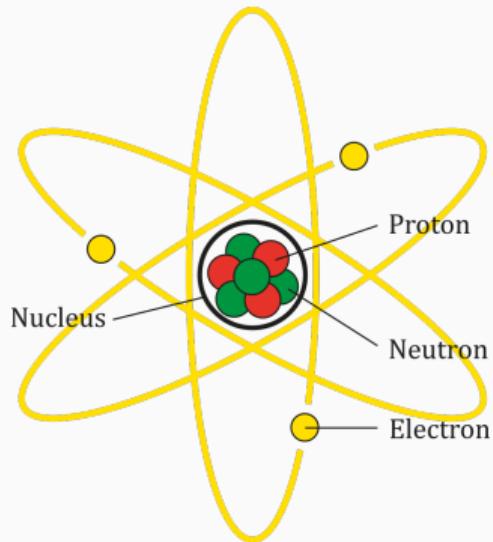
✗ Too complex and impossible to solve exactly/analytically! Need computers to approximately solve the equations! → computational chemistry.

**~30% of high-performance computing** used for chemistry-related problems

# Computational chemistry

# How do we describe these phenomena?

## Atoms – the building blocks of nature

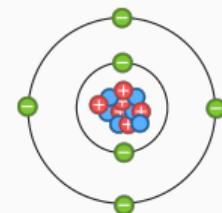
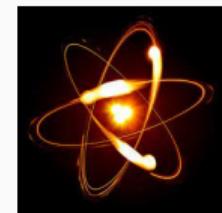


- If we knew the **position** and **motion** of all electrons and nuclei **at all times** we could describe the systems behavior and properties.
- Due to the size of the particles → **quantum effects**. We **can not** know the position and motion/momentum exactly at the same time. Heisenberg uncertainty relation/particle-wave duality.
- We can use **quantum mechanics** and write down an equation to describe the behavior of the system!

# Ingredients – what do we need?

We want an equation to describe the behavior of our system. How it evolves with time.

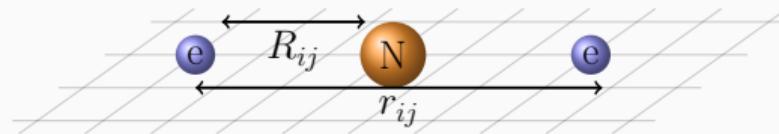
1. Nuclei **much heavier** than electrons (1000 fold) → assume nuclei fixed!
2. Motion of electrons → **kinetic energy**
3. Negative charged electrons attracted to positive charged nuclei
4. Negative charged electrons repel each other! ⚡  
→ movement and position of all electrons depend on each other! It is a **correlated problem**!



# Schrödinger equation

Ingredients to describe the behavior of the electrons of our system

$$\hat{H} = T_{\text{Kinetic}}(\mathbf{r}) + V_{\text{Attraction}}(\mathbf{r}, \mathbf{R}) + V_{\text{Repulsion}}(\mathbf{r}, \mathbf{r}')$$



Current state of all the electrons at time  $t$  described by the so-called wavefunction:

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_n; t)$$

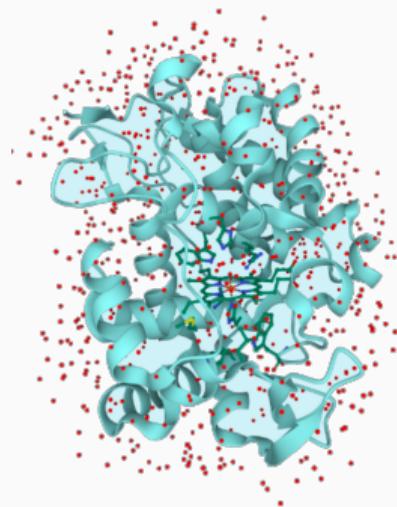
Schrödinger equation describes the change of the system with time  $t$ :

$$i \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = \hat{H} \Psi(\mathbf{r}, t)$$

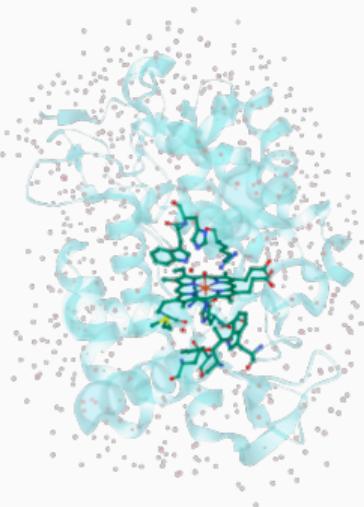
# The case for quantum computing

# Problem: Nature is very complex

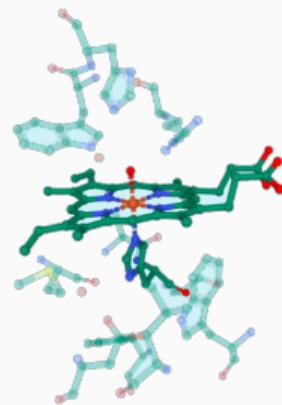
Cytochrome c: enzyme that eliminates toxic radicals ( $O_2^-$ ,  $H_2O_2$ ) produced by cells



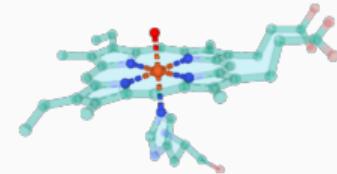
Cytochrome c in solution



Binding site



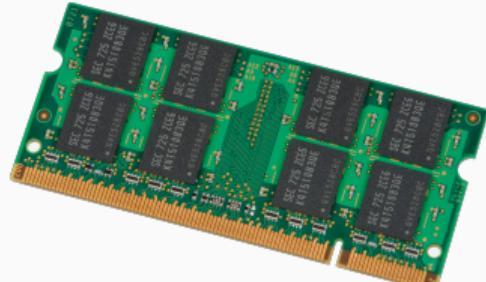
Heme group



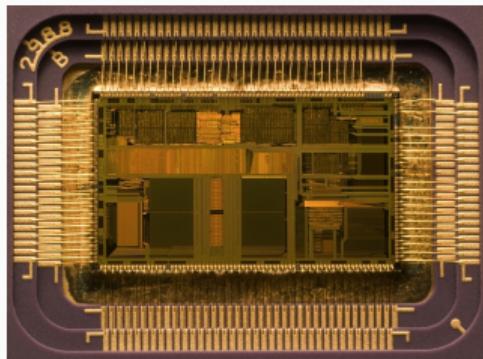
Iron cluster

Exact solution scales **exponential!**  $> 20$  electrons  $>\sim 100$  GB information!  
→ can not even store wavefunction in computer memory

# How is information stored and handled on a computer?



RAM

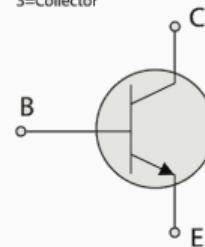


CPU

- Modern electronics are based on **transistors**, which can be seen as electronic switches that are either “off” or “on”; **0** or **1**.  
→ A logical state with **two** possible values: **a bit**.
- These **bits** of information can either store data (RAM/harddrive) or control operations (CPU)

## Transistor

2N  
2222F  
7590  
1 2 3

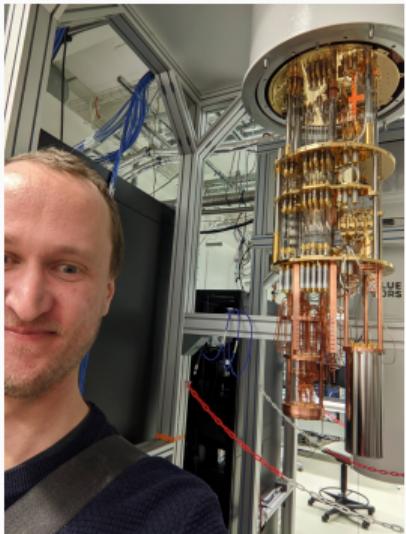


1=Emitter  
2=Base  
3=Collector

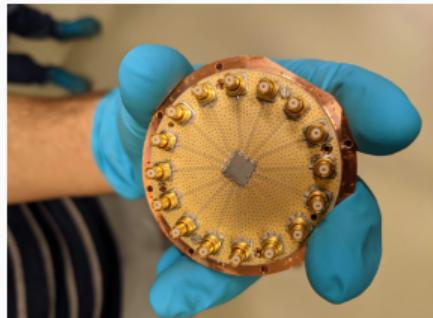
0011  
0101  
0110  
1001  
1010  
1100  
...

# of states

# Quantum Bits – Qubits

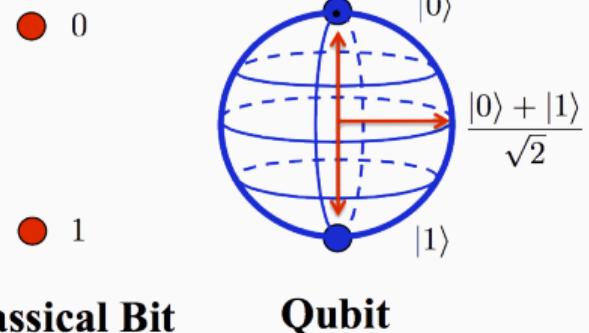


@ Chalmers

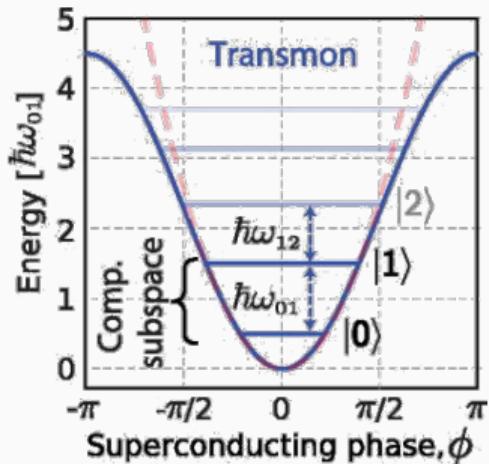


3 qubit device @Chalmers

Qubits can be both  $|0\rangle$  and  $|1\rangle$ .



