Quantum Computing and Energy Storage Research

By Christopher Glenn

Batteries

- Batteries are a critical piece of modern technology
- Typically rely on chemical processes

Chemistry

- Quantum properties
  - Electron orbitals
  - Ground state
- Implications for batteries
  - Energy density
  - Charging/discharging speed

Classical Chemical Modeling

- Goal
  - Solving the Schrödinger equation, calculate ground state and associated energy
- Methods
  - Density functional theory (DFT)
  - Quantum Monte Carlo
  - Tensor network

Classical Chemical Modeling

- Density functional theory
  - Looks at one-body density rather than the many-body wave function
    - Only needs three spatial coordinates
  - Is able to handle reasonably large systems
  - Has been used successfully in lithium-ion battery development
    - Equilibrium cell voltages
    - Voltage curves
    - Ionic mobility
    - Stability (thermal and electrochemical)
  - Depends on certain approximation and assumptions

Classical Chemical Modeling

- Problems
  - DFT
    - Depends on approximations and assumptions
    - Requires knowledge of computational methods, limits, and electrochemistry
    - Reaching limits of certain aspects of battery research
  - Other algorithms
    - Quantum Monte Carlo and tensor network methods are refinable, BUT
    - Massive computing costs

Quantum Chemical Modeling

- Goal: to solve for the ground state eigenvalue E_G and the ground state (the eigenvector) of a Hamiltonian H, as shown here:

$$H|\Phi_G\rangle = E_G|\Phi_G\rangle$$

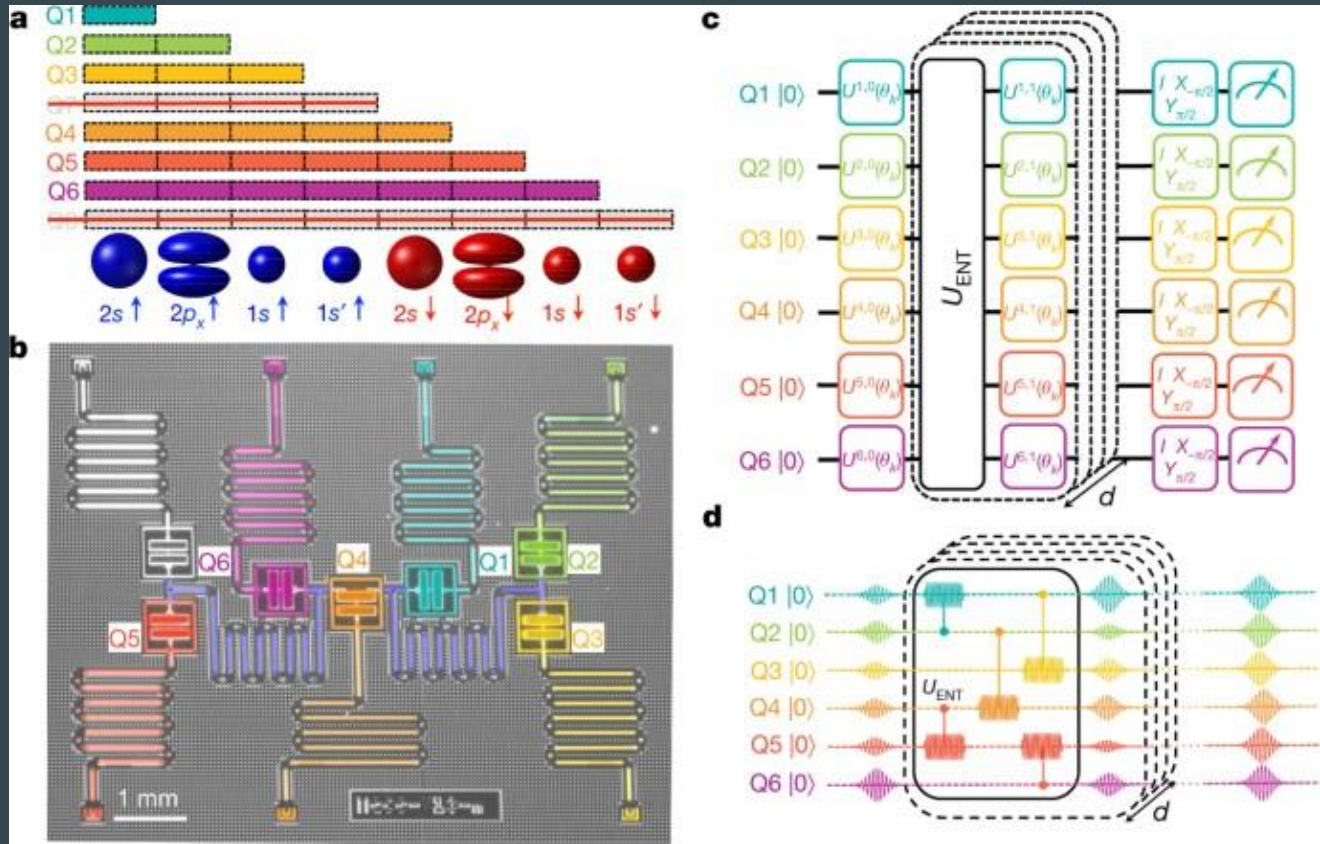
- Method:
  - Variational quantum eigensolvers (VQEs)

