基于超导量子线路的多体系统模拟

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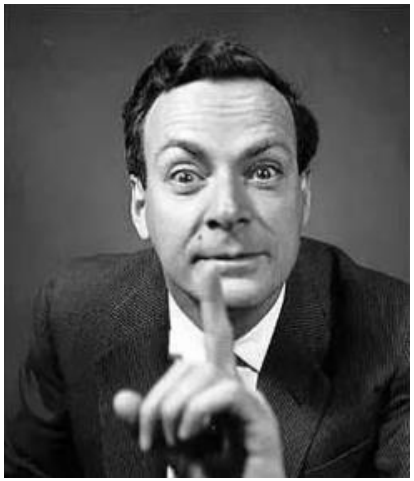
THEORETICAL PHYSICS DIVISION

为什么需要量子计算机？

...nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy...



by Richard Feynman

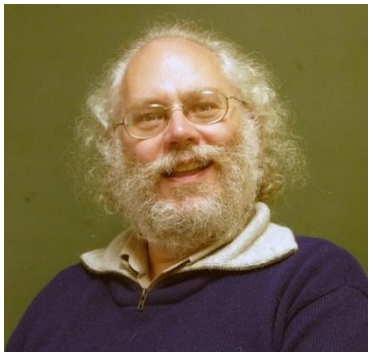
Simulating Physics with Computers

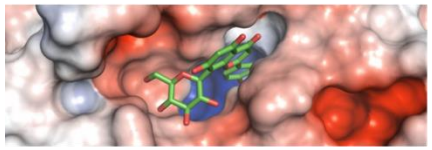
Richard P. Feynman

Department of Physics, California Institute of Technology, Pasadena, California 91107

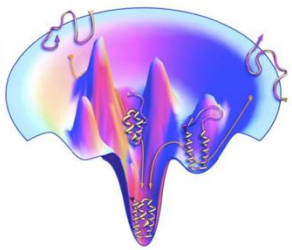
Received May 7, 1981

舒尔算法是由美国数学家彼得·舒尔（Peter Shor）于1994年提出的量子算法。该算法能够利用量子计算机在多项式时间内完成大整数的质因数分解，而经典计算机解决这一问题需要指数时间。这一特性直接威胁到广泛使用的RSA加密体系。

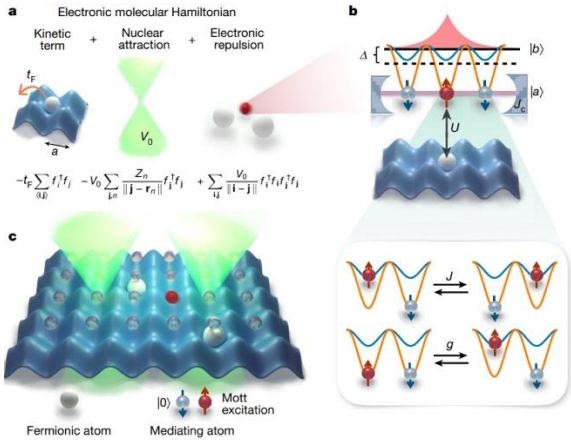




药物设计 化学计算
优化问题 材料研究



量子计算的种类与特点



J. Argüello-Luengo et al., Nature 574, 215(2019)

模拟量子计算

量子退火机

数字量子计算

量子计算机 vs 经典计算机

特性	经典计算机	量子计算机
信息单元	比特（0或1）	量子比特（叠加态）
运算方式	串行处理	并行计算（利用叠加与纠缠）
适用问题	通用计算、逻辑判断	特定复杂问题（如优化、模拟）
成熟度	高度成熟	实验阶段，尚未完全实用化

量子计算系统架构

DiVincenzo准则

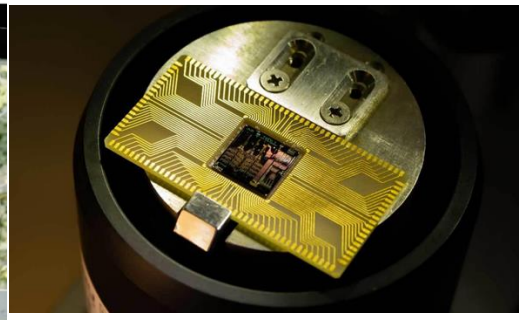
1. 系统比特可以拓展。
2. 量子态可以初始化。
3. 系统具有较长的相干时间。
4. 拥有一套通用量子门操作。
5. 末态信息可以被测量。

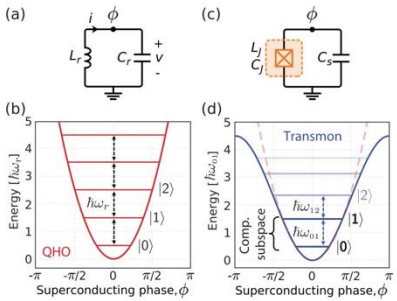
超导量子计算系统

1. 超导量子芯片
2. 测控线路
3. 稀释制冷机
4. 测控电子学
5. 测控软件
6. 量子应用软件

量子计算机的种类

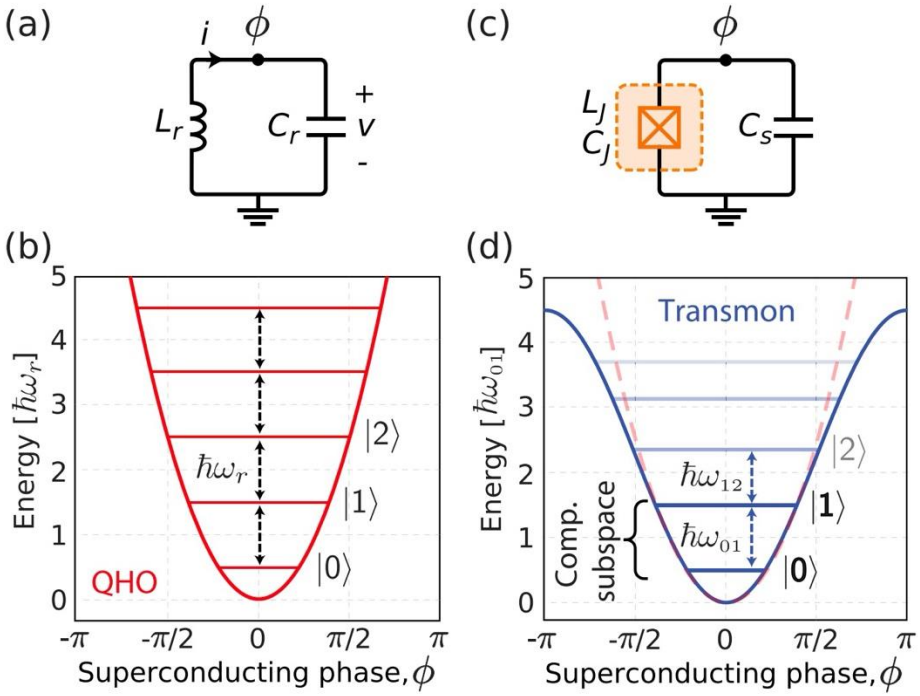
超导量子计算
离子阱量子计算
中性原子量子计算
光量子计算
半导体量子计算
核磁量子计算
金刚石色心量子计算
.....



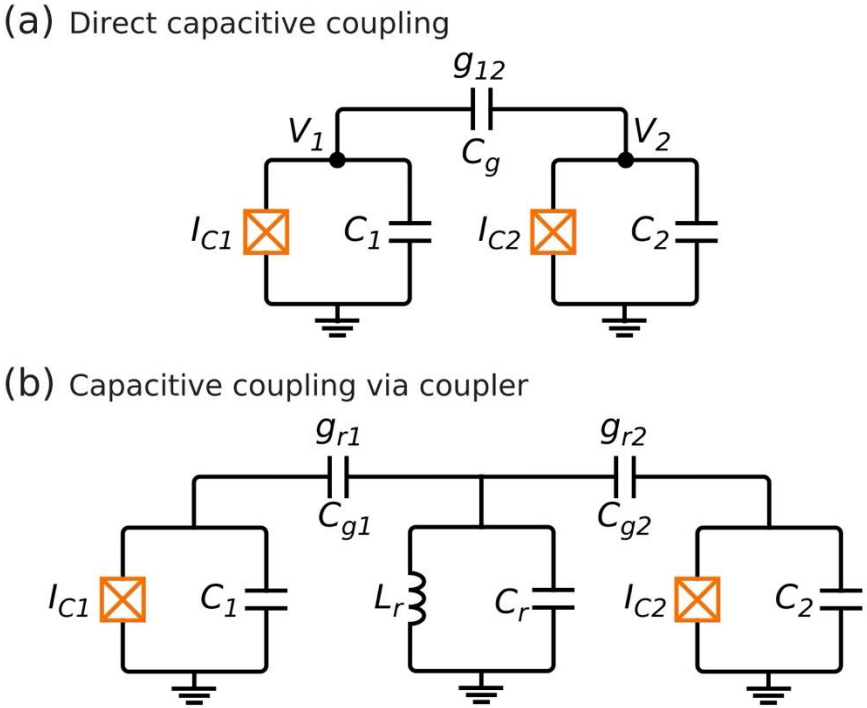


稀释制冷机内部主要包含制冷盘、测控线路和超导量子芯片。超导量子芯是由超导量子比特组成的，超导比特是一个近似二能级系统，由基态（0态）和第一激发态（1态）组成。

超导量子比特的结构



超导量子比特的实现

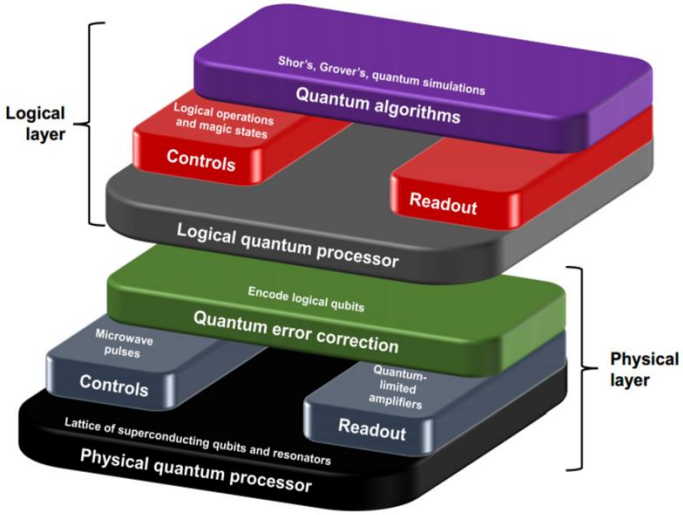


超导量子比特的耦合

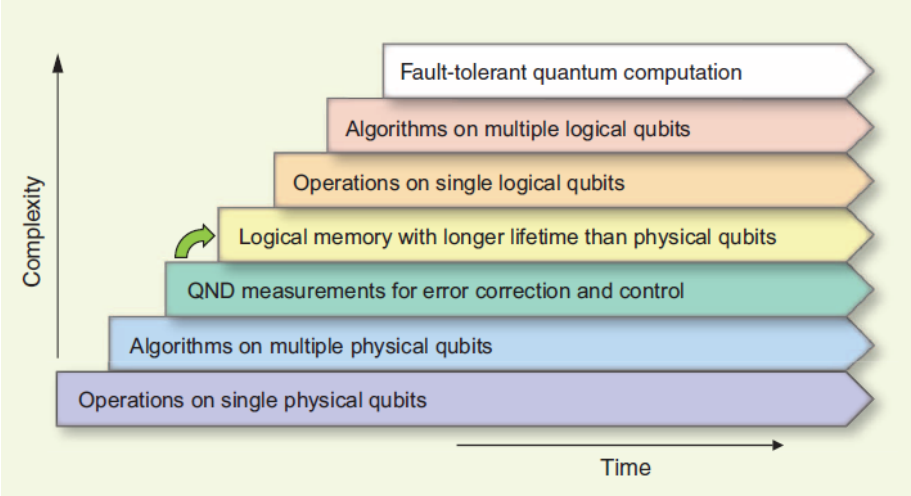
谷歌主要走的是可调耦合路线，更容易获得高保真度的门。
IBM主要走的是固定频率路线，稳定性高，适合云计算。