Qubits rely on quantum effects → very fragile, easily influenced by environmental effects/noise. Need to isolate and cool them close to absolute zero! Only few of them...



# Quantum Computing

Quantum bits (qubits) can be in a **superposition** of both  $|0\rangle$  and  $|1\rangle$

Bringing together **two** qubits:

$$|\Psi\rangle = \overbrace{(|0\rangle + |1\rangle)}^{\text{qubit 1}} \otimes \overbrace{(|0\rangle + |1\rangle)}^{\text{qubit 2}} = |00\rangle + |01\rangle + |10\rangle + |11\rangle \quad 4 \text{ states}$$

**Three** qubits:

$$\begin{aligned} |\Psi\rangle &= \overbrace{(|0\rangle + |1\rangle)}^{\text{qubit 1}} \otimes \overbrace{(|0\rangle + |1\rangle)}^{\text{qubit 2}} \otimes \overbrace{(|0\rangle + |1\rangle)}^{\text{qubit 3}} \\ &= |000\rangle + |001\rangle + |010\rangle + |100\rangle + |011\rangle + |101\rangle + |110\rangle + |111\rangle \quad 8 \text{ states} \end{aligned}$$

$n$  qubits can encode exponentially many ( $2^n$ ) states.

→ Need new **quantum algorithms** to use this potential advantage!

## Part II

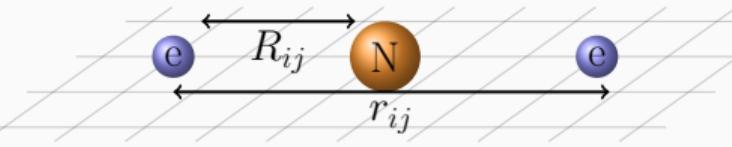
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# *Ab Initio* Quantum Chemistry – Electronic Structure Theory

All necessary information of a quantum system contained in electronic molecular Hamiltonian (Born-Oppenheimer approx. and atomic units)

$$\hat{H} = \underbrace{-\frac{1}{2} \sum_i \nabla_{\mathbf{r}_i}^2}_{\text{kinetic energy of } e^-} + \underbrace{\frac{1}{2} \sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}}_{e^- - e^- \text{ repulsion}} - \underbrace{\sum_{I,j} \frac{Z_I}{|\mathbf{R}_I - \mathbf{r}_j|}}_{\text{Potential}}$$



**Electronic properties:** Ground- and low-lying excited state properties, energy differences, polarization, response functions, ...

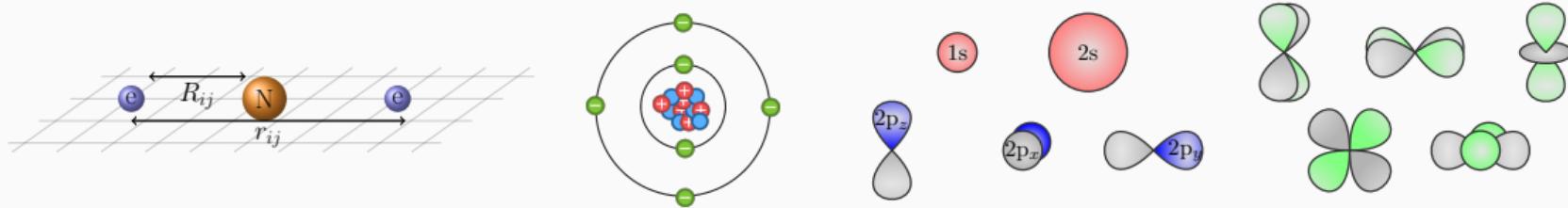
**Target:** High / “chemical accuracy” to ensure predictability, interpretability and comparison with experimental results

**Task:** Solve the Schrödinger equation derived from first principles:

$$\hat{H} |\Psi(\mathbf{r}_1, \dots, \mathbf{r}_n)\rangle = E_0 |\Psi(\mathbf{r}_1, \dots, \mathbf{r}_n)\rangle$$

# *Ab Initio* Quantum Chemistry – Electronic Structure Theory

We have to choose a numerical **basis/orbitals** to perform our calculations in! In comp. chemistry: orbitals are smooth, “atomic-like” orbitals (for each atom):

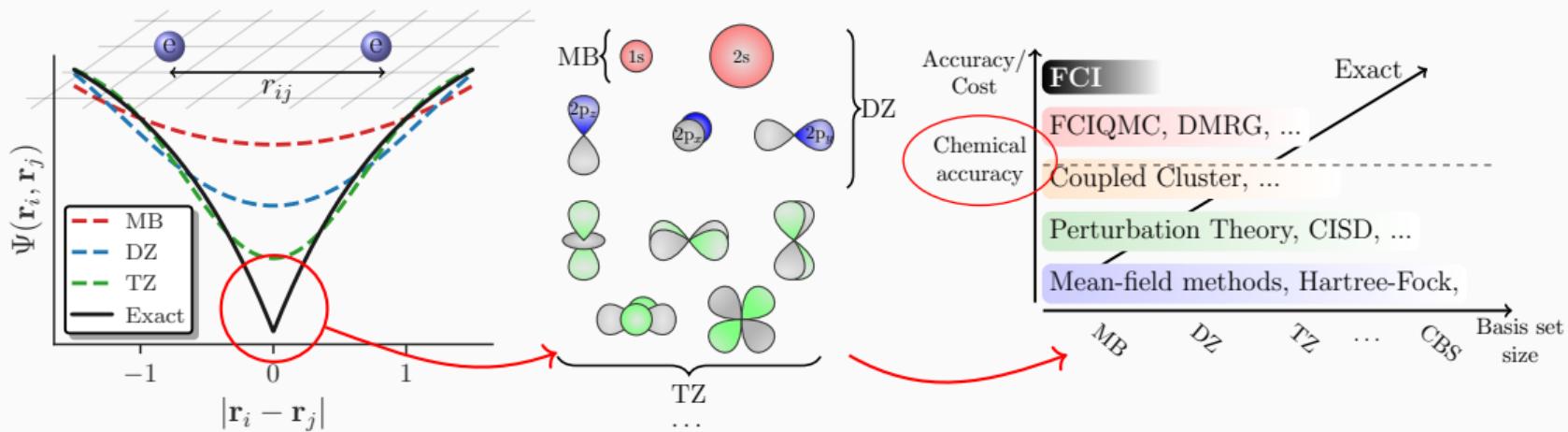


For accurate results we need **dozens to hundreds** of orbitals per atom!

# Problems for accurate description: Cusp condition

**Cusp condition:** Singularity of Coulomb potential,  $\frac{1}{r_{ij}}$ , for  $r_{ij} = 0$   
→ sharp cusp of exact wavefunction  $\Psi(\{\mathbf{r}\})$  at electron coalescence ( $r_{ij} = 0$ )

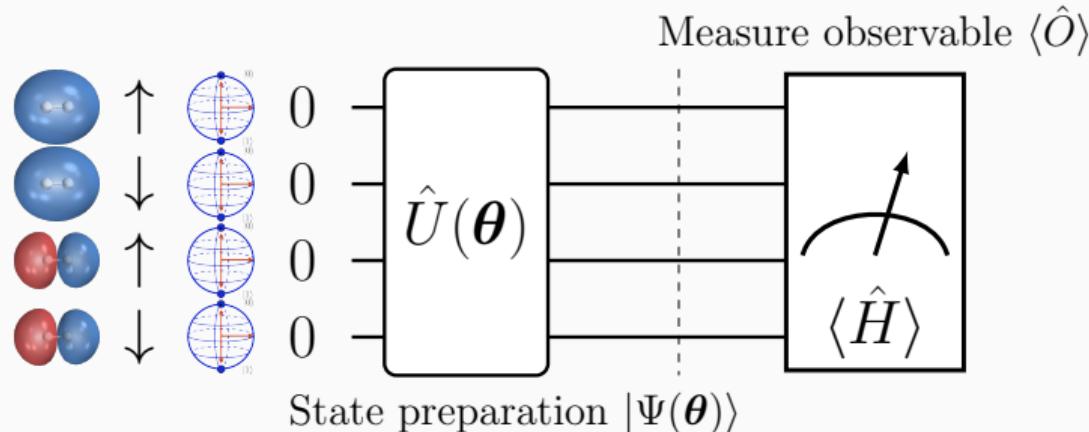
$$\hat{H} = - \sum_{I,j} \frac{Z_I}{|\mathbf{R}_I - \mathbf{r}_j|} - \frac{1}{2} \sum_i \nabla_{\mathbf{r}_i}^2 + \frac{1}{2} \sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}, \quad \hat{H} |\Psi(\{\mathbf{r}\})\rangle = E_0 |\Psi(\{\mathbf{r}\})\rangle$$



# Digital Quantum Simulation/Computation

1. Map fermionic Hamiltonian onto quantum hardware/qubits
2. Use quantum algorithms to solve the problem at hand

**Circuit model:** Lines/wires represent qubits encoding the **occupation** (0-1) of the associated spin-orbital. Similar to classical circuits (AND, OR, ...) we can act with **operations/gates** on one or more qubits. For quantum computers have to be **reversible/unitary operations**  $\hat{U}(\theta)$   $\rightarrow$  prepare **entangled** target state  $|\Psi(\theta)\rangle$ .