Quantum Chemical Modeling

- Variational Quantum Eigensolver
  - Quantum optimization
  - The algorithm:
    - Quantum computer prepares trial states based on parameters
    - Expectation value of the energy estimated
    - Expectation passed to a classical optimizer, which generates improved parameters
    - Repeat

Quantum Chemical Modeling: IBM (2017)

- IBM
- $U_{ENT} = \exp(-iH_0\tau)$, where H_0 is a drift Hamiltonian and τ is the evolution time
- In between the entanglement gates are single-qubit Euler rotations implemented as a combination of Z and X gates, $U^{q,i}(\boldsymbol{\theta}) = Z^q_{\theta_1^{q,i}} X^q_{\theta_2^{q,i}} Z^q_{\theta_3^{q,i}}$



Quantum Chemical Modeling: IBM (2017)

- The full circuit is described as shown. Here, $\boldsymbol{\theta}$ represents the Euler angles.

$$|\Phi(\boldsymbol{\theta})\rangle = \prod_{q=1}^{N} [U^{q,d}(\boldsymbol{\theta})] \times U_{\mathrm{ENT}} \times \prod_{q=1}^{N} [U^{q,d-1}(\boldsymbol{\theta})] \times \cdots \times U_{\mathrm{ENT}} \times \prod_{q=1}^{N} [U^{q,0}(\boldsymbol{\theta})]|00\ldots0\rangle$$

Quantum Chemical Modeling: IBM (2017)

- Models describing:
  - H_2
  - LiH
  - BeH_2

Quantum Classical Modeling: IBM (2020)

- IBM Q Valencia (5-qubit quantum computer)
- Modeling:
  - LiH
  - H_2S
  - LiSH
  - Li_2S
- Working with Daimler

Quantum Classical Modeling: IBM (2020)

- Used quantum and classical

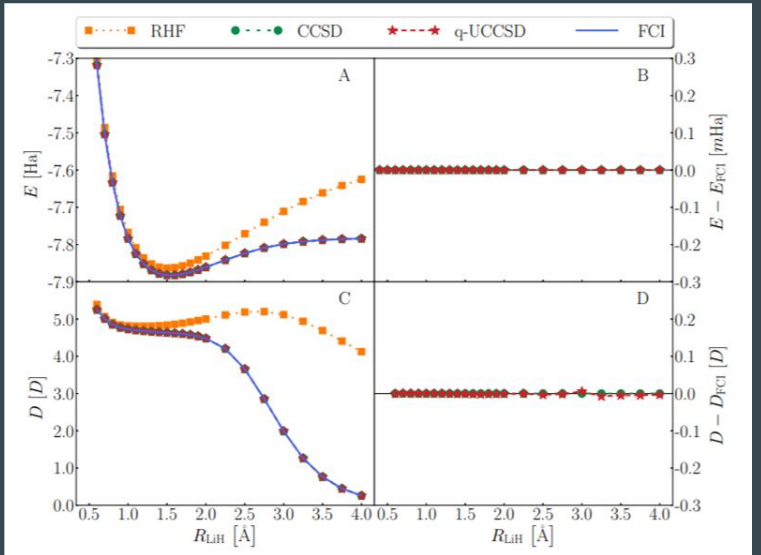


FIG. 2. Fig. 2 Calculations for lithium hydride, LiH. (A) Dissociation curve (ground state energy in Hartrees, as a function of interatomic distance, in angstroms) from RHF, CCSD, q-UCCSD and FCI. (B) Deviation from FCI energy, for CCSD and q-UCCSD, in millihartrees. (C) Dipole moment (in Debye) as a function of interatomic distance, in angstroms). (D) Deviation from FCI dipole moment, for CCSD and q-UCCSD, in Debye. Ha and D denote Hartree and Debye respectively.