P. Krantz, et al., Appl. Phys. Rev. **6**, 021318 (2019).

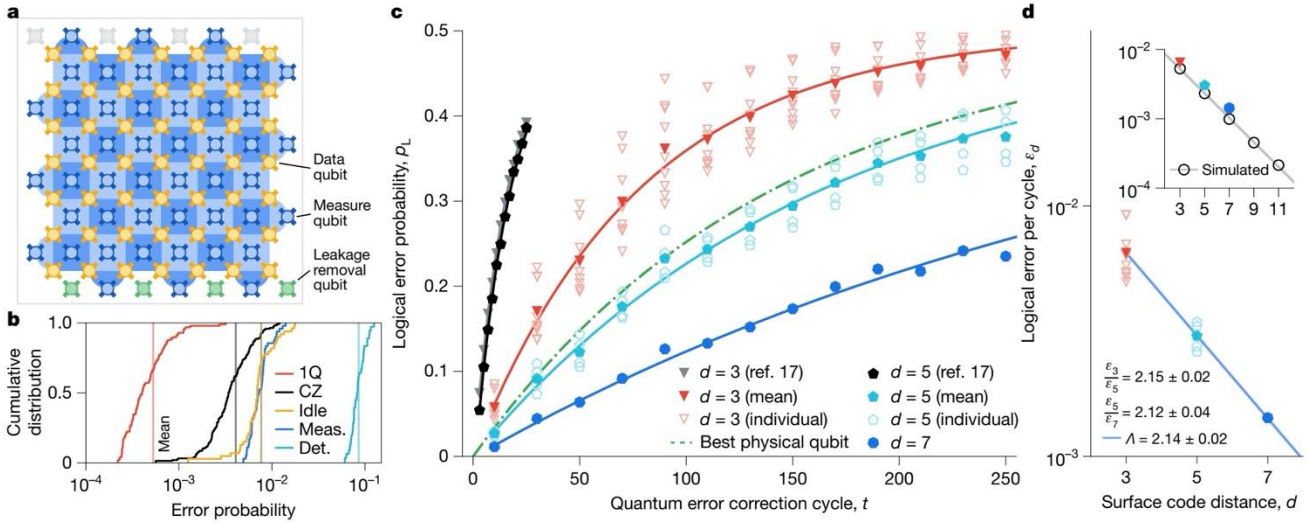
量子计算的发展路线



量子计算机需要纠错机制实现低错误率。



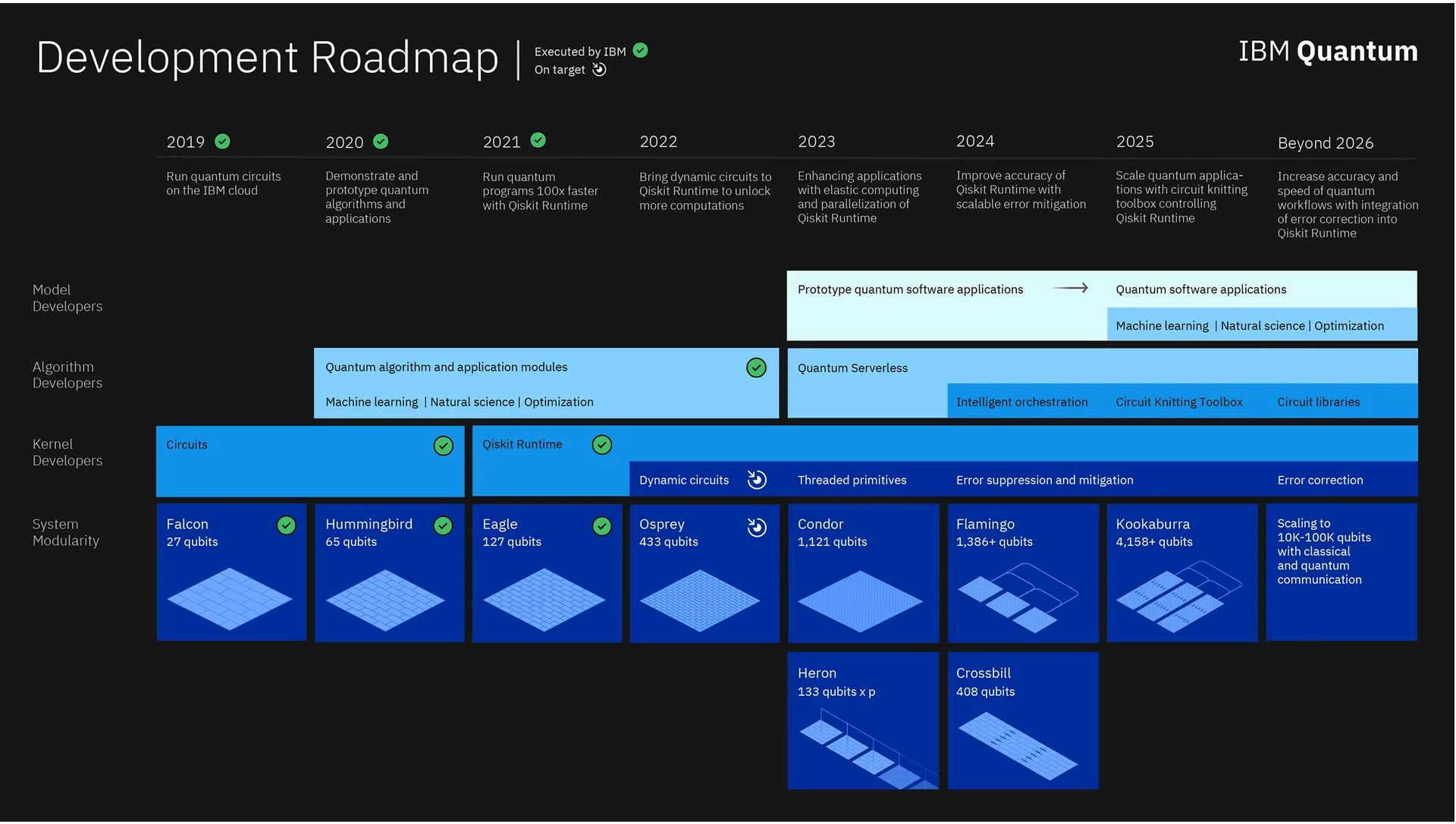
目前大致处于4–5阶段。



近期，谷歌量子计算团队实现了距离等于7的表面码纠错演示工作，并成功达到了表面码纠错阈值。

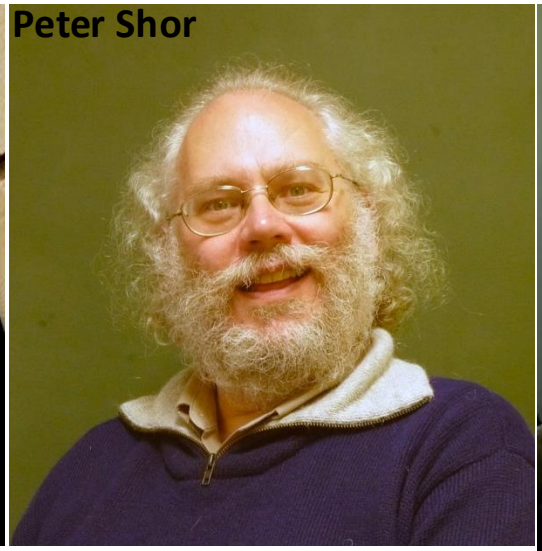
Google AI quantum, nature, **638**, 920 (2025).
M. H. Devoret, et al., Science **339**, 1169 (2013).

IBM的发展规划

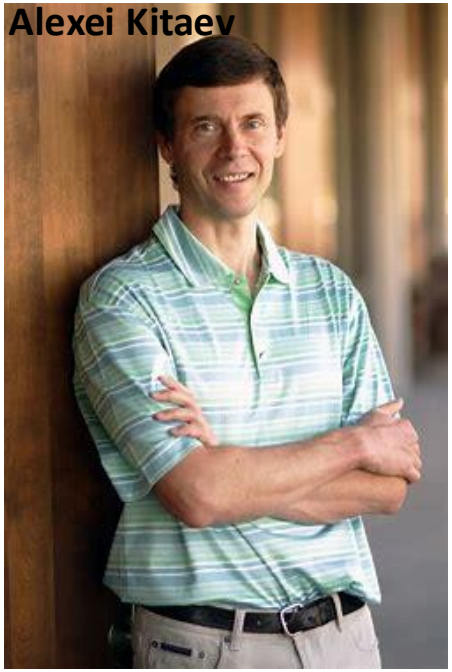

Development Roadmap
Executed by IBM
On target
IBM Quantum
2019
Run quantum circuits on the IBM cloud
2020
Demonstrate and prototype quantum algorithms and applications
2021
Run quantum programs 100x faster with Qiskit Runtime
2022
Bring dynamic circuits to Qiskit Runtime to unlock more computations
2023
Enhancing applications with elastic computing and parallelization of Qiskit Runtime
2024
Improve accuracy of Qiskit Runtime with scalable error mitigation
2025
Scale quantum applications with circuit knitting toolbox controlling Qiskit Runtime
Beyond 2026
Increase accuracy and speed of quantum workflows with integration of error correction into Qiskit Runtime
Model Developers
Prototype quantum software applications
Quantum software applications
Machine learning | Natural science | Optimization
Algorithm Developers
Quantum algorithm and application modules
Machine learning | Natural science | Optimization
Quantum Serverless
Intelligent orchestration
Circuit Knitting Toolbox
Circuit libraries
Kernel Developers
Circuits
Qiskit Runtime
Dynamic circuits
Threaded primitives
Error suppression and mitigation
Error correction
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
Heron
133 qubits x p
Crossbill
408 qubits

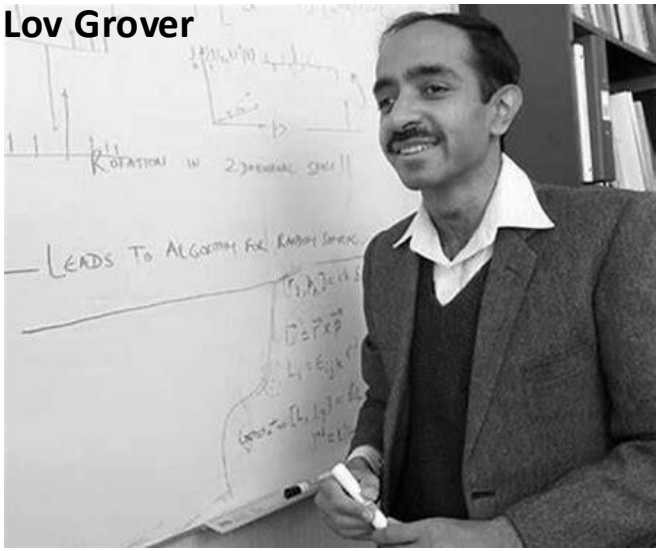
量子算法的发展

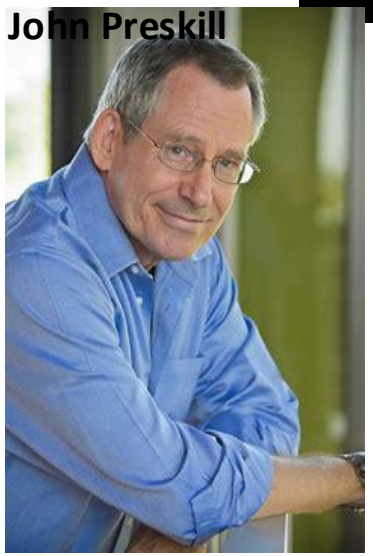
David Deutsch


Peter Shor

Seth Lloyd


Alexei Kitaev

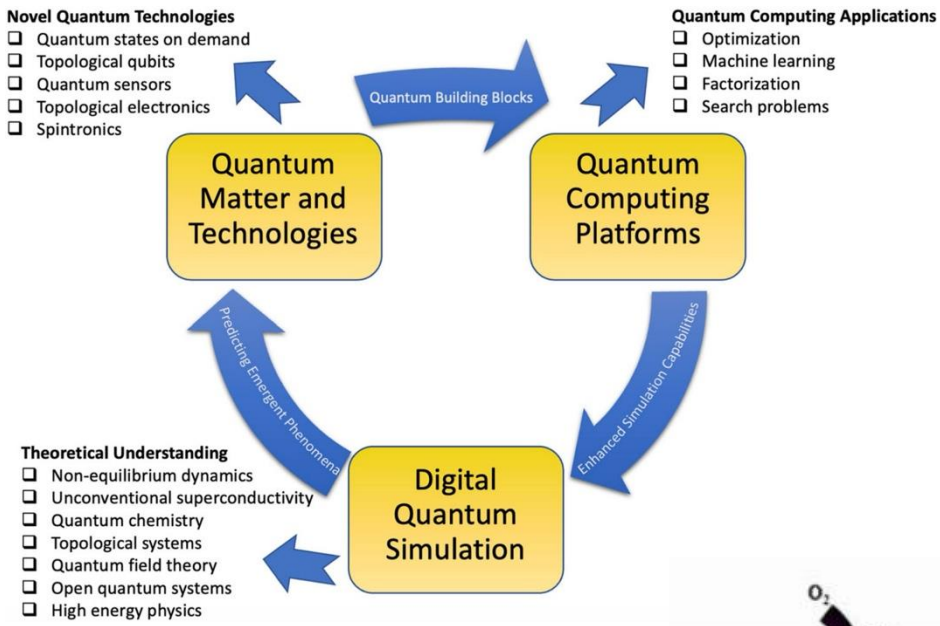

Lov Grover

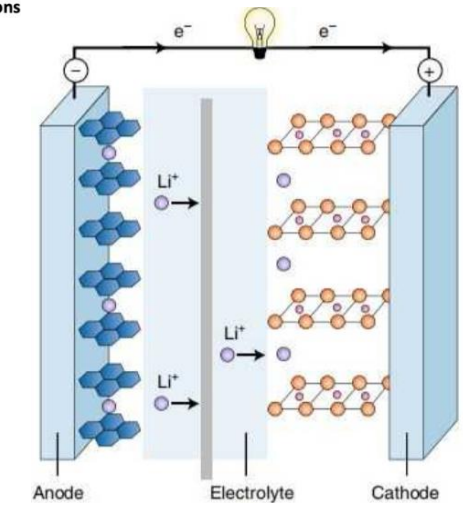

John Preskill

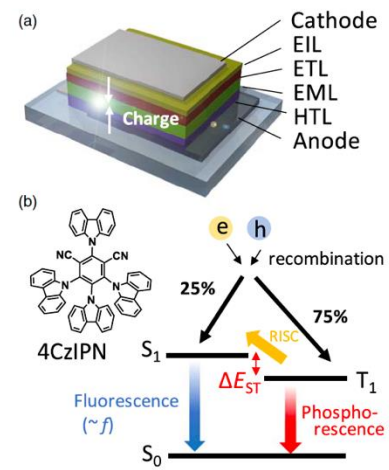
应用算法举例

1. many-body physics
   (QPE, VQE，QITE，AFQMC，PQE)
2. quantum cryptography (Shor)
3. linear algebra (HHL,VQLS,VQSVD)
4. machine learning (QPCA,QSVM,QNN)
5. optimization (QAOA)
6. .....

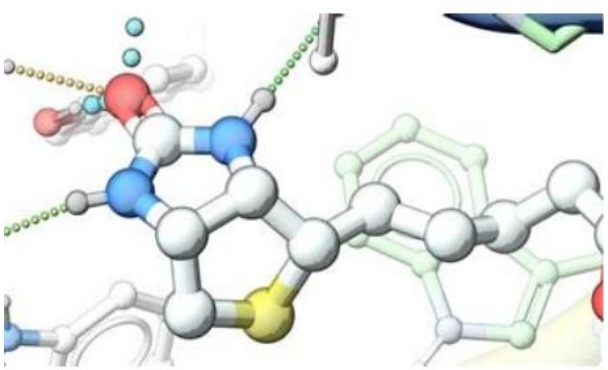
计算化学的应用领域

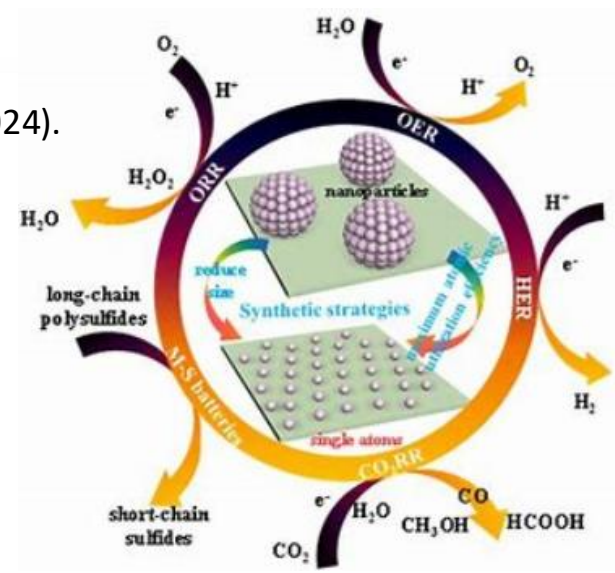


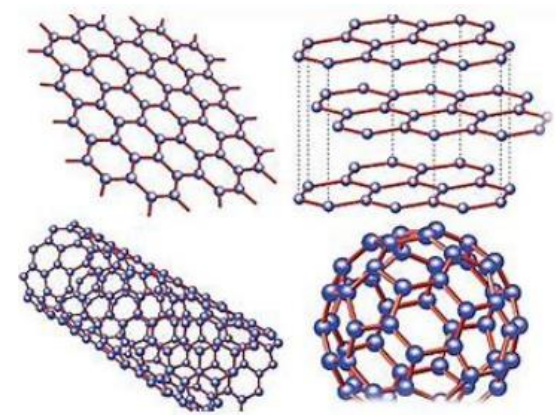




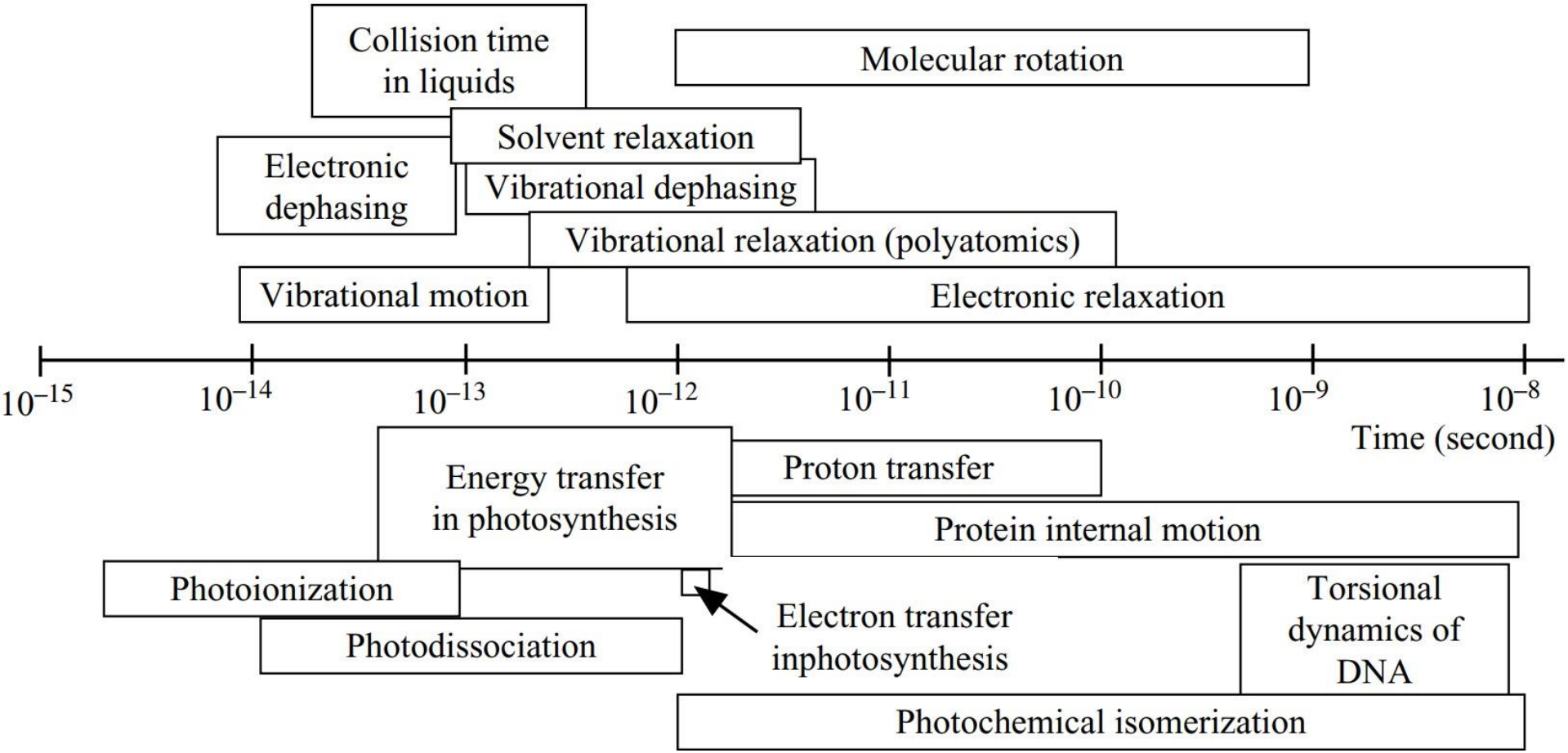
B. Fauseweh, nat. comm., **15**, 2123 (2024).