# Development Roadmap

Executed by IBM   
On target 

IBM Quantum

	2019 	2020 	2021 	2022 	2023	2024	2025	2026+
Model Developers	Run quantum circuits on the IBM cloud	Demonstrate and prototype quantum algorithms and applications	Run quantum programs 100x faster with Qiskit Runtime	Bring dynamic circuits to Qiskit Runtime to unlock more computations	Enhancing applications with elastic computing and parallelization of Qiskit Runtime	Improve accuracy of Qiskit Runtime with scalable error mitigation	Scale quantum applications with circuit knitting toolbox controlling Qiskit Runtime	Increase accuracy and speed of quantum workflows with integration of error correction into Qiskit Runtime
Algorithm Developers					Prototype quantum software applications  → Quantum software applications Machine learning   Natural science   Optimization			
Kernel Developers	Circuits 	Qiskit Runtime 	Dynamic circuits 	Threaded primitives 	Error suppression and mitigation	Intelligent orchestration	Circuit Knitting Toolbox	Circuit libraries
System Modularity	Falcon 27 qubits 	Hummingbird 65 qubits 	Eagle 127 qubits 	Osprey 433 qubits 	Condor 1,121 qubits 	Flamingo 1,386+ qubits 	Kookaburra 4,158+ qubits 	Scaling to 10K-100K qubits with classical and quantum communication

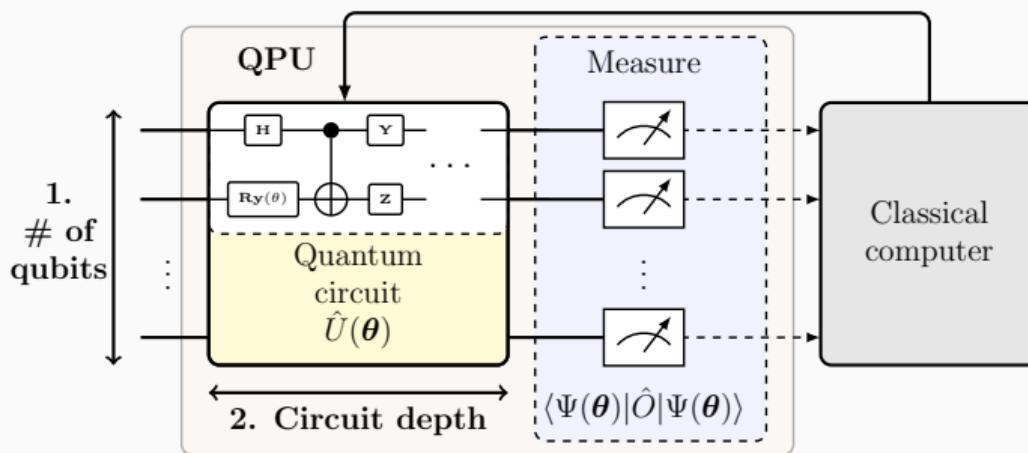
Chalmers next-gen chip: 25 qubits, compared to **billions** of transistors in current CPUs! Only small problems currently tractable on quantum devices

# Overview: Quantum Chemistry on Quantum Computers

Current quantum hardware has many problems still: **noise, decoherence and limited number of qubits** – noisy intermediate-scale quantum (NISQ) era

## Hybrid quantum-classical approach:

Update parameters  $\theta$

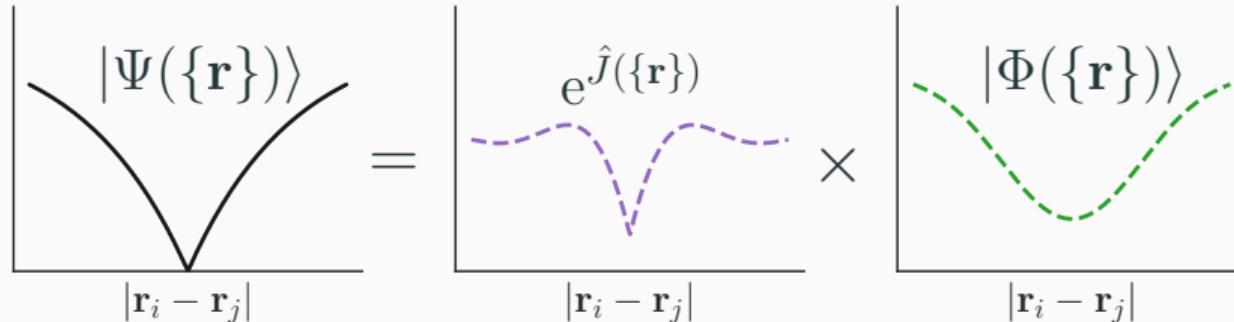


- Use pros of both classical and quantum hardware
- Use **short-depth quantum circuits** that fit current hardware
- Can **improve on classical estimates** by non-classical states
- Store quantum state with **exponentially fewer resources**

Need two qubits per orbital → only very small, inaccurate chemistry calculations possible!

# Reducing hardware requirements with the transcorrelated method

## Cusp Condition – Explicitly Correlated Ansatz



Describe the cusp exactly and capture part of correlation with a **correlated (Jastrow) wavefunction Ansatz**

$$|\Psi(\{\mathbf{r}\})\rangle = e^{\hat{J}} |\Phi(\{\mathbf{r}\})\rangle, \quad \text{with} \quad \hat{J}(\{\mathbf{r}\}) = \sum_{i < j} J_{ij} u(\mathbf{r}_i, \mathbf{r}_j),$$

where  $J_{ij}$  are optimizable parameters and  $u(\mathbf{r}_i, \mathbf{r}_j)$  polynomials dependent on the electron positions.  $J_{ij}$  optimizable with, e.g. Variational Monte Carlo (VMC)

# Similarity Transformation – Transcorrelated (TC) Method

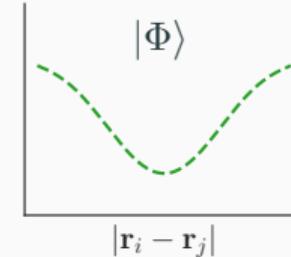
Incorporate the Ansatz into the Hamiltonian:

Instead of  $\hat{H} |\Psi\rangle = E |\Psi\rangle$  solve the similarity transformed/transcorrelated (TC) problem

$$\hat{H} |\Psi\rangle = E |\Psi\rangle, \quad \text{with} \quad |\Psi\rangle = e^{\hat{J}} |\Phi\rangle$$

$$e^{-\hat{J}} \rightarrow | \quad \hat{H} e^{\hat{J}} |\Phi\rangle = E e^{\hat{J}} |\Phi\rangle, \quad (\hat{J}^\dagger = \hat{J})$$

$$(e^{-\hat{J}} \hat{H} e^{\hat{J}}) |\Phi\rangle = E e^{-\hat{J}} e^{\hat{J}} |\Phi\rangle = E |\Phi\rangle$$



Baker-Campbell-Hausdorff (BCH) exp. to obtain TC Hamiltonian:

$$\bar{H} = e^{-\hat{J}} \hat{H} e^{\hat{J}} = \hat{H} + [\hat{H}, \hat{J}] + \frac{1}{2!} [[\hat{H}, \hat{J}], \hat{J}] + \dots \xrightarrow{0}$$

For the **molecular Hamiltonian** the BCH exp. terminates at 2nd order

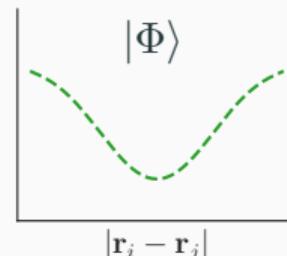
# The Similarity Transformed TC Hamiltonian

## Consequences:

- Transcorrelated  $\bar{H}$  is not Hermitian!  $\rightarrow$  loss of variational principle
  - Additional 3-body terms in  $\bar{H}$
- $\rightarrow$  Ansatz-based **quantum imaginary time evolution**<sup>†</sup> can handle both drawbacks on quantum hardware

## Benefits:

**More accurate results with smaller basis sets/less qubits!**



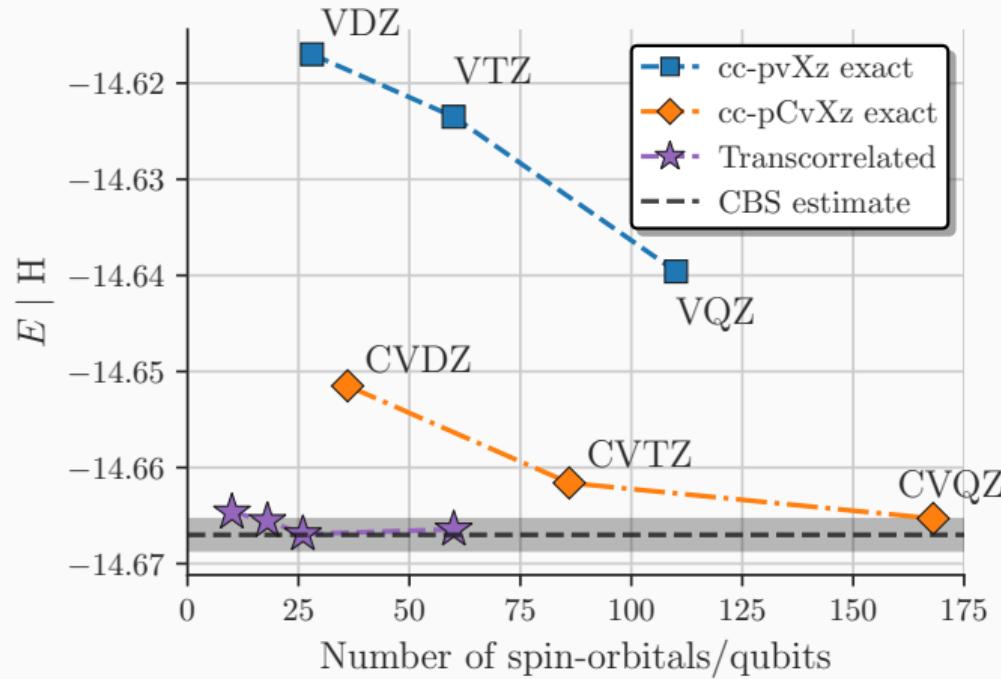
<sup>†</sup>McArdle, *et al.*, npj Quantum Information **5**, 75, 2019; McArdle and Tew, arxiv:2006.11181; \*Haupt, Hosseini, López Ríos, WD, Cohen and Alavi, arxiv:2302.13683, 2023