Quantum Classical Modeling: IBM (2020)

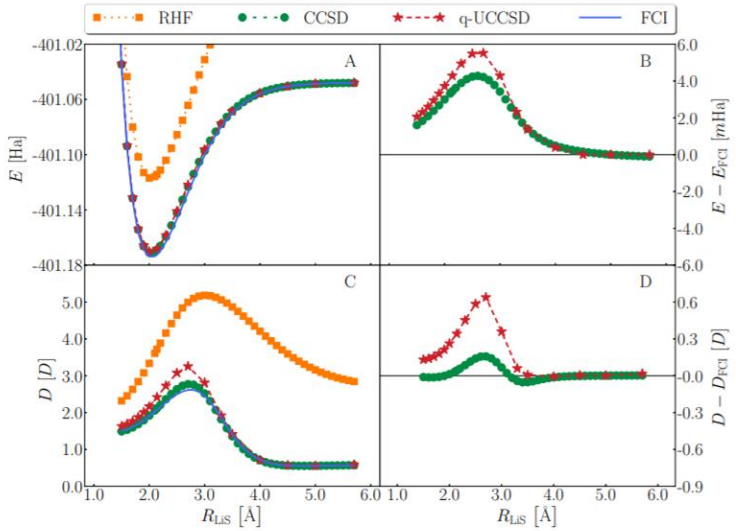


FIG. 5. Simulations of lithium hydrogen sulfide, LiSH, when breaking the Li-S bond. (A) Dissociation curve (ground state energy in Hartrees as a function of interatomic distance, in angstroms) from RHF, CCSD, q-UCCSD and FCI. (B) Deviation from FCI energy, for CCSD and q-UCCSD, in millihartrees. (C) Dipole moment (in Debye) as a function of interatomic distance, in angstroms). (D) Deviation from FCI dipole, CCSD and q-UCCSD, in Debye. Ha and D denote Hartree and Debye respectively.

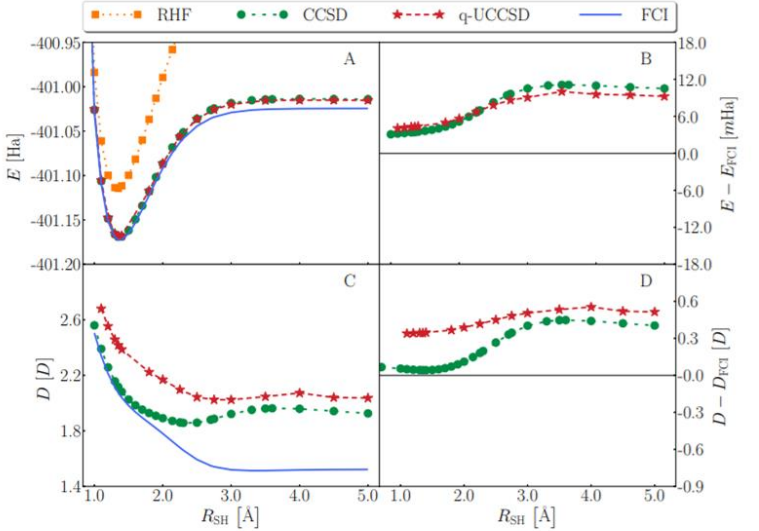


FIG. 6. Simulations of lithium hydrogen sulfide, LiSH, when breaking the S-H bond. (A) Dissociation curve (ground state energy in Hartrees as a function of interatomic distance, in angstroms) from RHF, CCSD, q-UCCSD and FCI. (B) Deviation from FCI energy, for CCSD and q-UCCSD, in millihartrees. (C) Dipole moment (in Debye) as a function of interatomic distance, in angstroms). (D) Deviation from FCI dipole, CCSD and q-UCCSD, in Debye. Ha and D denote Hartree and Debye respectively.

Conclusion

- Classical algorithms able to model chemical properties and reactions
  - Approximation or computationally expensive
- Quantum computing has potential to improve speed and accuracy
- Applications and interest
  - Samsung and Honeywell
  - Daimler and IBM

Sources

- https://www.nature.com/articles/nature23879
- https://arxiv.org/abs/2001.01120
- https://www.ibm.com/blogs/research/2020/01/next-gen-lithium-sulfur-batteries/
- https://www.ibm.com/blogs/research/2017/09/quantum-molecule/
- https://www.engadget.com/samsung-honeywell-quantum-computing-battery-160016217.html
- https://www.sciencedirect.com/science/article/pii/S254243511830182X