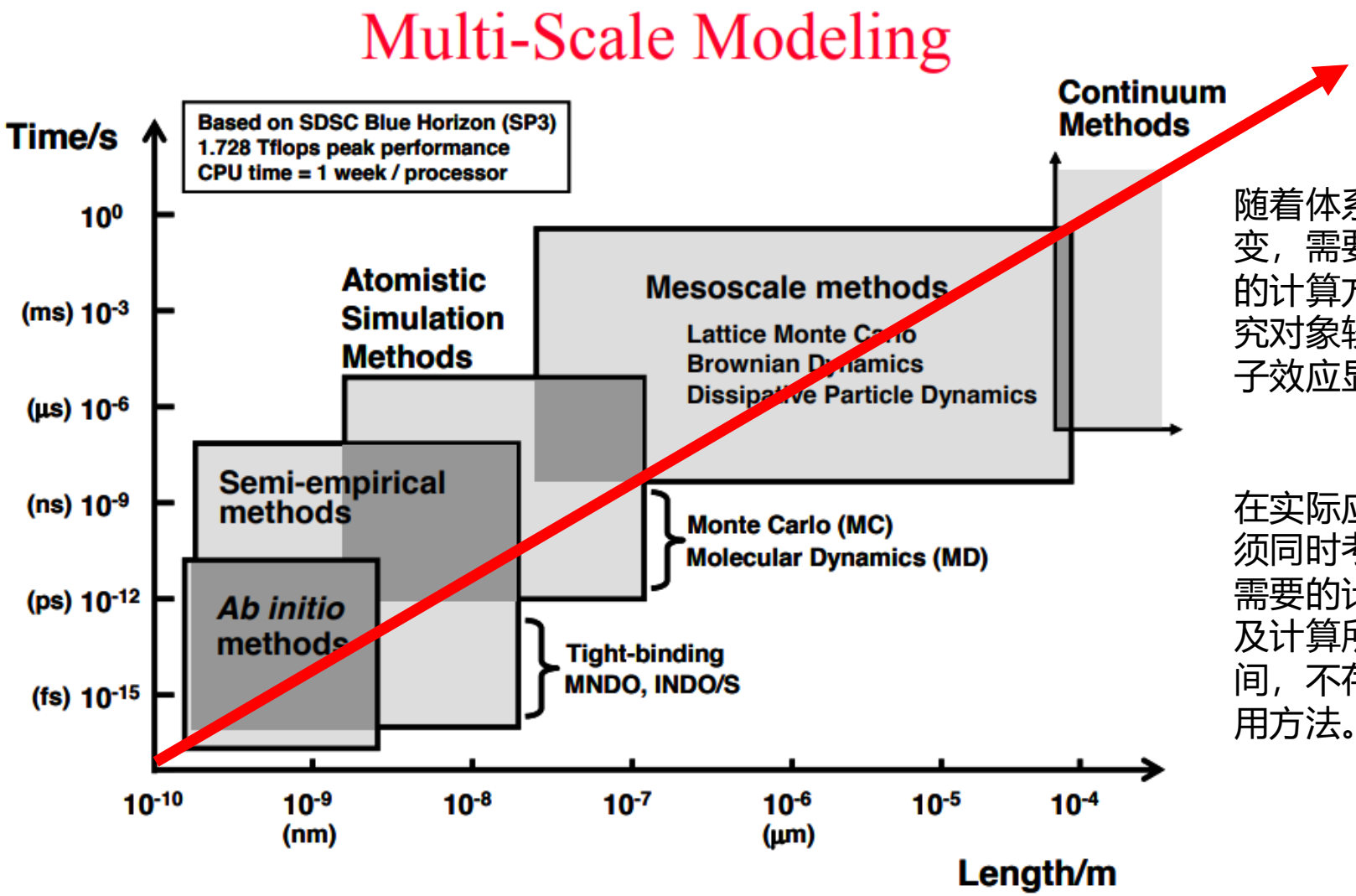


典型分子现象的时间尺度



G. R. Fleming and P. G. Wolynes, Physics Today, p. 36, May 1990

不同时间-空间尺度现象对应的计算方法

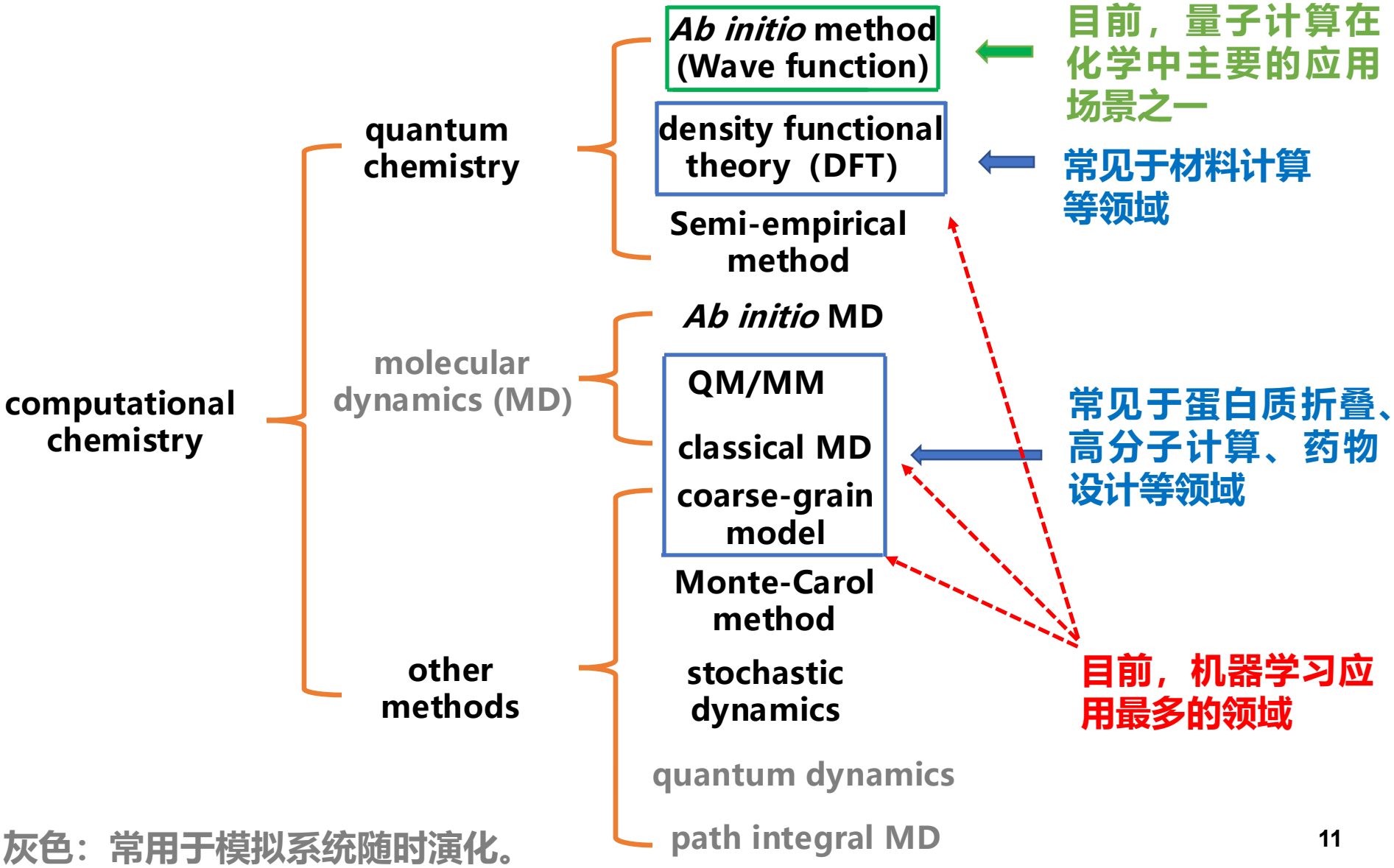


随着体系尺度的改变，需要选取不同的计算方法，当研究对象较小时，量子效应显著增加。

在实际应用中，必须同时考虑体系所需要的计算精度以及计算所花费的时间，不存在一个通用方法。

F.R. Hung, K.E. Gubbins, and S. Franzen, *Chemical Engineering Education*, Fall 2004

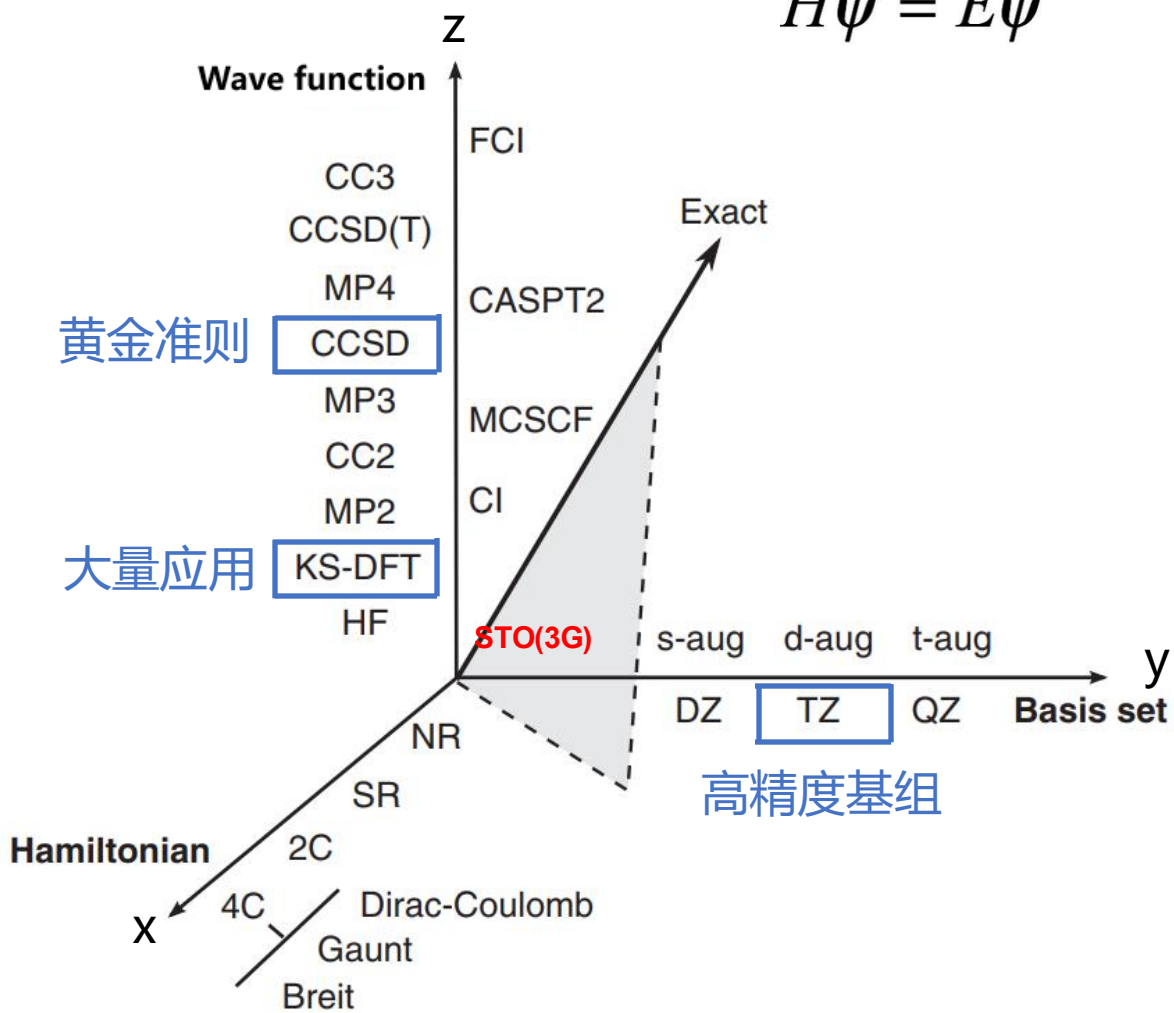
计算化学/物理的分支



灰色：常用于模拟系统随时演化。

量子化学问题的计算

$$\hat{H}\psi = E\psi$$



量子计算化学常用组合：
NR+STO(3G)+UCCSD

谷歌的工作：
NR+STO(3G)+HF

经典算法复杂度：

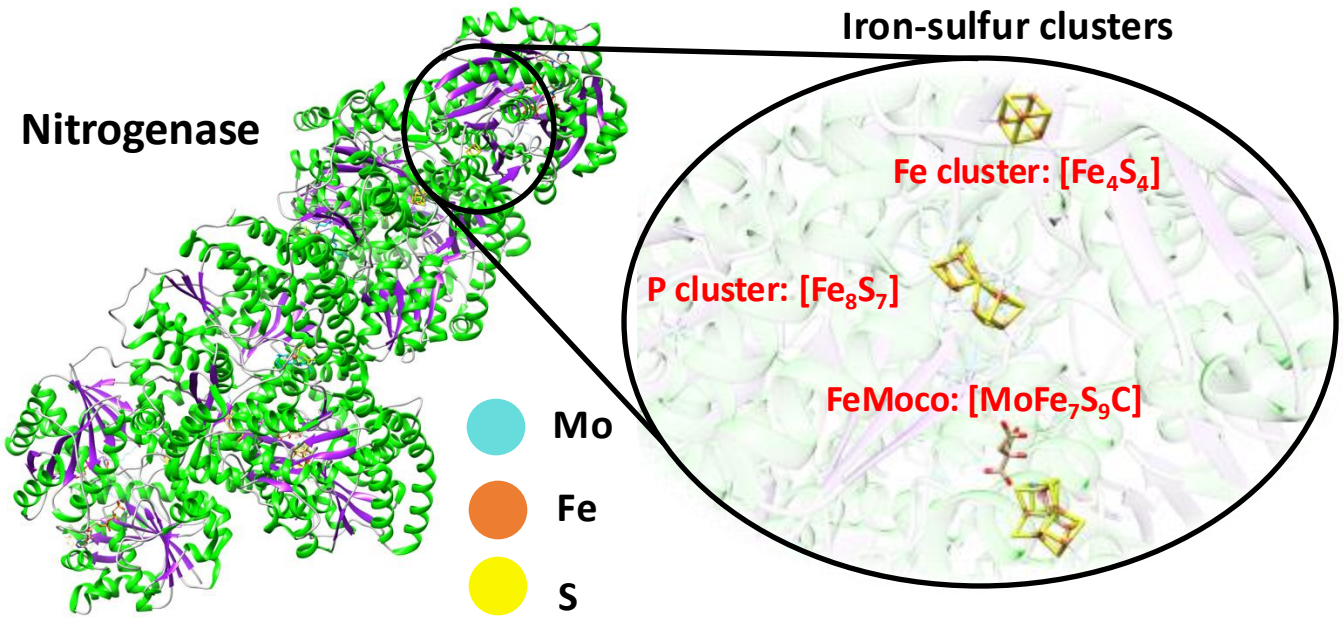
HF: N^4
DFT: $N^{3\text{-}4}$
MP2: N^5
CCSD: N^7
FCI: exp

量子相位估计（QPE）在某些具体问题中可以使基态计算具有指数优势。

A. Aspuru-Guzik, A. D. Dutoi, et al., Science 309, 1704 (2005)

经典计算 vs. 量子计算

$$N_2 + 8H^+ + 8e^- + 16ATP \rightarrow 2NH_3 + H_2 + 16ADP + 16P_i$$



目前观点认为量子计算可以有效处理固氮酶等强关联系统的计算问题。

Z. Li, et al., Nat. Chem. 11, 1026 (2020)

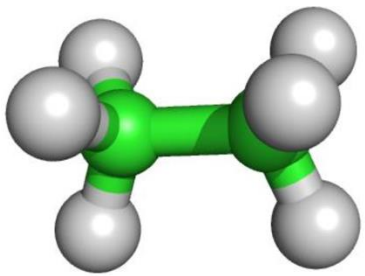
D. Berry, et al., Quantum 3, 208 (2019)