Applications: Reducing the number of qubits for  
chemistry

# Beryllium atom

**Beryllium atom** – exact simulation of a quantum device (no noise)

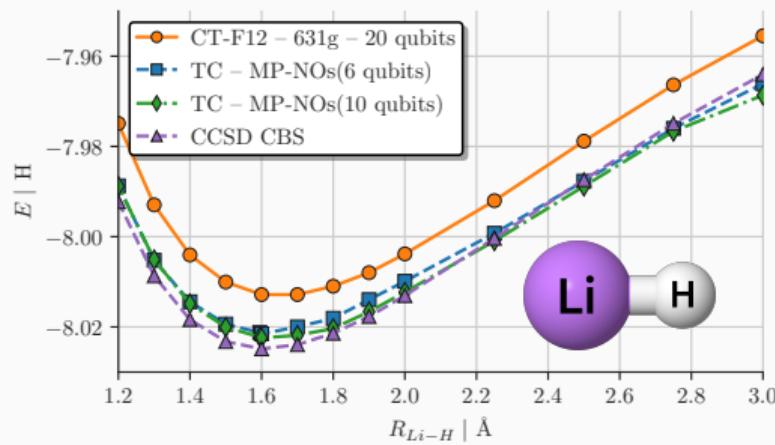
**Goal:** complete basis set (CBS) limit → full description to compare with experiment



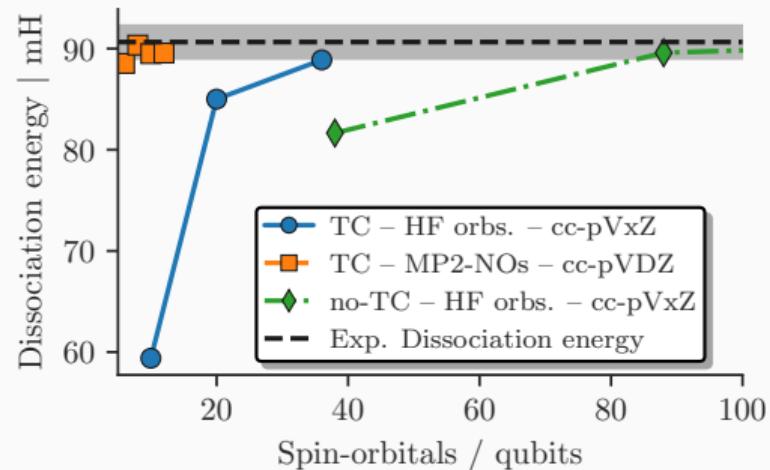
# Lithium hydride – LiH

**Lithium hydride** – exact, noiseless simulation of quantum device

“Standard basis sets” not optimized for the TC method → use pre-optimized orbitals, e.g. natural orbitals from perturbation theory calculation (MP2-NOs)



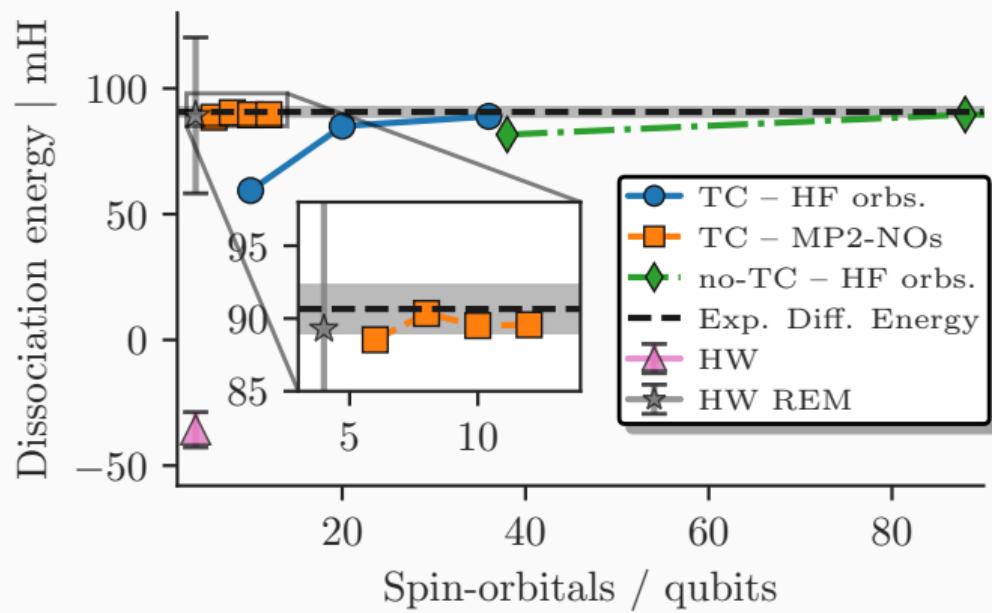
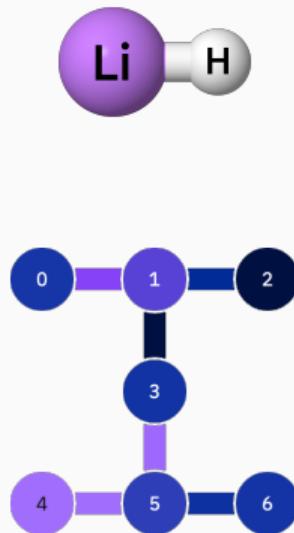
Error wrt. CBS result vs bond distance



Experimental<sup>†</sup> dissociation energy  
Order of magnitude less qubits!

# LiH – Experiment on IBM Quantum devices

Hardware (HW) experiment: lithium hydride dissociation energy on `ibm_lagos`

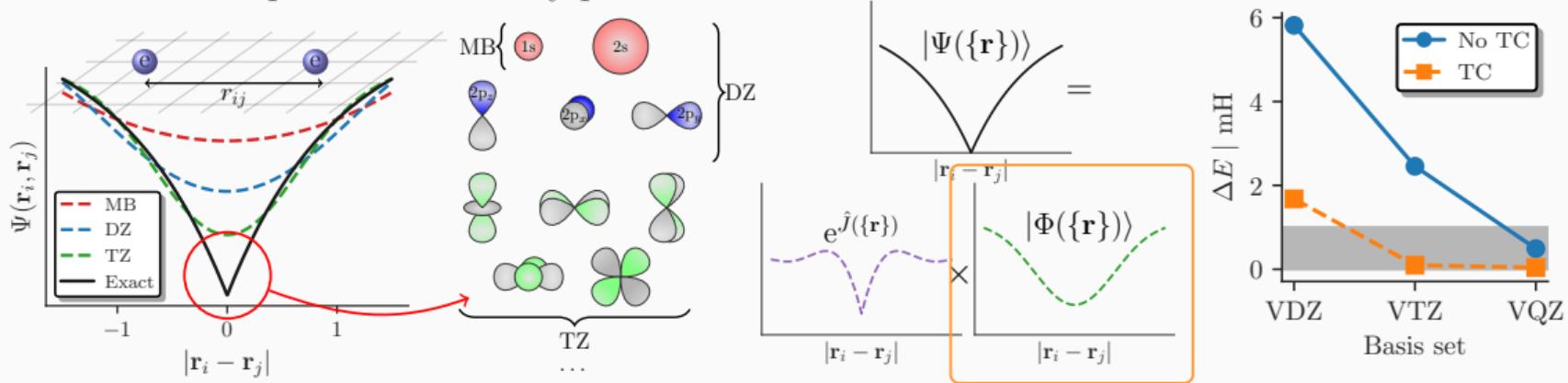


Large effect of noise! Error mitigation techniques\* to reduce effect of noise.

## Conclusions and outlook

# Conclusion – Transcorrelated Approach on Quantum Hardware

- The **TC method** partially transfers electronic correlations from the wavefunction into the Hamiltonian, **capturing the cusp condition**.
- **Reduce qubit requirements and circuit depth**, due to accurate results with a small basis sets.
- **Extends applicability of current and near-term quantum devices** to more relevant quantum chemistry problems.



# Workshop – Frontiers of near-term quantum computing



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The workshop aims to bring together researchers from the fields of **computer science, quantum information and chemistry**: <https://tinyurl.com/frontiers-of-qc>.

**29th August – 1st September, 2023, Gothenburg, Sweden**

## Confirmed speakers:

- Ivano Tavernelli
- Sophia Economou
- Sevag Gharibian
- Richard Kueng
- Xiao Yuan
- Christian Gogolin
- Zoë Holmes
- Stefan Knecht
- Jakob Kottmann
- Panagiotis Barkoutsos
- Ashley Montanaro
- Anand Natarajan
- Pauline Ollitrault
- Benjamin Brown
- Francesco Tacchino
- Juani Bermejo-Vega
- David Muñoz Ramo
- Tony Metger

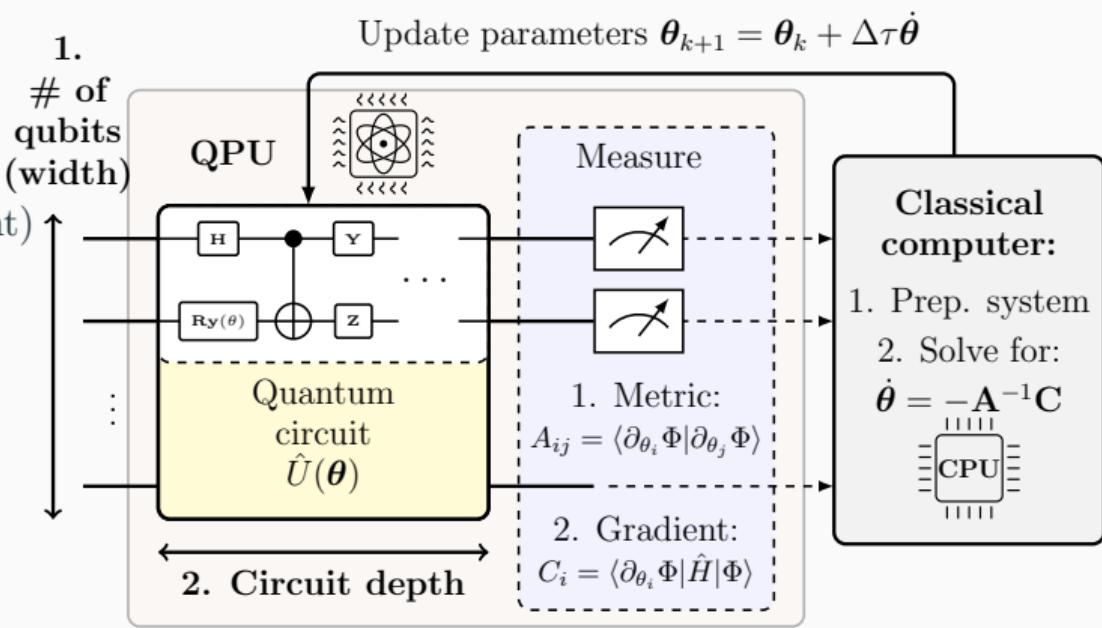
Thank you for your attention!

# How to solve non-Hermitian problems on quantum hardware

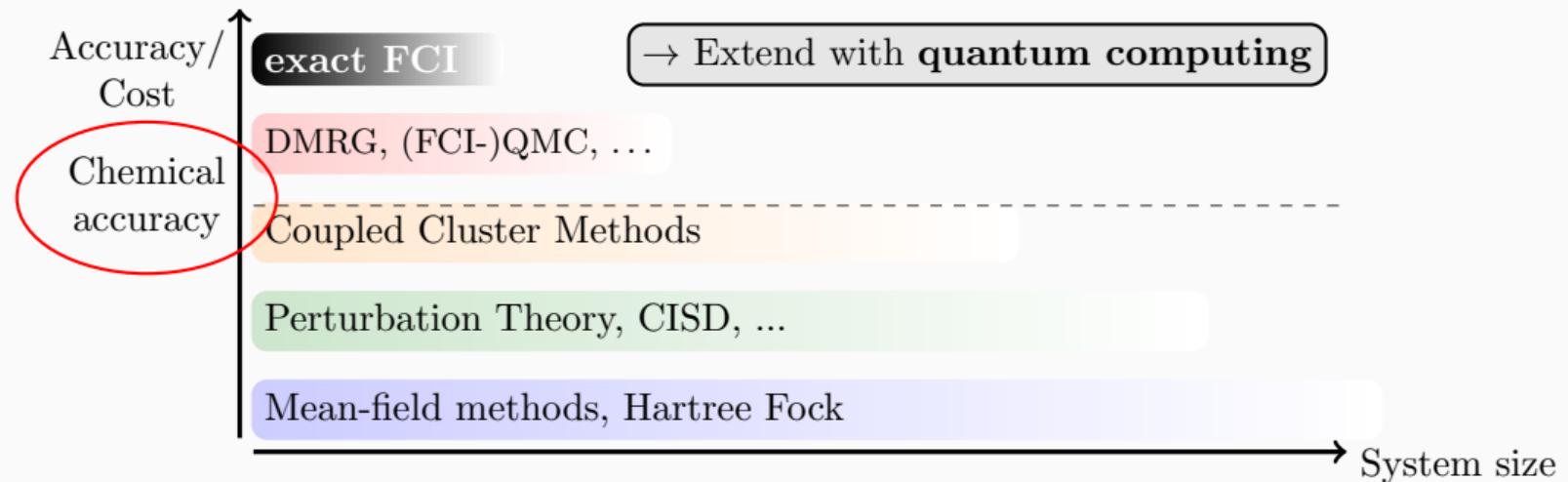
Since the TC Hamiltonian is **non Hermitian**, VQE not applicable!

→ Use Ansatz-based Variational **Quantum Imaginary Time Evolution\***

- Based on imaginary-time Schrödinger equation
- Projector method to obtain (right) eigenvector
- Allows to formulate non-unitary time evolution as minimization
- Applicable to non-Hermitian problems



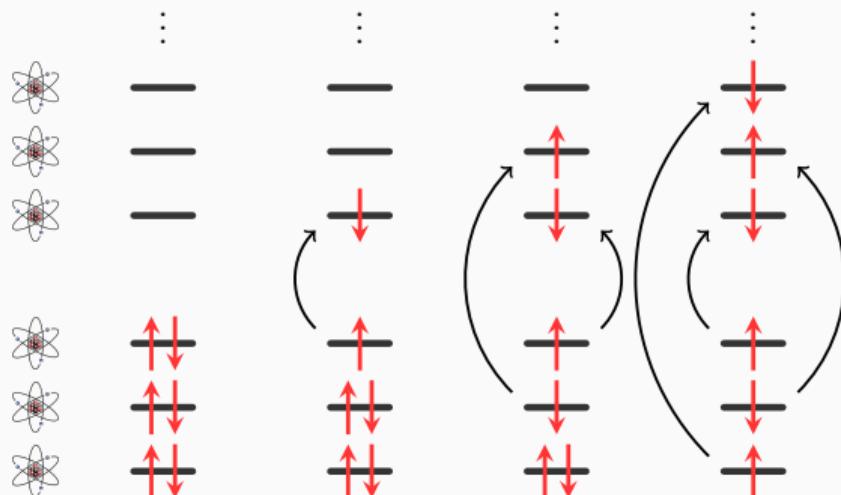
# Hierarchy of methods



Highly accurate methods only applicable to **very small** system sizes.  
Current quantum computing calculations/experiments use small/**minimal basis sets** far from experimental results, due to **limited number of qubits**

# Exponential scaling of Full Configuration Interaction

There is a long history and wide variety of computational approaches in chemistry



Mol.	#electrons	#states
$H_2$	2	4
$LiH$	4	36
$Be_2$	8	4900
$H_2O$	12	$\sim 8 \cdot 10^5$
$C_2H_4$	16	$\sim 16 \cdot 10^6$
$F_2$	18	$\sim 2 \cdot 10^9$

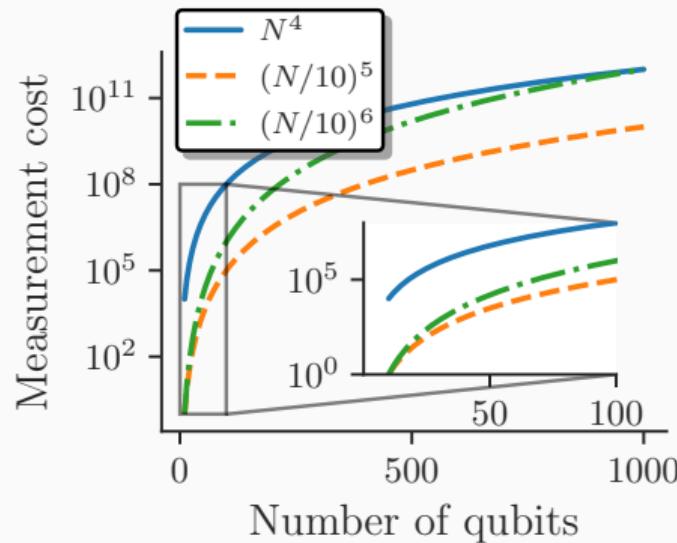
$> 20$  electrons  $> \sim 100$  GB information!

→ can not even store wavefunction in computer memory

# Scaling of TC – Measurement Cost

$$\bar{H} = \sum_{pq,\sigma} h_q^p a_{p,\sigma}^\dagger a_{q,\sigma} + \frac{1}{2} \sum_{pqrs,\sigma\tau} \bar{V}_{rs}^{pq} a_{p,\sigma}^\dagger a_{q,\tau}^\dagger a_{s,\tau} a_{r,\sigma} - \frac{1}{6} \sum_{pqrstu,\sigma\tau\lambda} L_{stu}^{pqr} a_{p,\sigma}^\dagger a_{q,\tau}^\dagger a_{r,\lambda}^\dagger a_{u,\lambda} a_{t,\tau} a_{s,\sigma}$$

- Measurement formally scaling as  $N^6$ , with  $N$  being the number of orbitals
- Recently shown that  $N^6$ -scaling terms can be neglected to good accuracy\*
- Current work on  $N^4$ -scaling approximation
- Order of magnitude less orbitals: since also no core functions needed in basis set†
- Shorter circuit depth, due to more compact ground state!