Problem		Physical qubits		Execution time (h)	
System	Spin orbitals (N)	$p = 10^{-3}$	$p = 10^{-4}$	$p = 10^{-3}$	$p = 10^{-4}$
Hubbard model	72	1.4×10^6	4.4×10^5	4.6	2.6
Hubbard model	128	2.1×10^6	6.6×10^5	15	8.4
Hubbard model	200	3.2×10^6	8.9×10^5	40	21
Hubbard model	800	1.4×10^7	3.6×10^6	6.7×10^2	3.7×10^2
Electronic structure	54	1.4×10^6	3.9×10^5	0.82	0.43
Electronic structure	128	2.4×10^6	8.1×10^5	9.9	5.6
Electronic structure	250	4.4×10^6	1.2×10^6	58	30
Electronic structure	1024	2.0×10^7	4.8×10^6	2.7×10^3	1.4×10^3

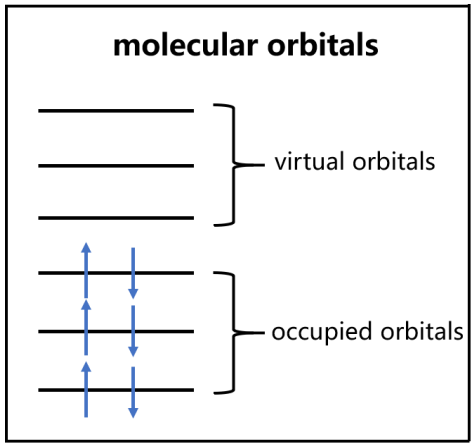
R. Babbush, et al., Phys. Rev. X 8, 041015 (2018)

变分量子本征求解器 (VQE)

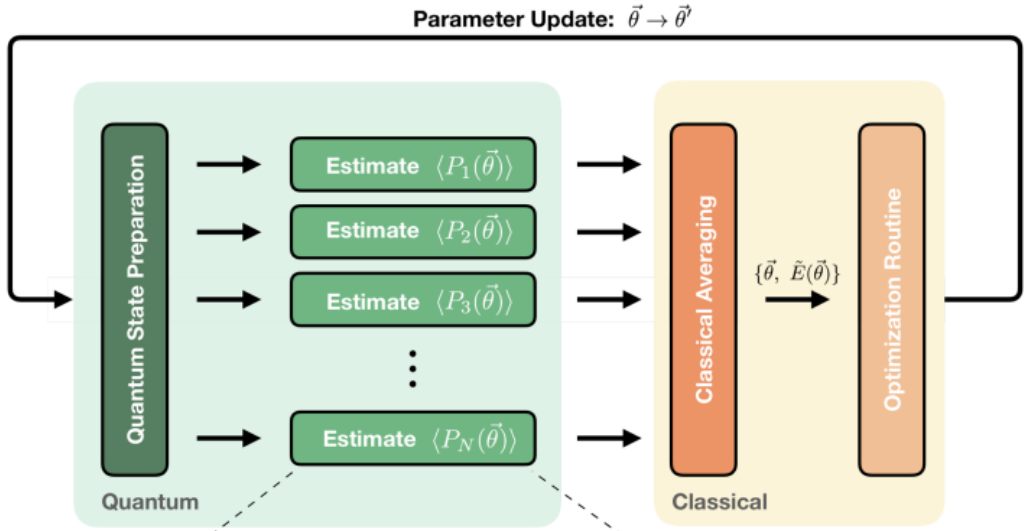
$$\hat{H}\psi = E\psi$$

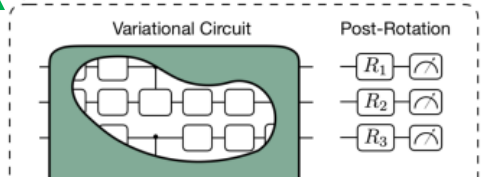


Born-Oppenheimer approximation
Single determinant approximation
Mean field approximation



Variational quantum eigensolver (VQE)





Encoding:
JW
Parity
BK

Ansatz:
Unitary couple cluster
Hardware-efficient ansatz
Tensor network

$$H = \sum_{p,q=1}^{K} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{p,q,r,s=1}^{K} h_{pqrs} a_p^\dagger a_q^\dagger a_s a_r$$

$$|\Phi(\boldsymbol{\theta})\rangle = U(\boldsymbol{\theta})|\Phi_0\rangle = e^{T(\boldsymbol{\theta}) - T^\dagger(\boldsymbol{\theta})}|\Phi_0\rangle$$

Y. Cao, et al, Chem. Rev., **119**, 10856 (2019).

一些量子计算化学实验

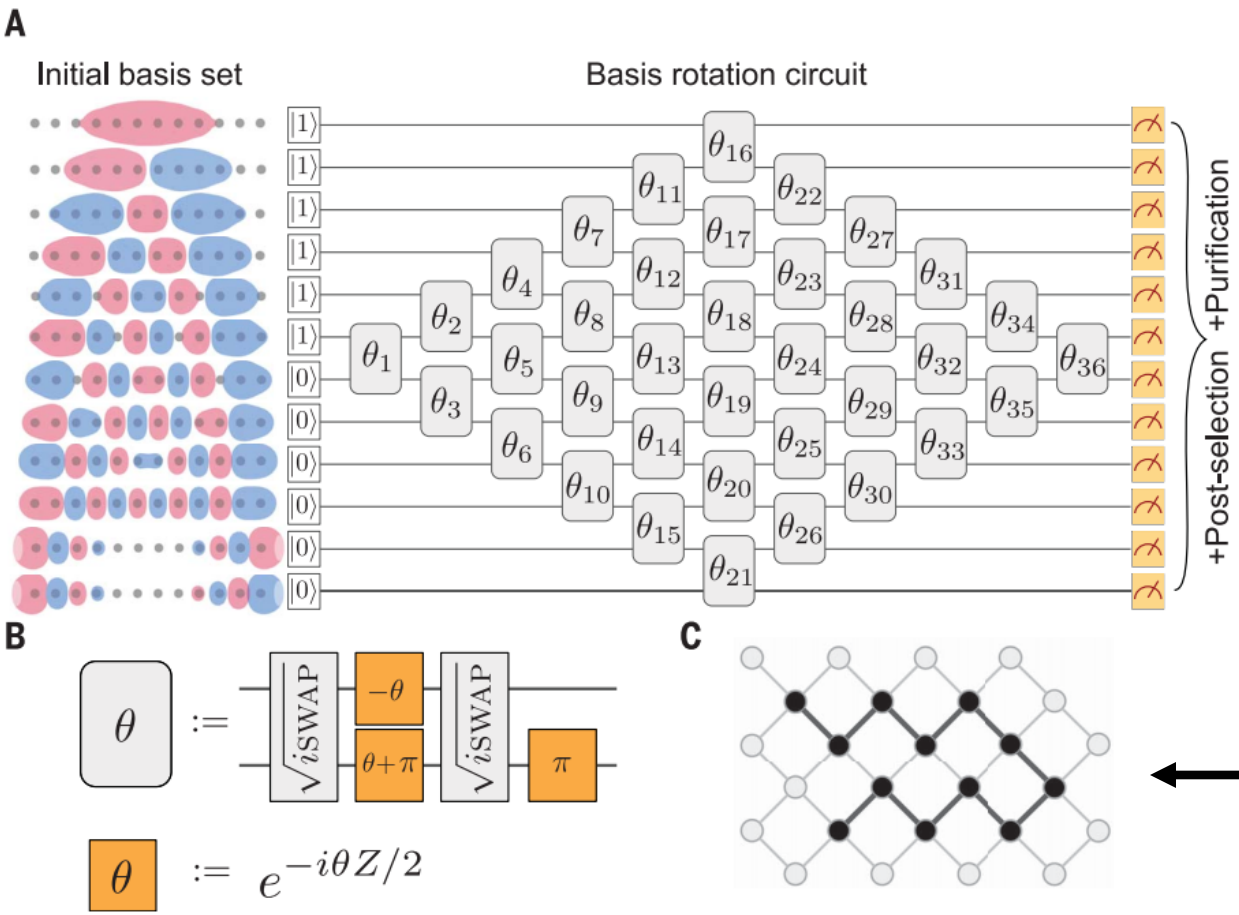
Table 2. Comparison between this work and previous publicly-reported VQE chemistry simulations on QPUs.

Year	Ansatz	System	# Qubits	# Parameters	2QGE[a]	Full VQE?	Error Mitigation?	Hardware Vendor
2022	oo-upCCD [this work]	Li_2O	12	72	12	Yes	Yes	IonQ
2022	upCCD[28]	Cyclobutene Ring	10	25	25	No	Yes	Google
2022	uCCSD[52]	$CH_3^{\cdot}$	6	4	7	No	Yes	Quantinuum
2022	YXXX[53]	oxazine derivatives	4	1	N/A[b]	Yes (superconducting), No (trapped-ion)	Yes	IBM, Quantinuum
2022	uCCSD-PBC[54]	crystalline iron model	2	1	2	Yes	Yes	IBM
2022	Entang. Forging[55]	H_3S^+	6	8	19	No	Yes	IBM
2022	Entang. Forging[56]	H_2O	5	3	11	Yes	Yes	IBM
2021	HEA[3]	LiH (dipole moment)	4	16	9	Yes	Yes	IBM
2021	HEA[27]	TADF	2	4	1	Yes	Yes	IBM
2021	qubit CC[34]	H_{10}	2	3	1	No	Yes	IonQ
2021	HEA[57]	Li_2O_4 model	2	4	1	Yes	Yes	IBM
2020	Hartree-Fock[14]	H_{12}	12	36	72	Yes	Yes	Google
2020	upCCD[15]	H_2O	3	3	6	Yes	No	IonQ
2019	HEA[26]	LiH	4	20	9	Yes	Yes	IBM
2019	reduced uCC[20]	NaH, KH, RbH	4	3	8	No	Yes	IBM, Rigetti
2018	uCCSD[19]	LiH	3	2	4	Yes	No	UInn
2018	uCCSD[44]	H_2 (excited states)	2	1	1	Yes	No	UCB, LBNL
2017	HEA[13]	BeH_2	6	30	5	Yes	No	IBM
2016	uCCSD[12]	H_2	2	1	2	No (scan)	No	UCSB
2014	uCCSD[11]	HeH^+	2	6	1	Yes	No	Univ. of Bristol

[a]2QGE: 2-qubit gate equivalents.
[b]The authors did not provide this in their paper.

L. Zhao, et al., npj Quantum Inf. **9**, 60 (2022)

Hartree-Fock方法



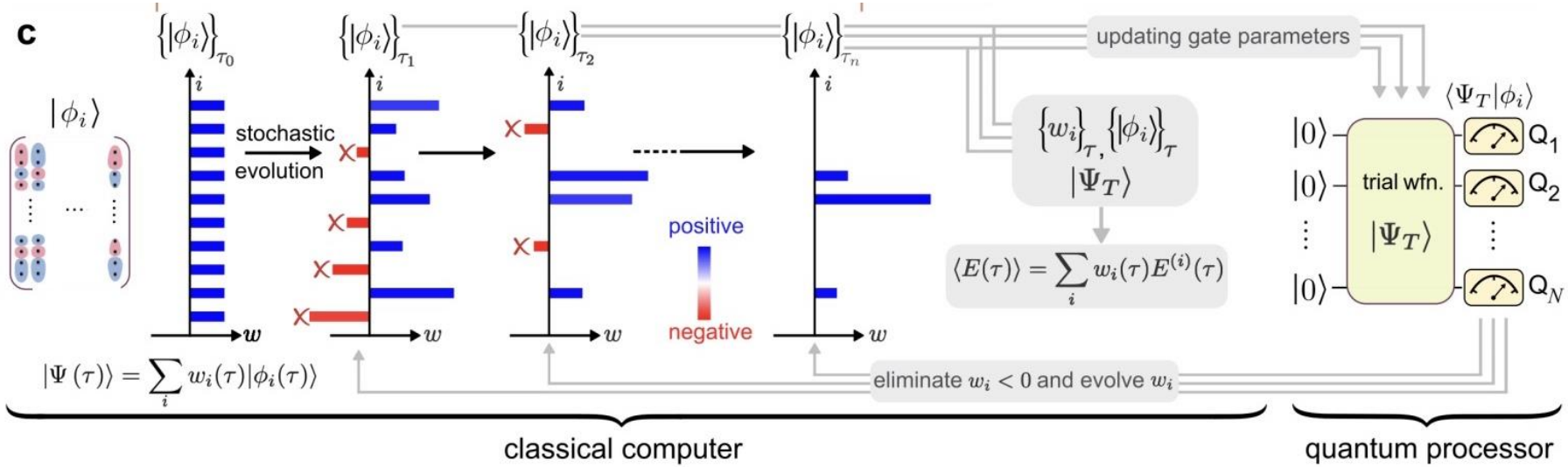
利用Givens rotation 实现矩阵对角化。

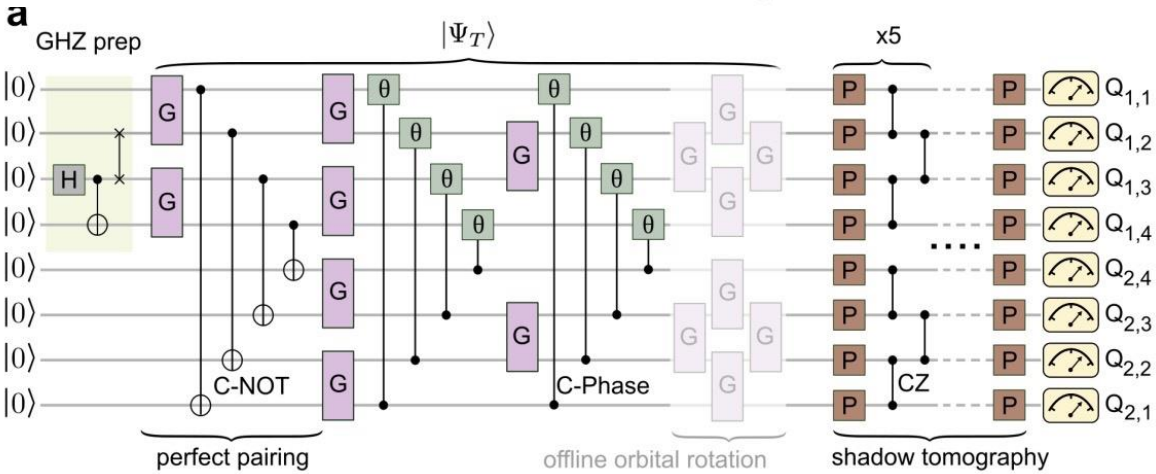
$$
\begin{pmatrix}
* & * & * & * & * & * & * & * & * \\
8 & * & * & * & * & * & * & * & * \\
7 & 9 & * & * & * & * & * & * & * \\
6 & 8 & 10 & * & * & * & * & * & * \\
5 & 7 & 9 & 11 & * & * & * & * & * \\
4 & 6 & 8 & 10 & 12 & * & * & * & * \\
3 & 5 & 7 & 9 & 11 & 13 & * & * & * \\
2 & 4 & 6 & 8 & 10 & 12 & 14 & * & * \\
1 & 3 & 5 & 7 & 9 & 11 & 13 & 15 & *
\end{pmatrix}
$$

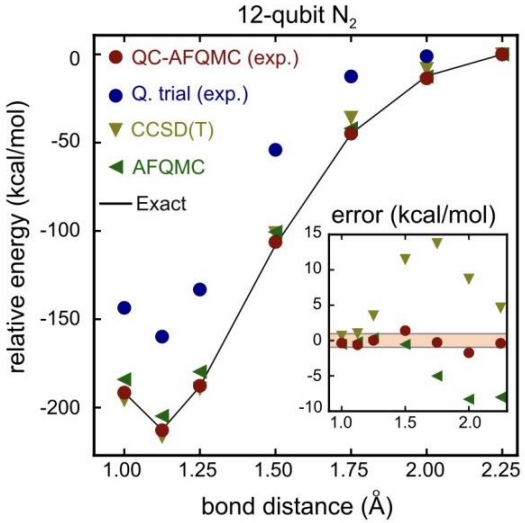
量子比特只需要线性相连

Google AI Quantum and Collaborators, Science, **369**, 1084 (2020)

辅助场量子蒙特卡洛（AFQMC）方法

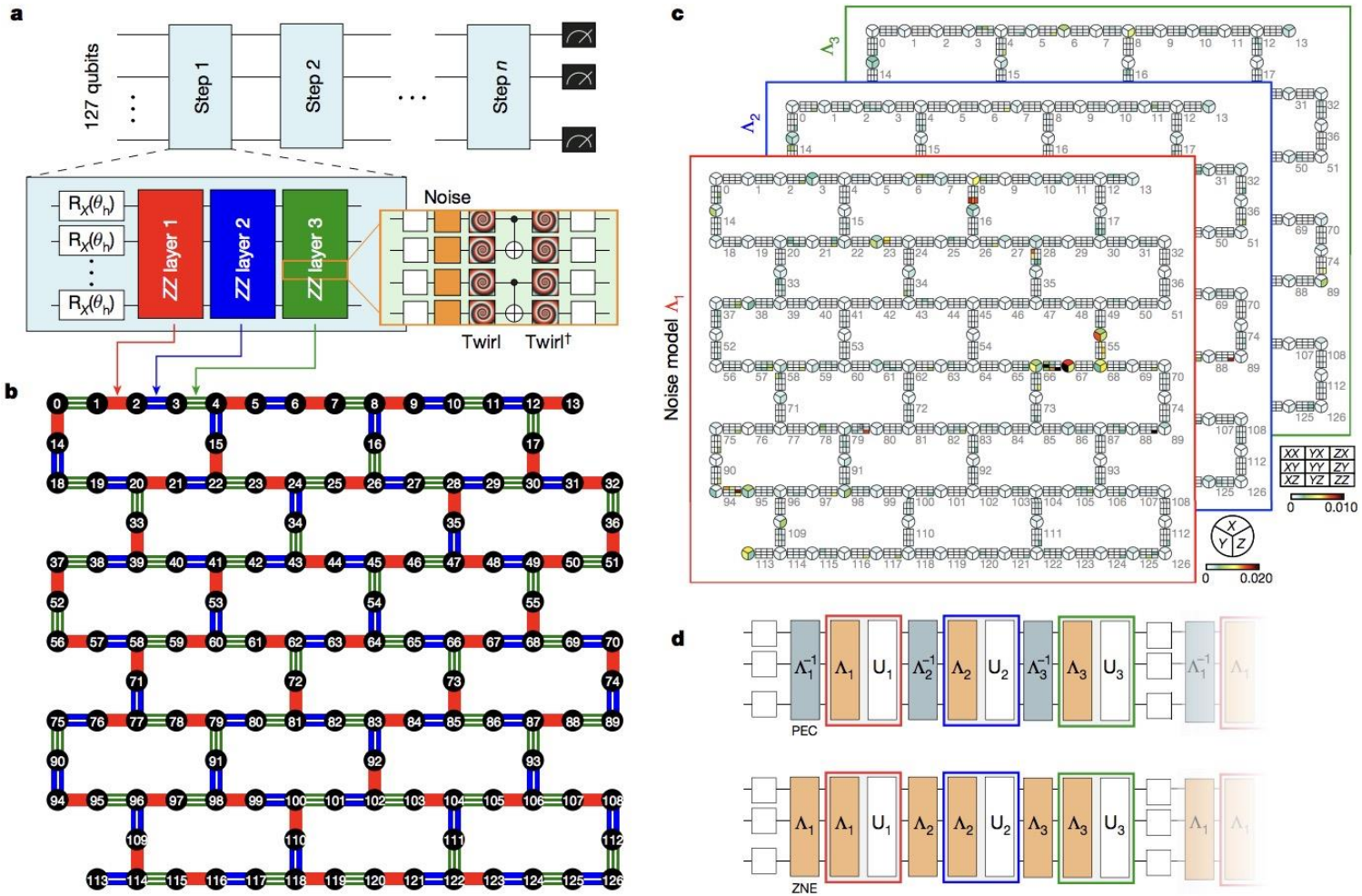






W. Huggins. et al., Nature, **603**, 416 (2022)

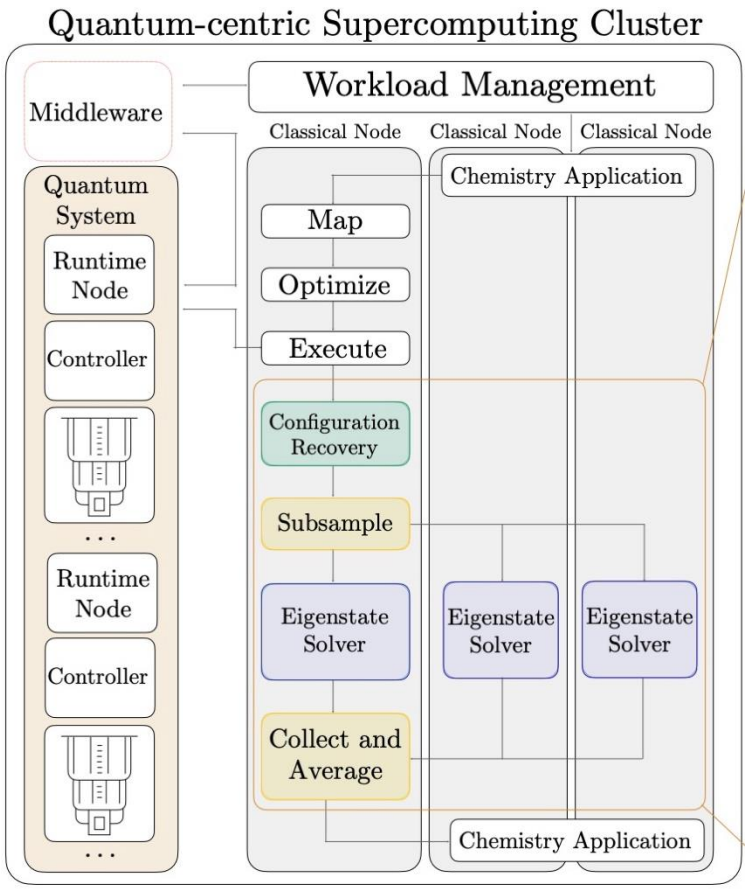
横场伊辛模型的模拟

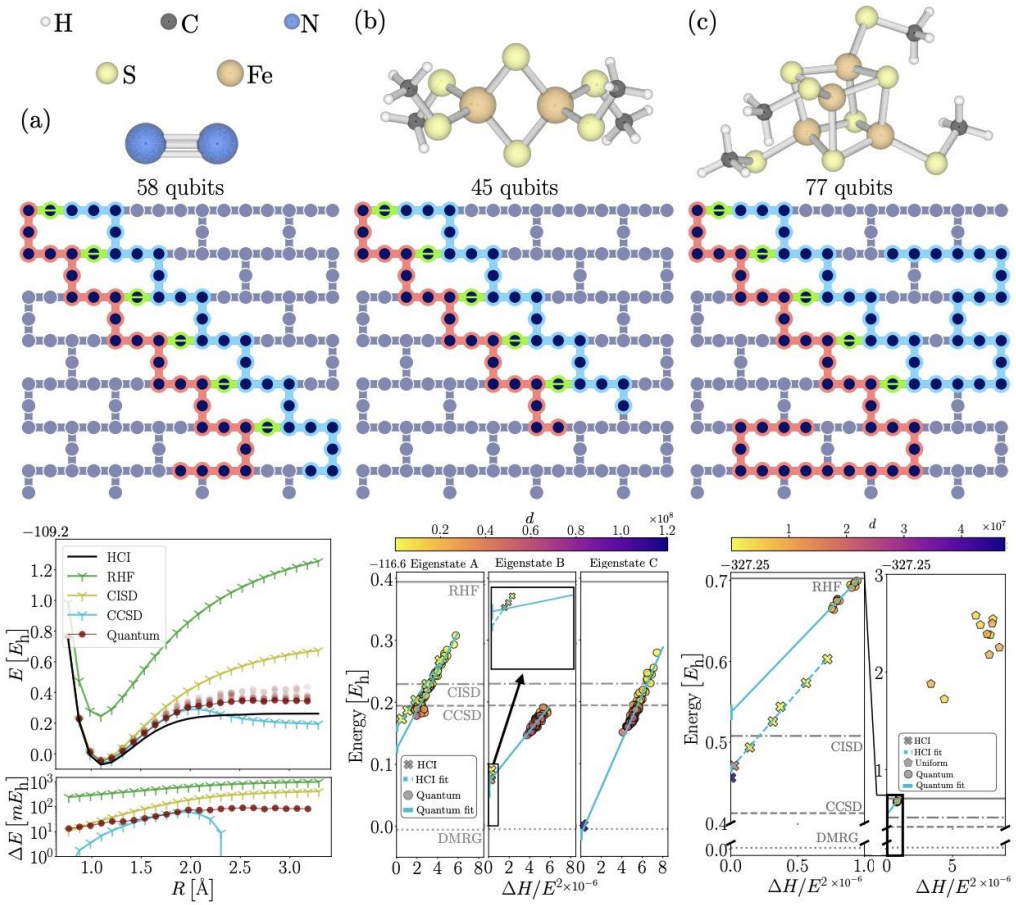


IBM实现了127比特的横场伊辛模型的含时演化模拟，该模拟是当前最大的多体系统演示实验。

IBM group, Nature, **618**, 500 (2023)

量子计算-超算结合的方案

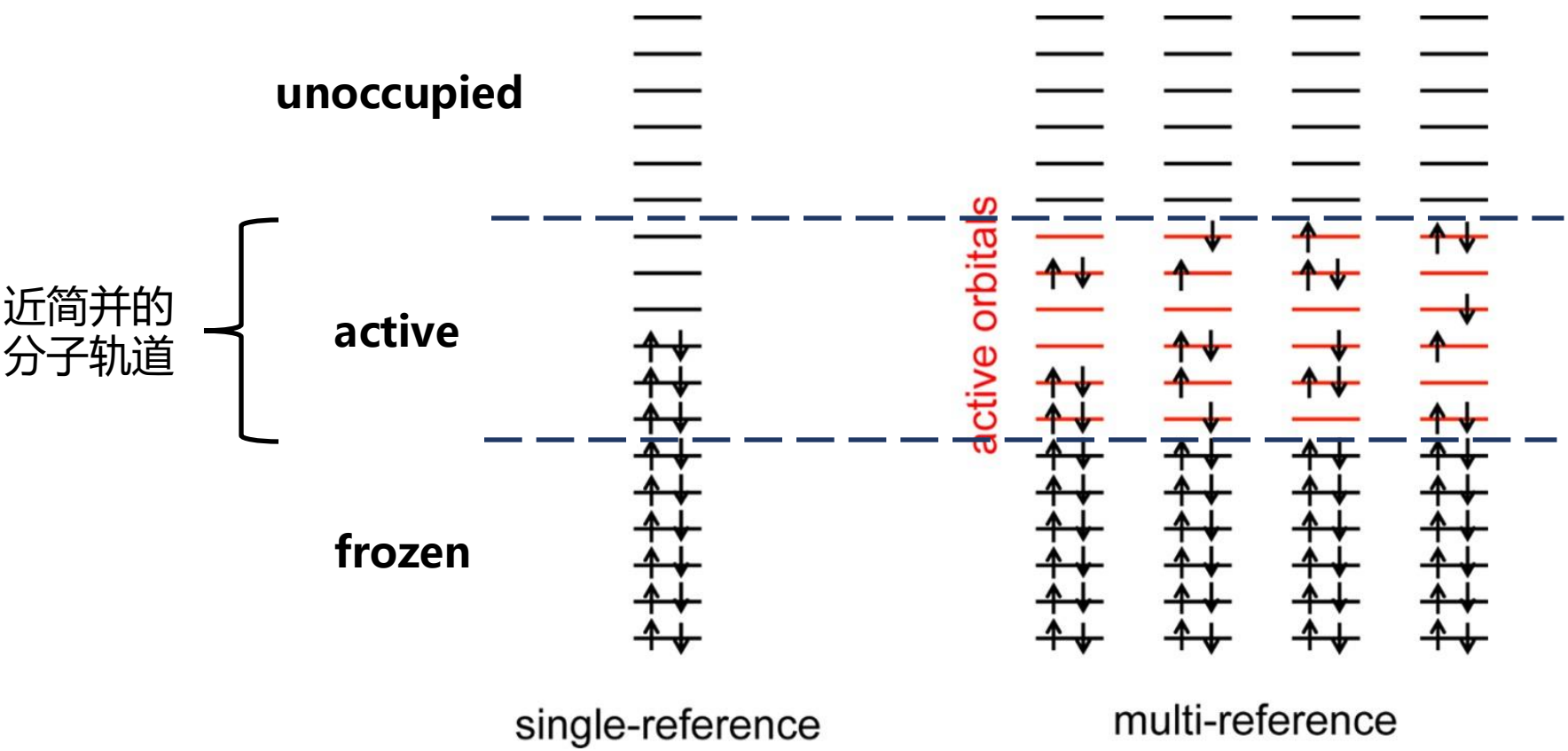




IBM实现了基于selective CI方法的量-超融合展示。其核心思想是利用量子计算机给出初始构象的猜测，利用超算进行优化。

J. Robledo-Moreno, et al., Nature, arXiv: 2405.05068 (2024)

多参考态量子计算方案



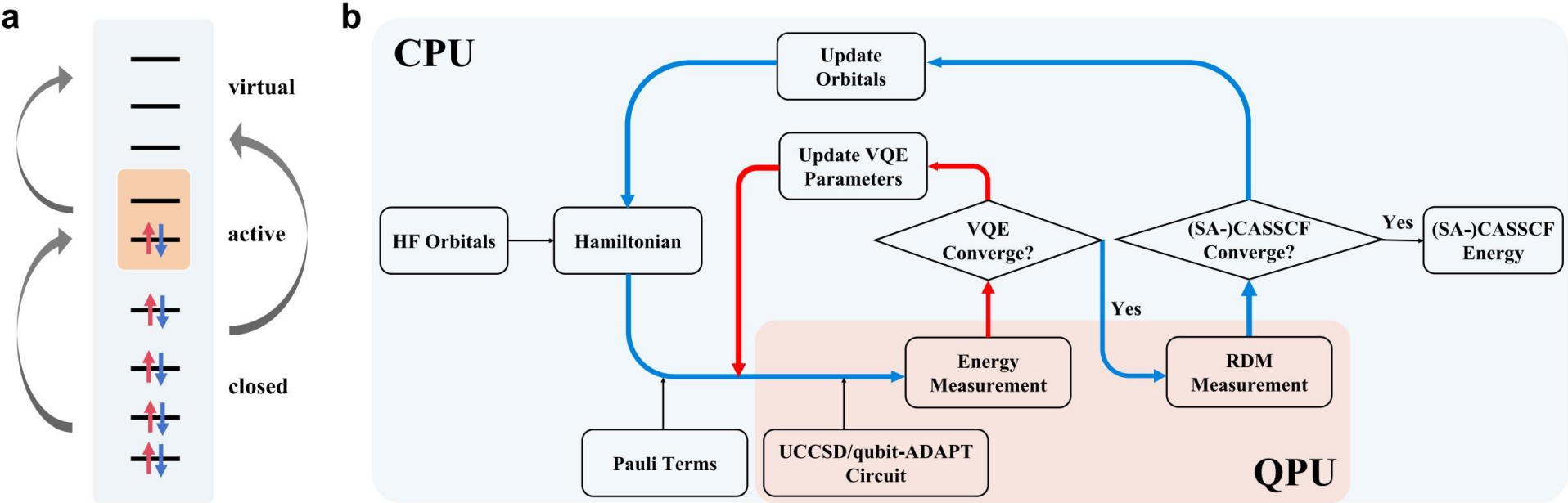
$$|CASSCF\rangle = |Active\rangle \otimes |Core\rangle = e^{-\sum_{pq} R_{pq} a_q^{+} a_p} \sum_n c_n |n\rangle$$