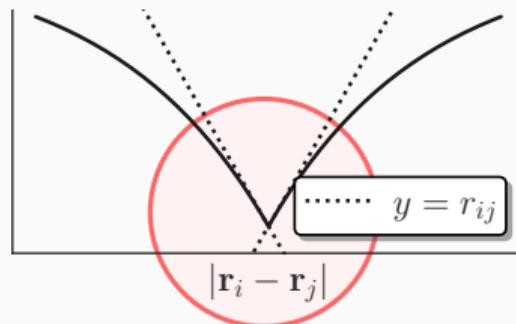
## Variational Quantum Monte Carlo to optimize Jastrow factors

Minimize variational energy, by optimizing trial wavefunction parameters  $J_{ij}$ :

$$E_{VMC} = \min_{\hat{J}(J_{ij})} \frac{\langle \Phi_0 | e^{\hat{J}} \hat{H} e^{\hat{J}} | \Phi_0 \rangle}{\langle \Phi_0 | e^{2\hat{J}} | \Phi_0 \rangle}, \quad |\Phi_T\rangle = e^{\hat{J}} |\Phi_0\rangle$$

- The choice of trial wavefunction is critical in VMC calculations → accuracy limited by  $|\Phi_T\rangle = e^{\hat{J}} |\Phi_0\rangle$ !
- Hartree-Fock state usually first starting point for  $|\Phi_0\rangle$ , but more elaborate/accurate states possible...
- Polynomial scaling  $\sim N^3$
- Such a VMC calculations to optimize  $J_{ij}$  with a HF state  $|\Phi_0\rangle = |\Phi_{HF}\rangle$  our **starting point** for the **transcorrelated method**

## Explicitly Correlated methods



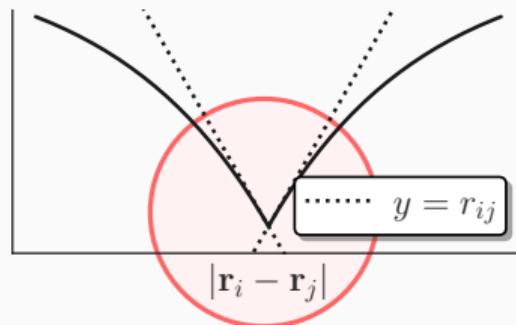
Linear behavior in electron-electron distance  $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$  for small  $r_{ij}$ !

**R12** methods\*:  $|\Psi\rangle = r_{ij} |\Phi\rangle$

**F12** methods<sup>†</sup>:  $|\Psi\rangle = f(r_{ij}) |\Phi\rangle, \quad f(r_{ij}) = \frac{1 - \exp(-\gamma r_{ij})}{\gamma}$

**Jastrow** Ansatz<sup>‡</sup>:  $|\Psi\rangle = e^{\hat{J}} |\Phi\rangle, \quad \hat{J} = \sum_{ij} J_{ij} g(\tilde{r}_{ij})$

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$$\exp(-x) \approx 1 - x + \mathcal{O}(x^2), \quad \tilde{r}_{ij} = \frac{r_{ij}}{1 + r_{ij}}, \quad \lim_{r_{ij} \rightarrow 0} \tilde{r}_{ij} \rightarrow 0, \quad \lim_{r_{ij} \rightarrow \infty} \tilde{r}_{ij} \rightarrow 1$$

\* Kutzelnigg, Theoretica chimica acta 68, 445 (1985); <sup>†</sup> Ten-no, J. Chem. Phys. 121, 117 (2004); <sup>‡</sup> Jastrow, Phys. Rev. 98, 1479 (1955);

## Non-Hermitian Hamiltonian – Problem for VQE

Since TC Hamiltonian is **non Hermitian**, variational algorithms like VQE not applicable

$$E_{\text{VQE}} = \min_{\theta} \langle \Psi(\theta) | \hat{H} | \Psi(\theta) \rangle$$

Our Approach:

Solve for the **right** eigenvector of non-Hermitian  $\bar{H}$  by **projection** with QITE:

$$|\Phi_0^R\rangle \propto \lim_{t \rightarrow \infty} e^{-t\bar{H}} |\phi^R\rangle, \quad \text{with} \quad \bar{H} |\Phi_0^R\rangle = E |\Phi_0^R\rangle,$$

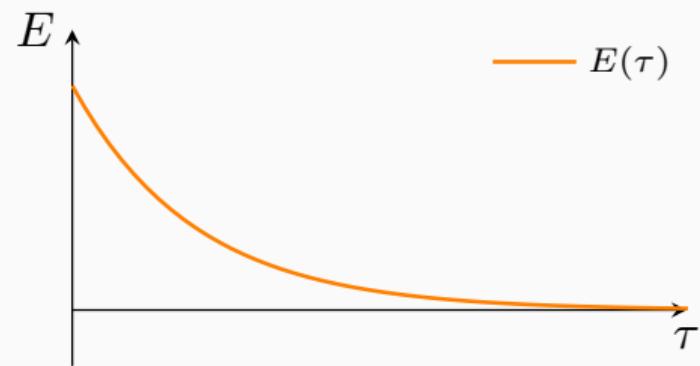
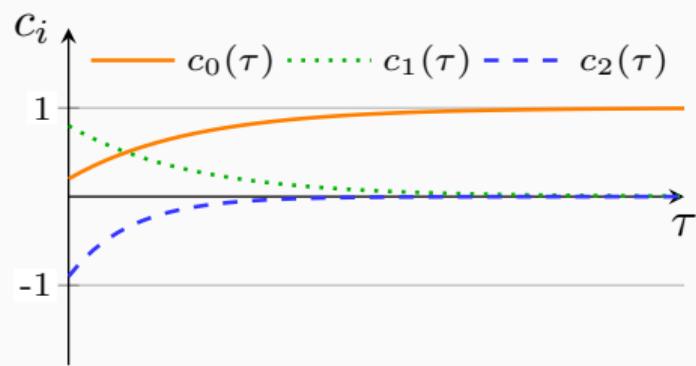
where  $|\Phi^R\rangle$  is a full expansion in SDs  $|\Phi^R\rangle = \sum_i c_i |D_i\rangle$

# Quantum Imaginary Time Evolution – QITE

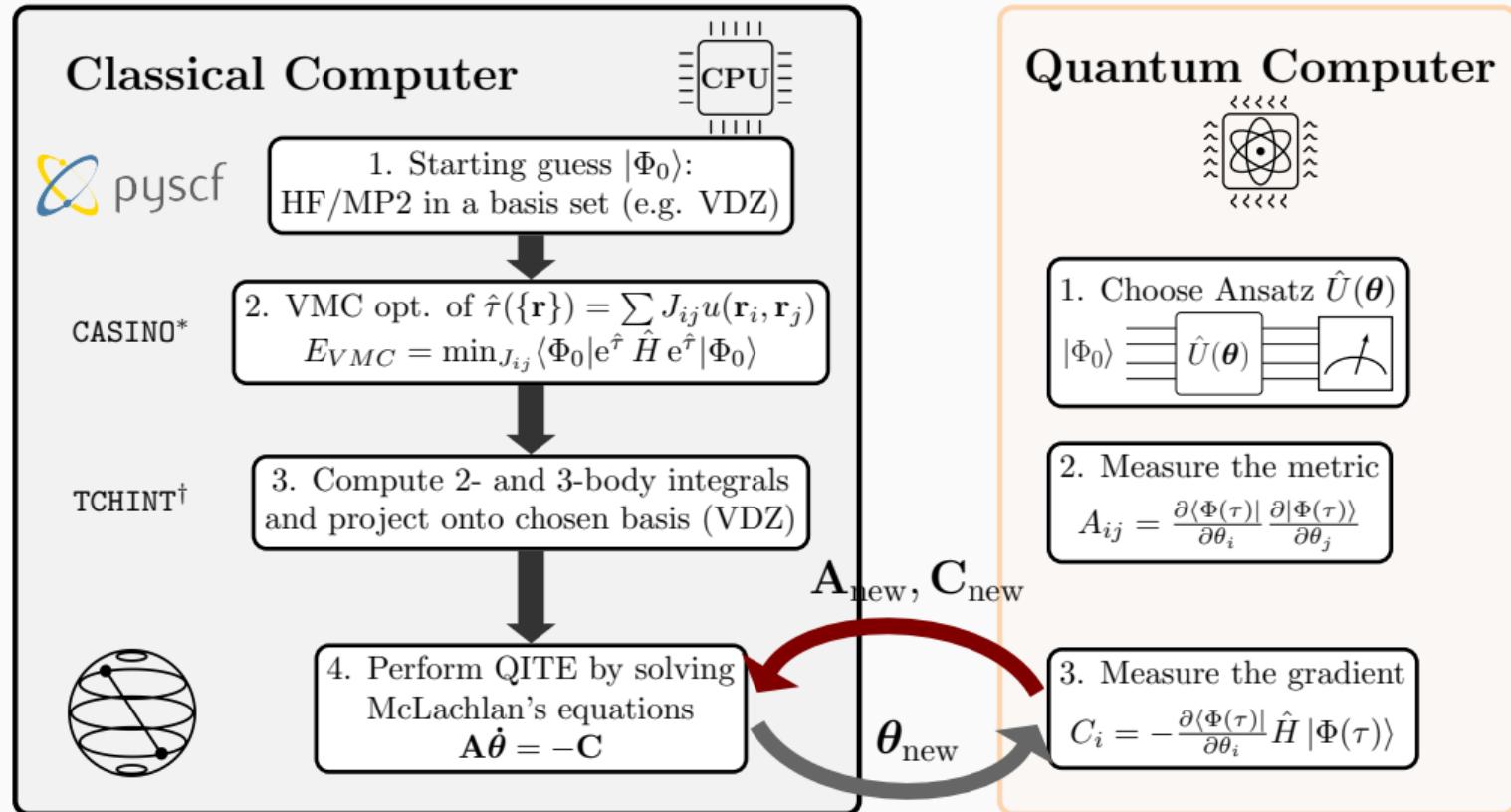
→ Solve for the **right** eigenvector of non-Hermitian  $\bar{H}$  by (quantum) imaginary-time evolution (QITE)

$$i \frac{\partial |\Psi\rangle}{\partial t} = \hat{H} |\Psi\rangle \quad \stackrel{\tau=it}{\rightarrow} \quad \frac{\partial |\Psi\rangle}{\partial \tau} = -\hat{H} |\Psi\rangle \quad \rightarrow \quad |\Psi(\tau)\rangle = N(\tau) e^{-\hat{H}\tau} |\Psi(0)\rangle$$