量子经典混合CASSCF的计算流程

CASSCF体系总能量为

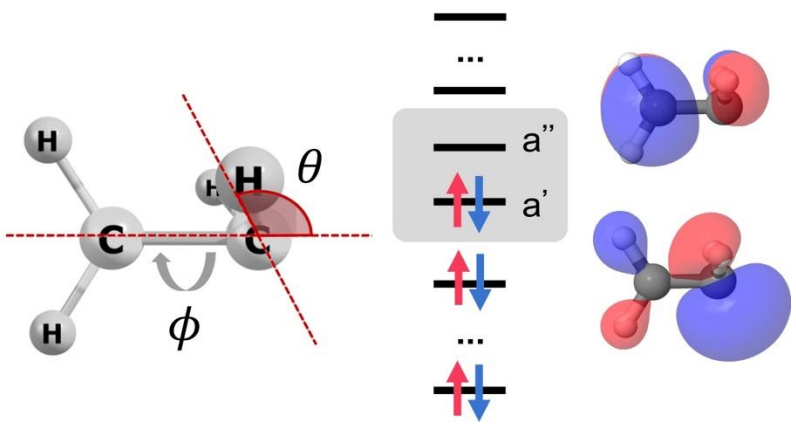
$$E = \langle CASSCF | \hat{H} | CASSCF \rangle = \sum_{pq} h_{pq}\gamma_{pq} + \sum_{pqrs} g_{pqrs}\Gamma_{pqrs} + E_{nuc}$$

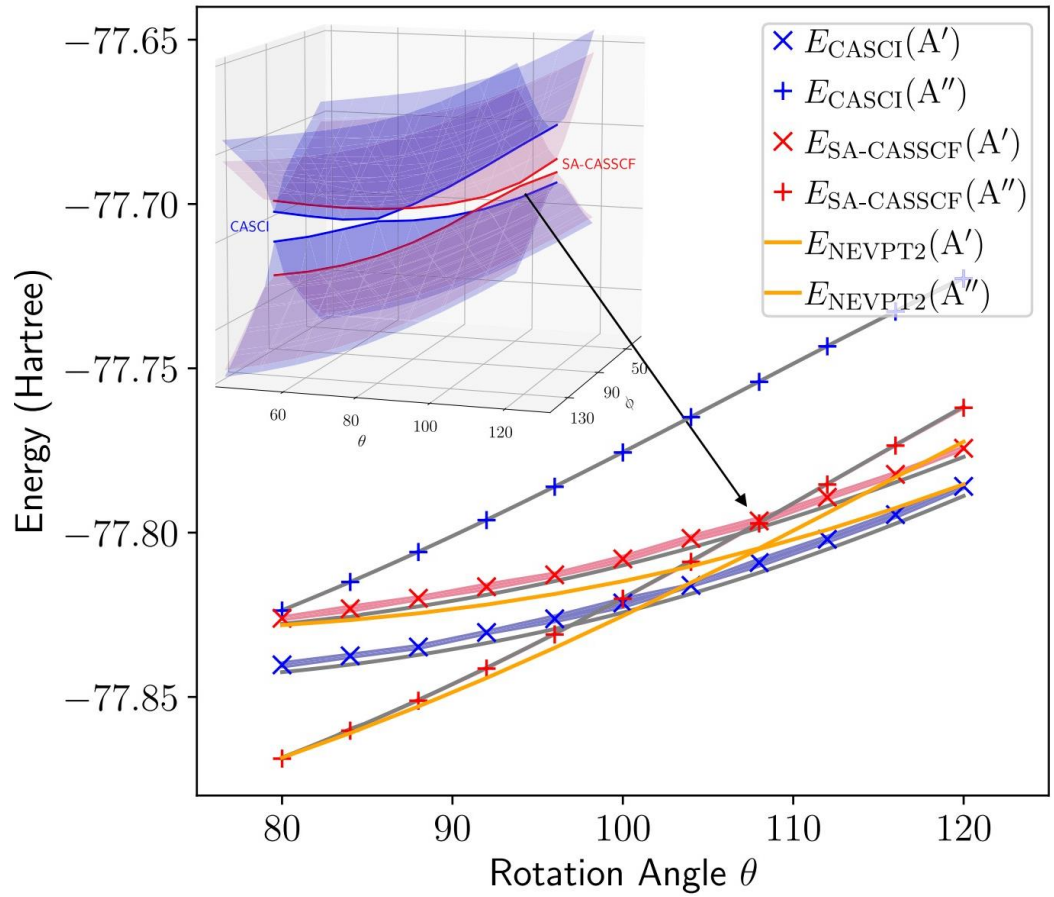
VQE-SA-CASSCF



S. Zhao, et al., J. Phys. Chem. Lett. **15**, 7244 (2024).

乙烯的计算





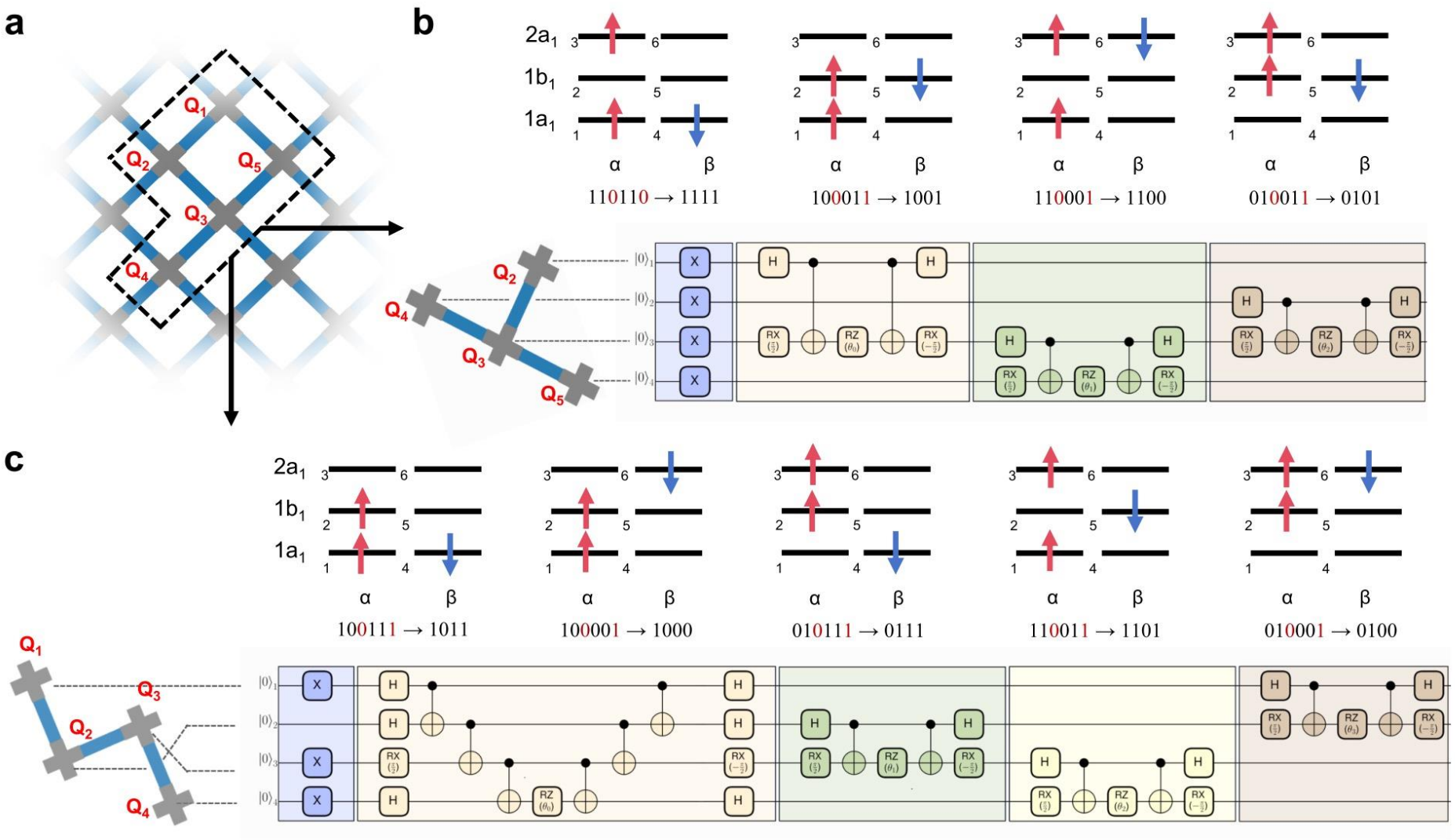
真实器件下，乙烯体系CASSCF与CASCI能量的相对关系被正确地重复出来。

真实器件下的VQE-SA-CASSCF定量复现了乙烯势能面的交叉点：

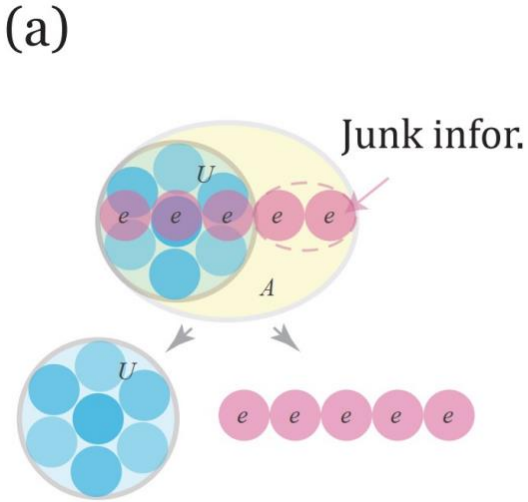
理论值：106.8度

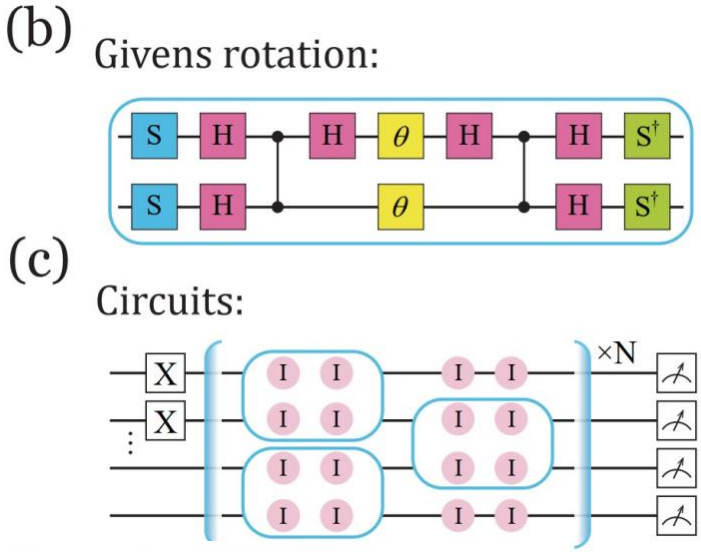
实验值：108.0度

H_3线路的映射

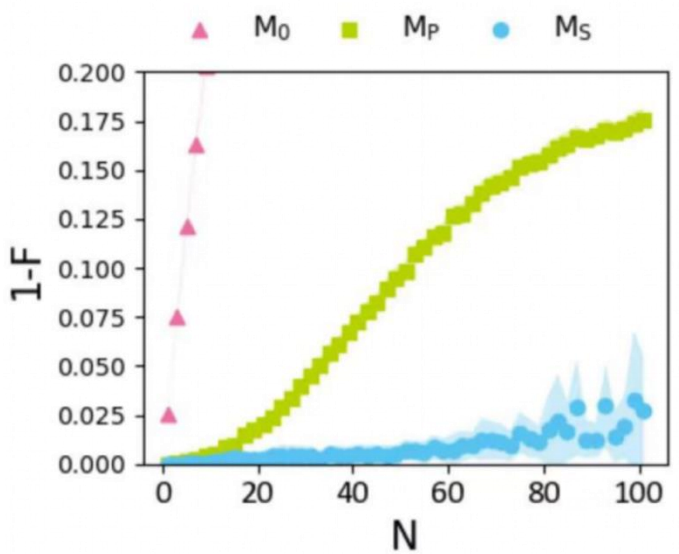

a
b
c
Q1
Q2
Q3
Q4
Q5
2a1
1b1
1a1
α
β
110110 → 1111
100011 → 1001
110001 → 1100
010011 → 0101
100111 → 1011
100001 → 1000
010111 → 0111
110011 → 1101
010001 → 0100

快速消除去极化噪声的方法





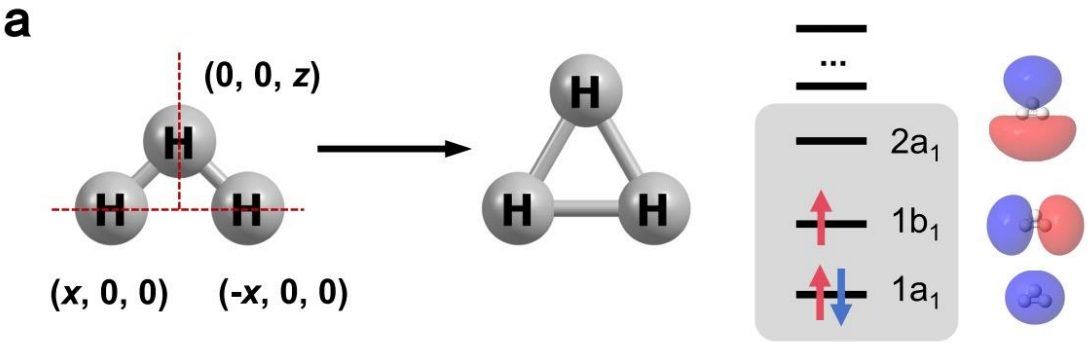
研究对象编码为比特后，可分为物理态与非物理态。
例：分子轨道编码（4个轨道，2个电子）

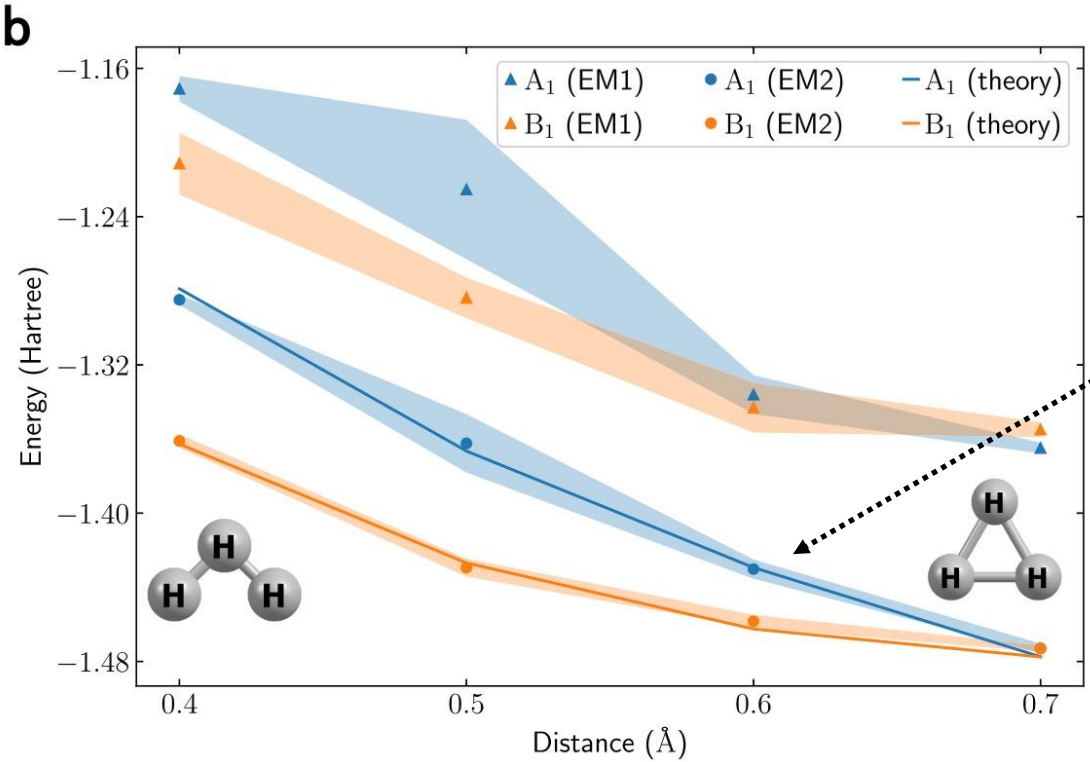


随着线路深度的增加，该方案可有效地降低态分布的错误率。

R. Wang, et al., arXiv: 2402.10480v1 (2024).

H_3的计算



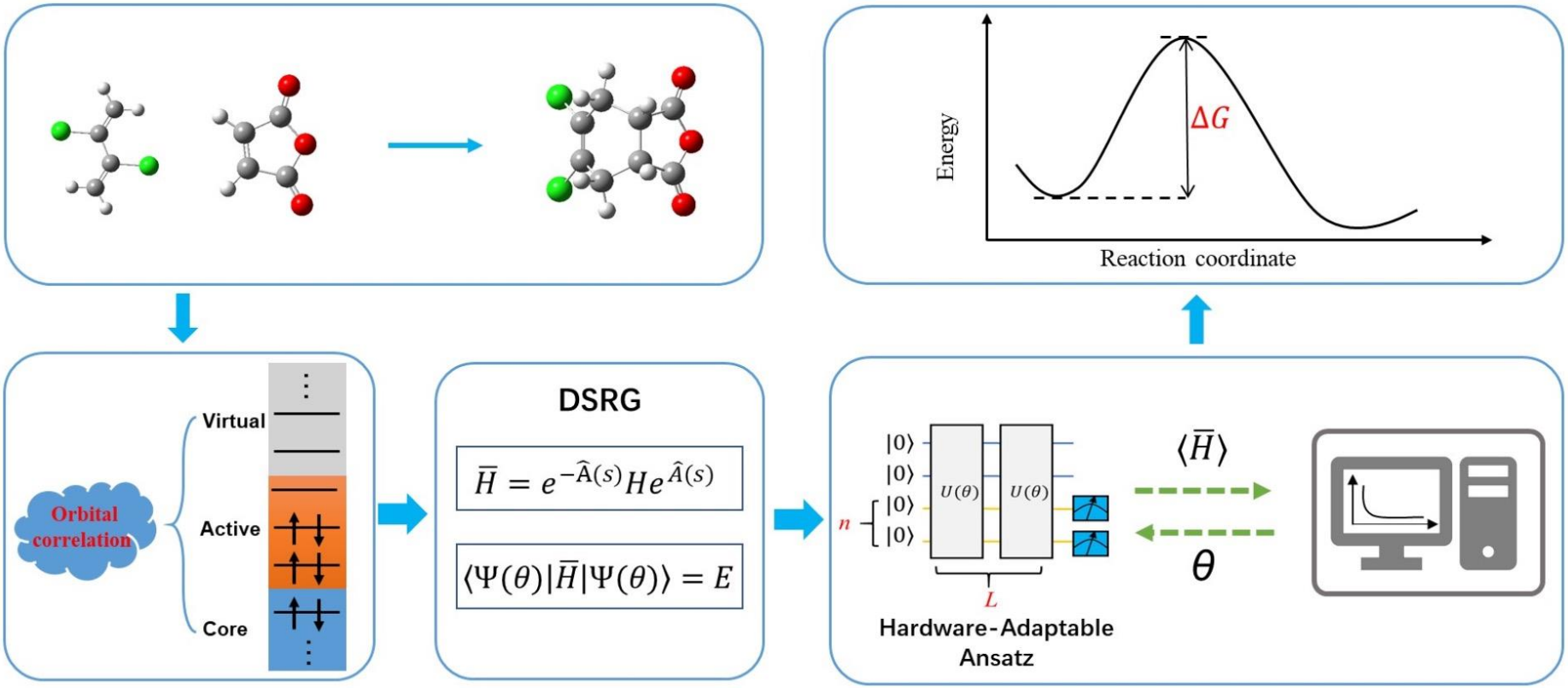


1. 常见的错误缓解（error mitigation）方案,如零噪声外推（ZNE）、概率消除（PEC）需要增加一个数量级的测量时间。

2. 这里使用新开发的基于系统对称性的概率分布重整，在不增加测量的前提下，把实验能量值优化到理论值附近。

基于量子云的量子化学计算

化学反应过渡态能量的计算

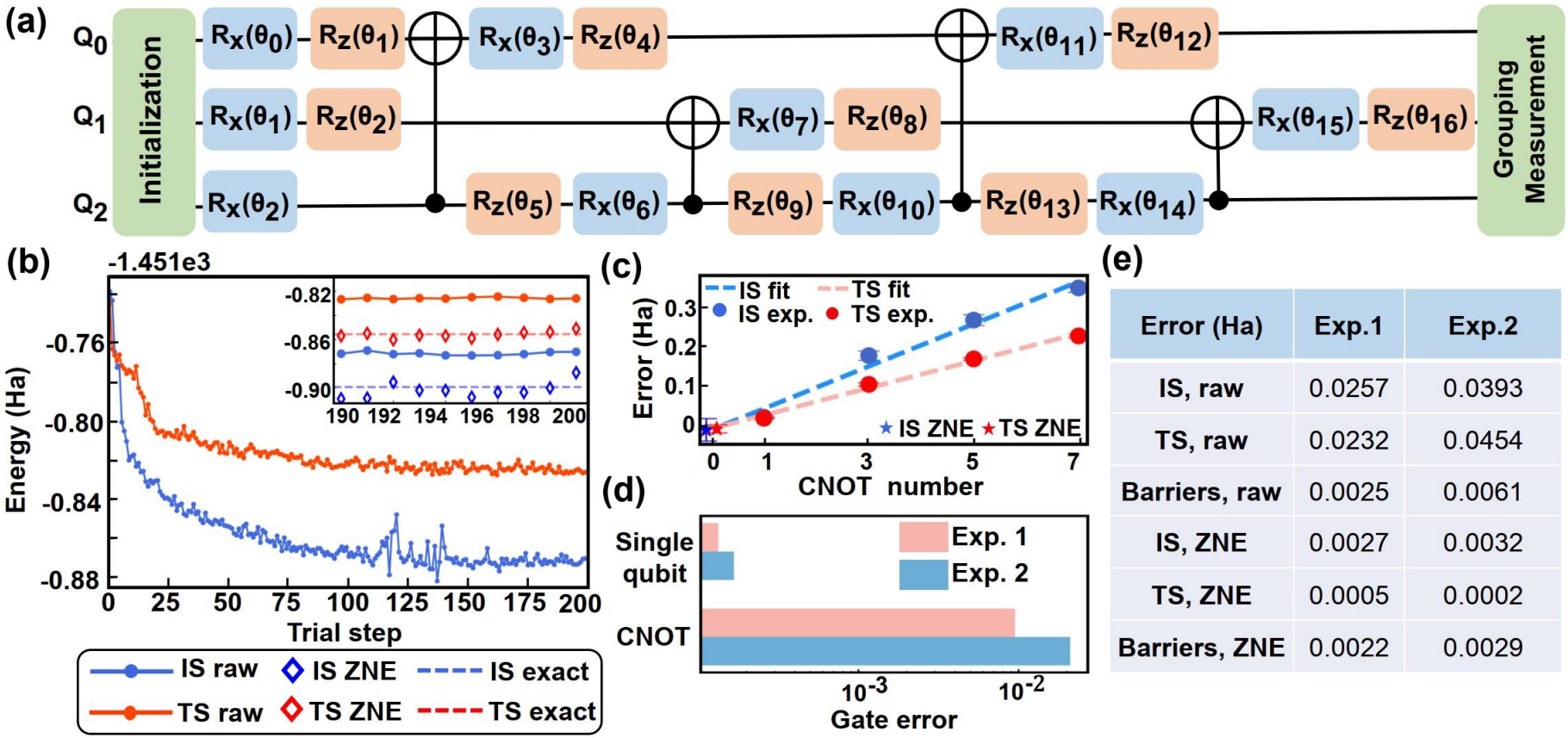


计算流程图：给定分子构象->获得波函数与哈密顿量->编码为量子线路并进行参数优化->获得反应势垒高度。

X. Zeng, et al., arXiv: 2404.14038v1 (2024).

基于量子云的量子化学计算

Baiwang云的计算结果

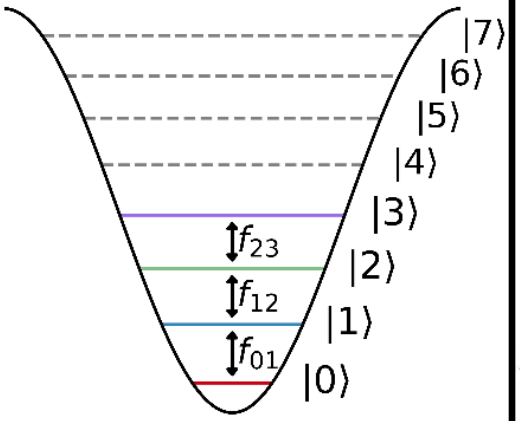


(e)

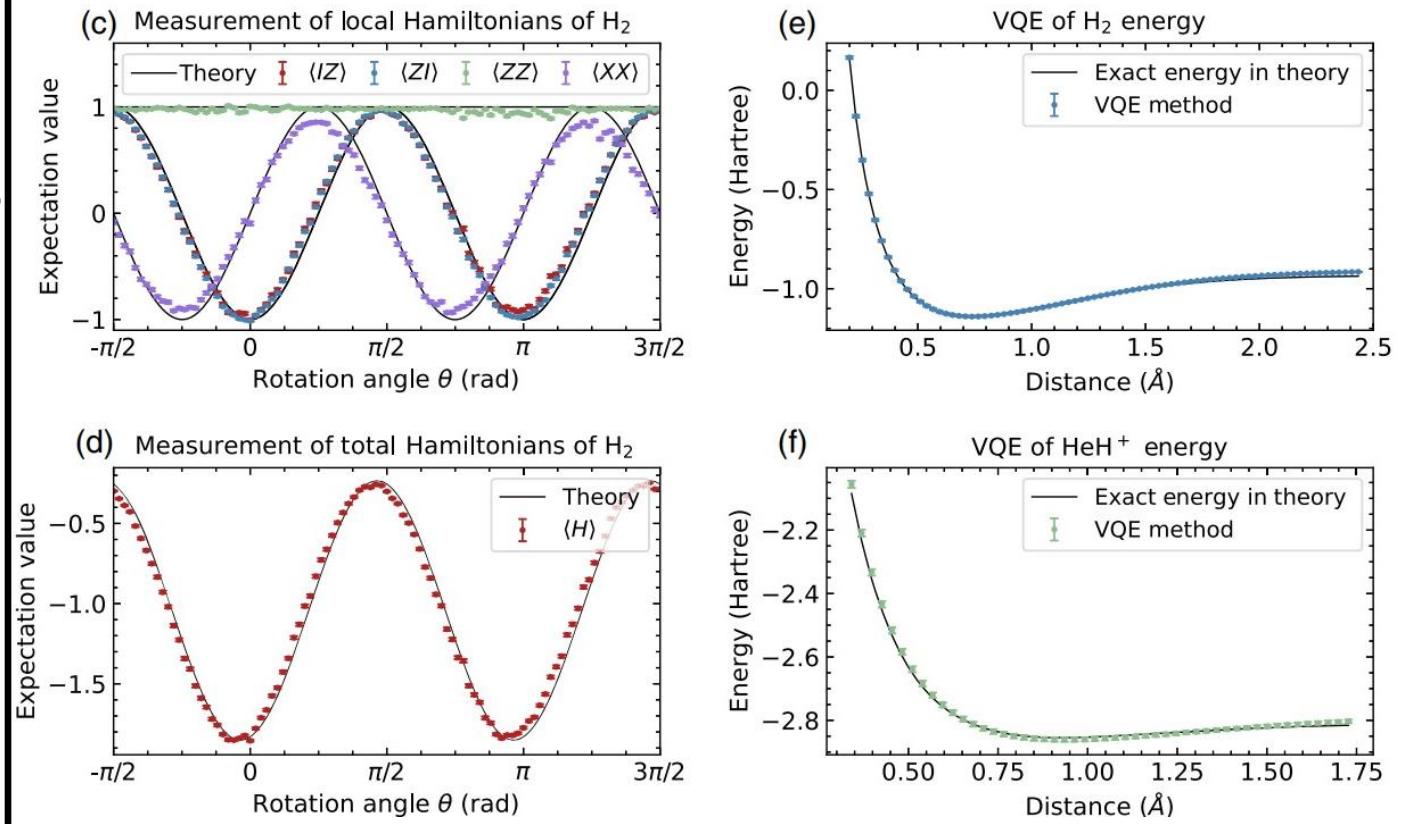
Error (Ha)	Exp.1	Exp.2
IS, raw	0.0257	0.0393
TS, raw	0.0232	0.0454
Barriers, raw	0.0025	0.0061
IS, ZNE	0.0027	0.0032
TS, ZNE	0.0005	0.0002
Barriers, ZNE	0.0022	0.0029

（a）需要优化的量子线路，包含17个变分参数。（b）能量优化过程。（c）对初态和过渡态进行外推。（d）所使用的门保真度。（e）能量计算的结果。

Quantum chemistry on qudit



4能级量子比特



实现了H_2、HeH^+的编码与基态势能面计算。

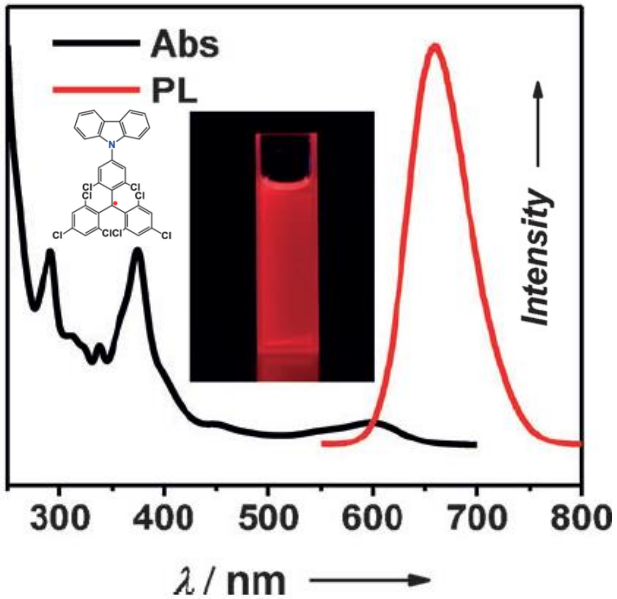
P. Liu, et al., Phys. Rev. X., **13**, 021028(2023)

分子响应性质的量子计算方案

dynamic polarizability

$$\alpha_{zz}(\omega) = \sum_{n>0} \left[\frac{\langle \Psi_0 | \hat{z} | \Psi_n \rangle \langle \Psi_n | \hat{z} | \Psi_0 \rangle}{\omega_{n0} - (\omega + i\gamma)} + \frac{\langle \Psi_0 | \hat{z} | \Psi_n \rangle \langle \Psi_n | \hat{z} | \Psi_0 \rangle}{\omega_{n0} + (\omega + i\gamma)} \right]$$

OLED



Q. Peng, A. Obolda, et al., Angew. Chem. Int. Ed. 54, 1 (2015)

	Classical	FT-era	NISQ-era
Ground state (eigenvalue problem)	DFT, WFT	QPE	VQE
Response properties (linear equation)	TD-DFT, WFT-LRT, etc.	HHL	VQLS

QPE for QC: A. Aspuru-guzik, et al., Science **309**, 1704 (2005)
VQE for QC: A. peruzzo, et al., Nat. comm. **5**, 4213 (2014)
HHL/VQLS for QC: our work
X. Cai, W. Fang, et al., Phys. Rev. Res. **2**, 033324(2020)
K.Huang#, X. Cai#, et al., J. Phys. Chem. Lett. **13**, 9114(2022)

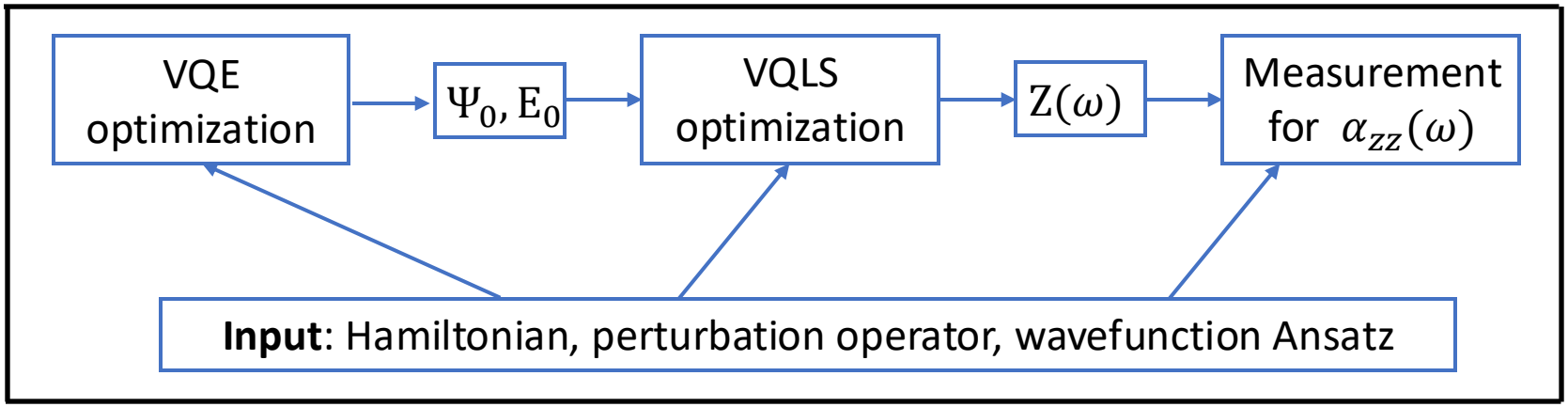
QPE: quantum phase estimation
VQE: variational quantum eigensolver
HHL: Harrow-Hassidim-Lloyd
VQLS: variational quantum linear system