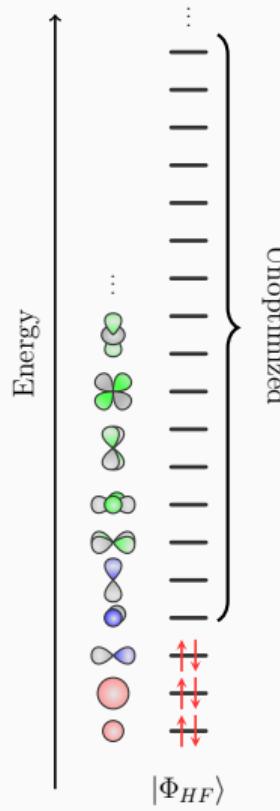
$$|\Psi(0)\rangle = \sum_i c_i(0) |\psi_i\rangle \quad \rightarrow \quad |\Psi(\tau)\rangle = e^{-\tau(\hat{H}-S_\tau)} \sum_i c_i(0) |\psi_i\rangle = \sum_i c_i(0) e^{-\tau(E_i-S_\tau)} |\psi_i\rangle$$



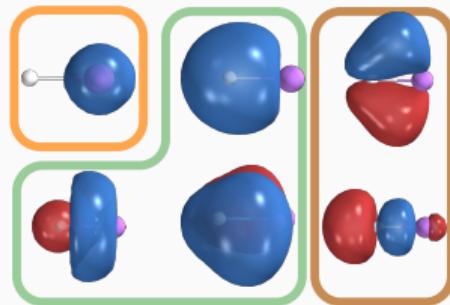
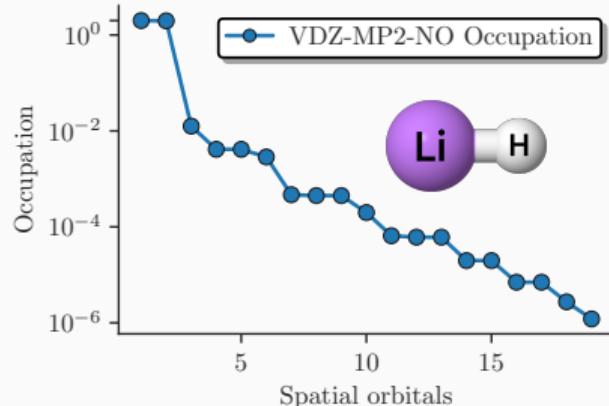
# Workflow



# (Virtual) orbital optimization



- “Standard basis sets” not optimized for the TC method
  - include effect of virtuals through orbital optimization / downfolding
  - e.g. natural orbitals (NO) from a “cheap” perturbation theory (MP2) calculation

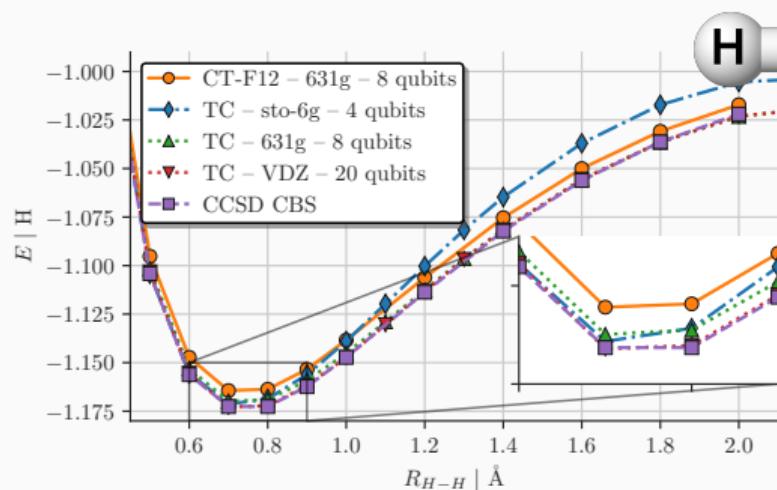


# Hydrogen molecule

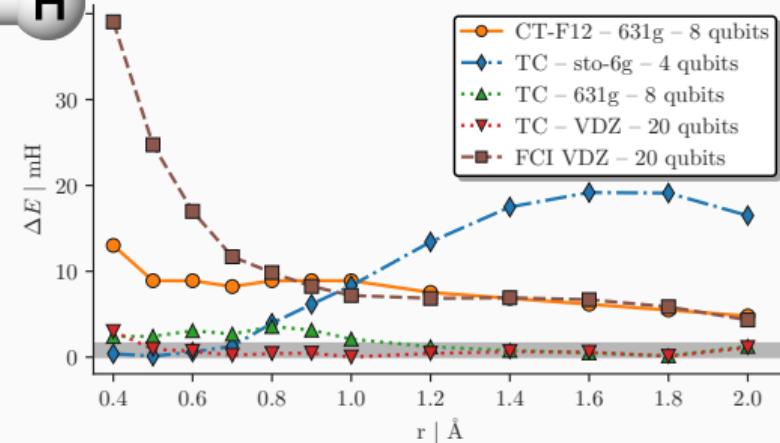
Favorite quantum chemistry test case: Hydrogen molecule – H<sub>2</sub>

CT-F12 approximated explicitly correlated method, by Motta *et al.*\*

Exact statevector simulation – UCCSD Ansatz



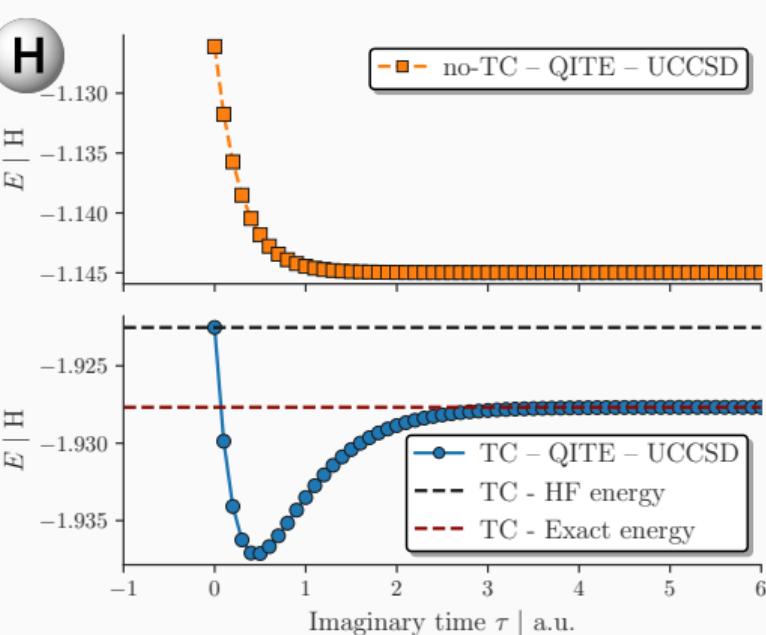
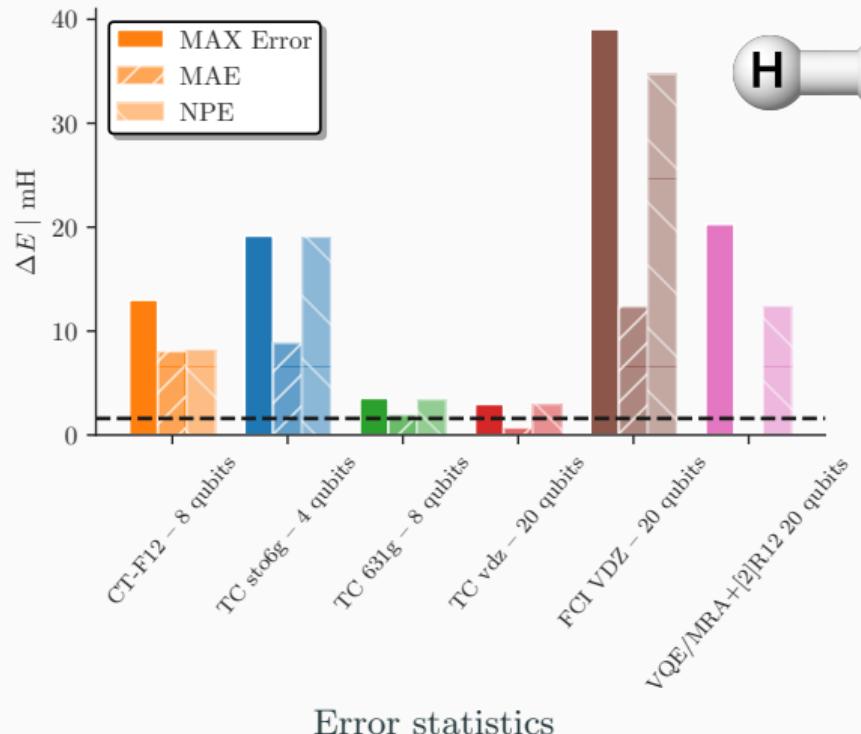
Energy vs. bond distance