利用VQLS 算法计算动态极化率

Comparation of VQE and VQLS

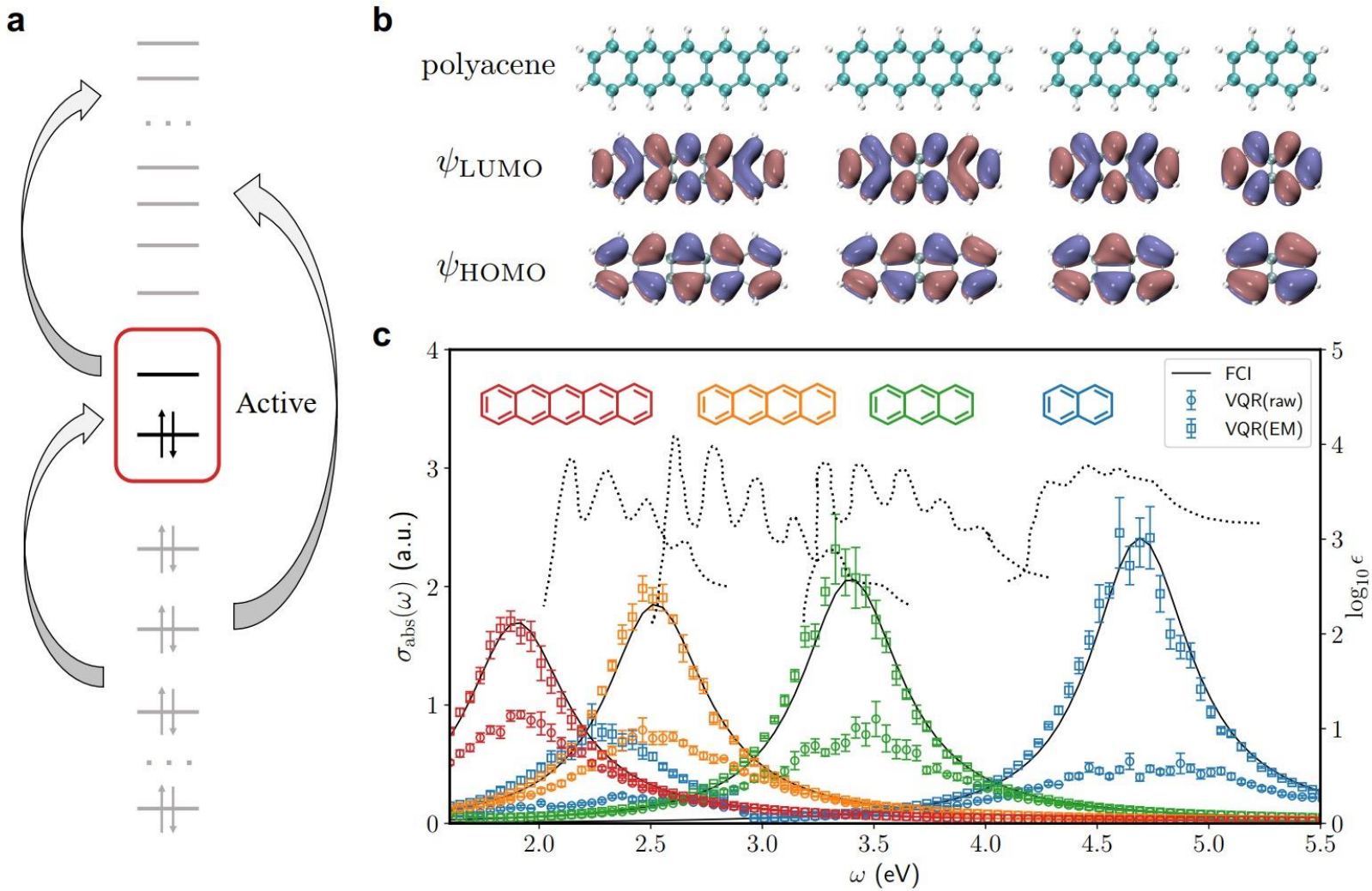
	Satisfied equation	Variational formulation
Ground state	$H\|\Psi\rangle = E\|\Psi\rangle$	$E(\theta) = \langle\Psi(\theta)\|H\|\Psi(\theta)\rangle$
Response state	$\hat{A}(\omega)\|Z(\omega)\rangle = \hat{z}\|\Psi_0\rangle$	$C_p(\theta) = I - \frac{\|\langle \mathbf{b}_{z\psi_0}\|\hat{A}(\omega)\|\mathbf{x}(\theta)\rangle\|^2}{\langle\mathbf{x}(\theta)\|\hat{A}(\omega)^\dagger\hat{A}(\omega)\|\mathbf{x}(\theta)\rangle}$

Flowchart of variational hybrid calculation of polarizablity



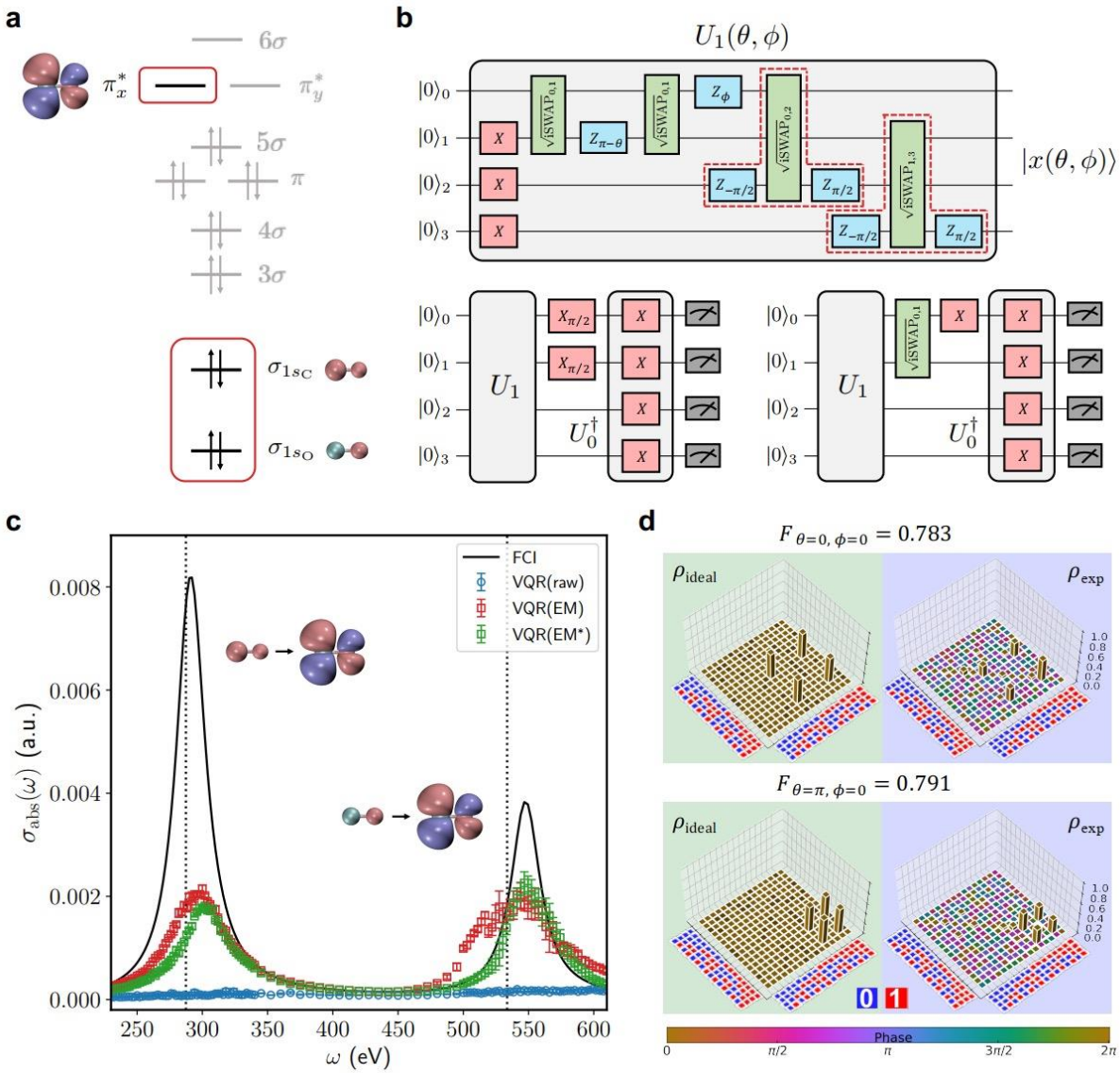
X. Xu, J. Sun, S. Endo, et al., Sci. Bull. **16**, 2181 (2021)

多并苯的紫外-可见光吸收谱



K.Huang, X. Cai, et al., J. Phys. Chem. Lett., **13**, 9114(2022)

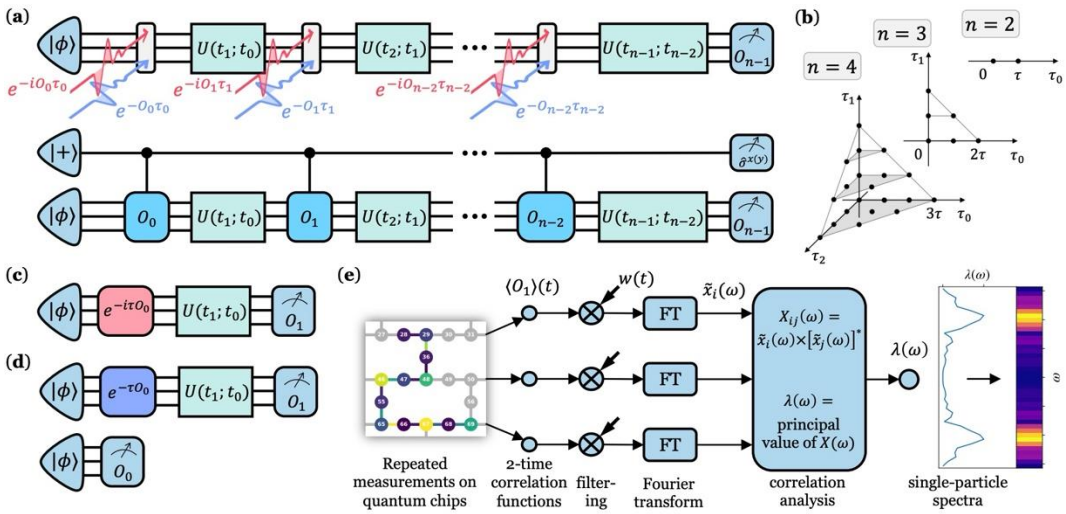
一氧化碳的X射线吸收谱

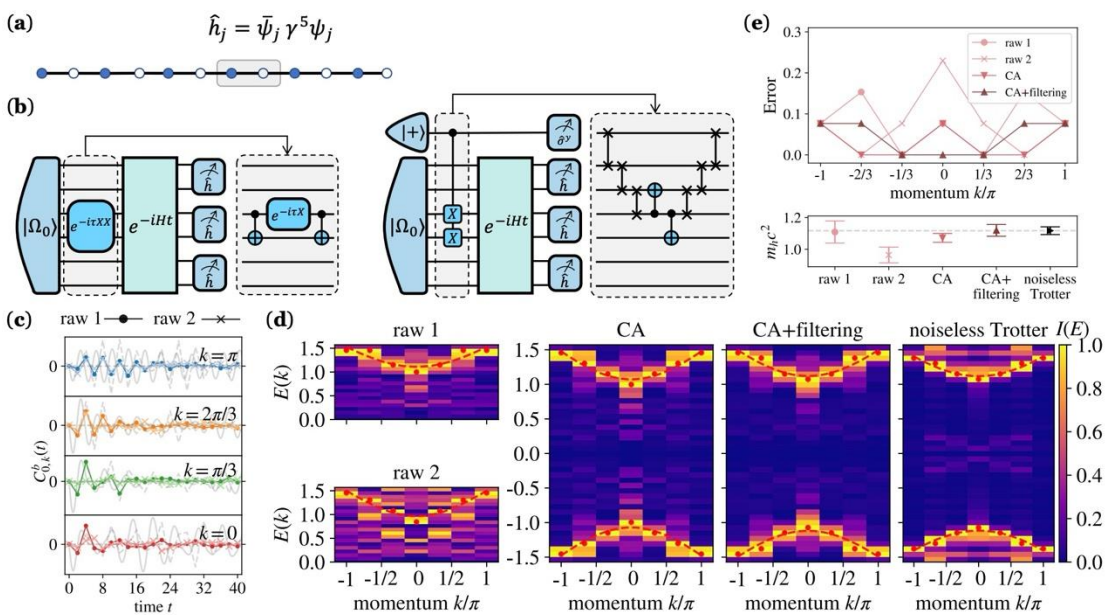


一氧化碳X射线吸收谱，使用Bravyi-Kitaev编码结合Z_2对称性。

K.Huang, X. Cai, et al., J. Phys. Chem. Lett. **13**, 9114(2022)

任意n-点时间关联函数的计算



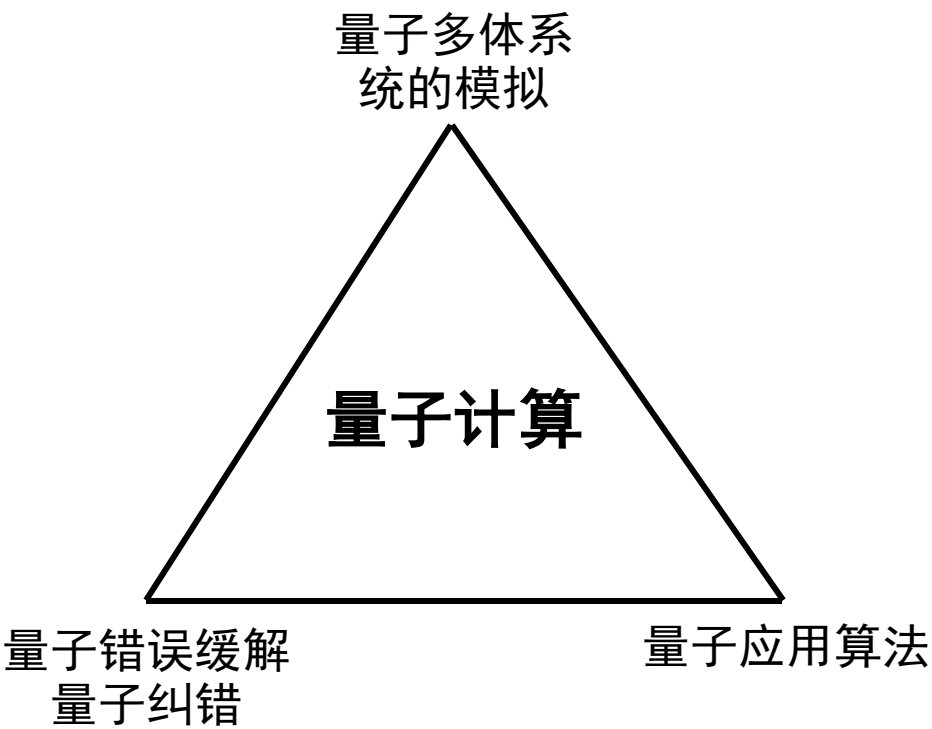


传统计算关联函数的方法需要引入辅助比特，如LCU等。对硬件拓扑结构的要求较高。

利用新的组合错误缓解方法，可以达到高精度的Schwinger model强子谱计算。

X. Wang, L. Xiong, et al., arXiv: 2504.12975 (2025)

总结



量子计算与高能物理的结合
格点场论的模拟
量子精密测量

量子多体系统的模拟
固氮酶
自旋玻璃
高温超导
光合作用
……

量子应用算法
VQE
QITE
QMC
QML
……

量子错误缓解
ZNE
PEC
PS
……

Thanks for attention