Error wrt. CBS result vs. bond distance

\*CT-F12: Motta *et al.*, Phys. Chem. Chem. Phys. **22**, 24270, 2020

# $H_2$ cont

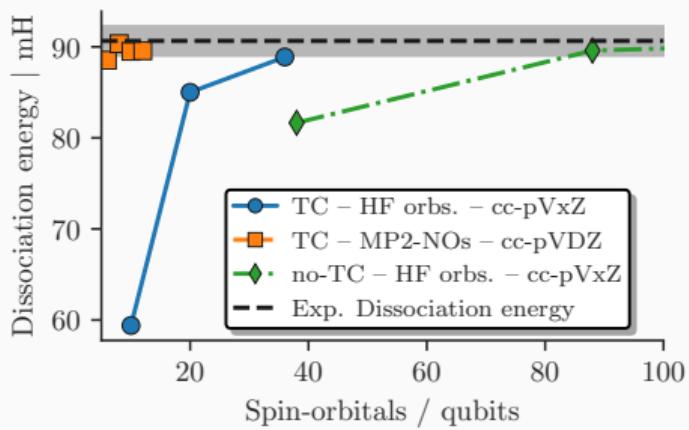
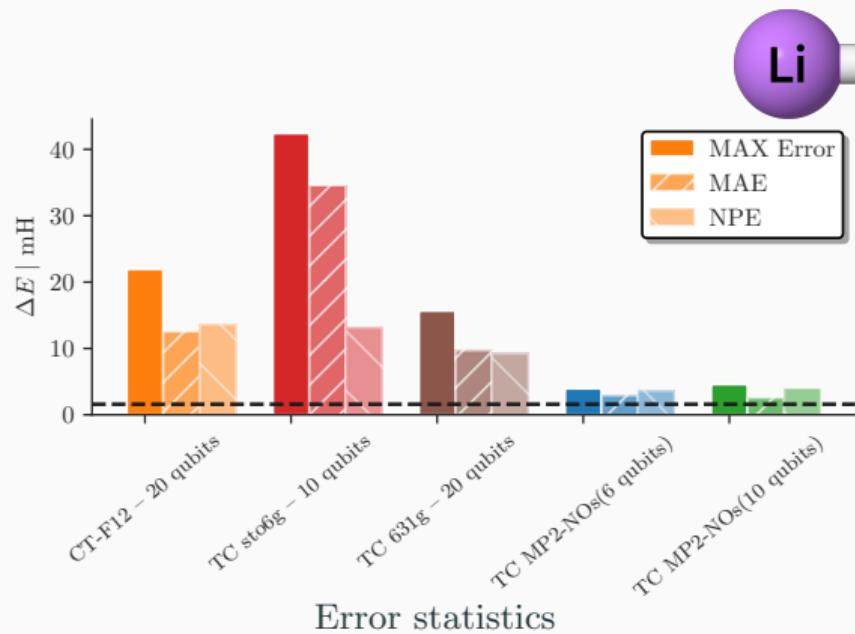


Error statistics

Imaginary time evolution – STO-6G – 0.7 Å

# LiH – Dissociation energy

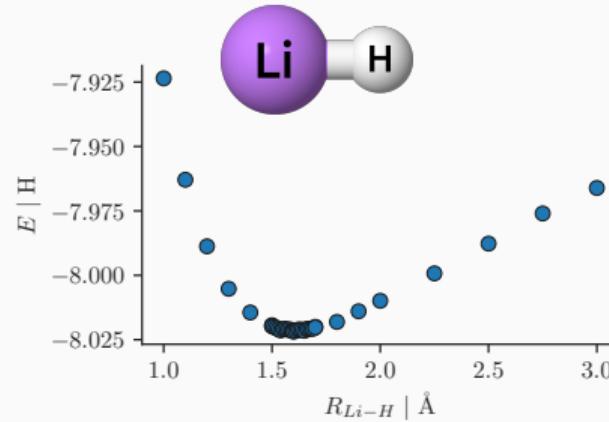
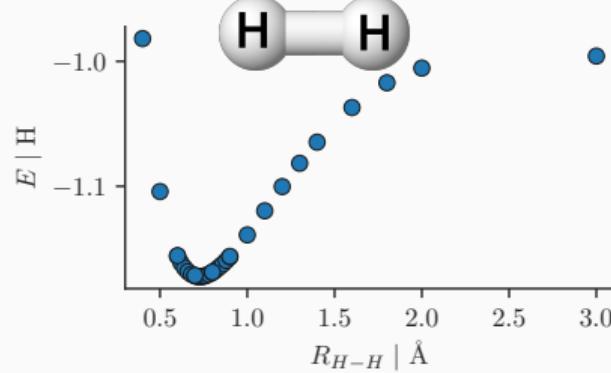
Error statistics and comparison to **experimental\*** dissociation energy



**Experimental dissociation energy**

\* Haeffler *et al.*, Phys. Rev. A, 1996, 53, 6, 4127 (1996)

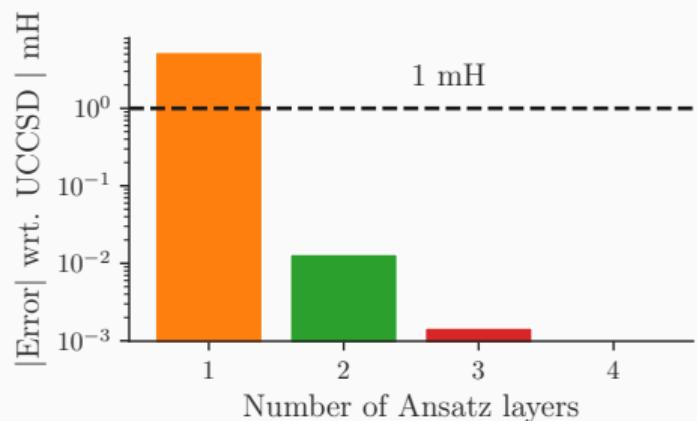
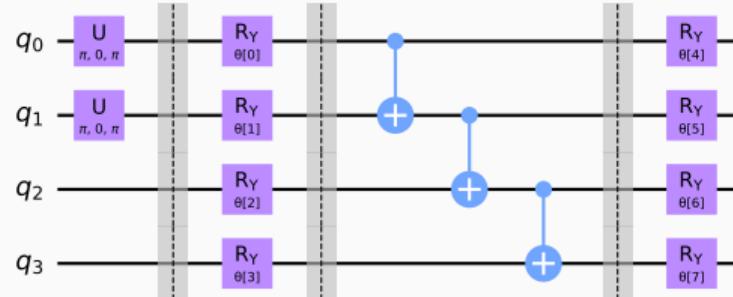
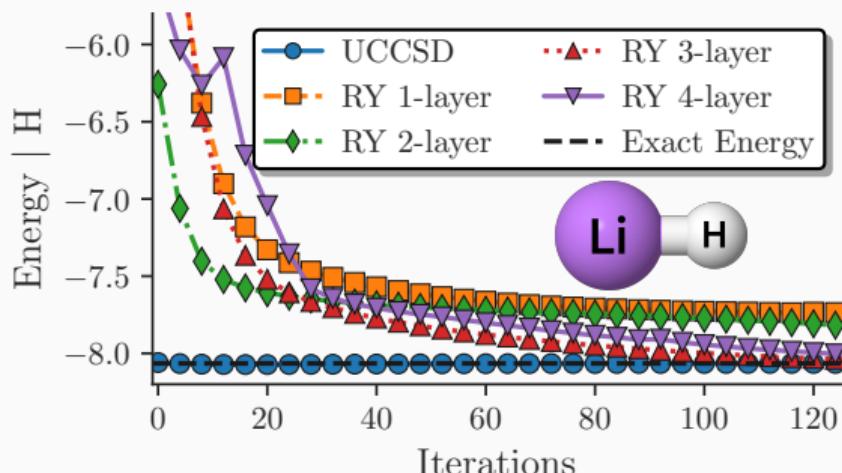
# Spectroscopic Constants



$\text{H}_2$				$\text{LiH}$					
	qubits	$R_e(\text{\AA})$	$D_0(\text{eV})$	$\omega_e(\text{cm}^{-1})$		qubits	$R_e(\text{\AA})$	$D_0(\text{eV})$	$\omega_e(\text{cm}^{-1})$
no-TC	4	0.73	3.67	4954		12	1.54	2.66	1690
	8	0.75	3.87	4297		22	1.67	1.80	1283
	20	0.76	4.19	4353		38	1.62	2.17	1360
TC	4	<b>0.74</b>	<b>4.69</b>	<b>4435</b>		<b>6</b>	<b>1.60</b>	<b>2.42</b>	<b>1377</b>
Exp.		<b>0.74</b>	<b>4.52</b>	<b>4401</b>			<b>1.60</b>	<b>2.47</b>	<b>1406</b>

# LiH – Hardware-efficient Ansatz

- LiH at equilibrium bond distance with 3 MP2 NOs.
- Hardware efficient RY Ansatz with linear entangling layer and parity encoding.
- Statevector simulation



# LiH – Hardware-efficient Ansatz – QASM Simulations

- Reference-state error mitigation (REM)\* (see Poster session I today – G00/292) or zero-noise extrapolation

