

# Harnessing Quantum Information Science for Enhancing Sensors in Harsh Fossil Energy Environments



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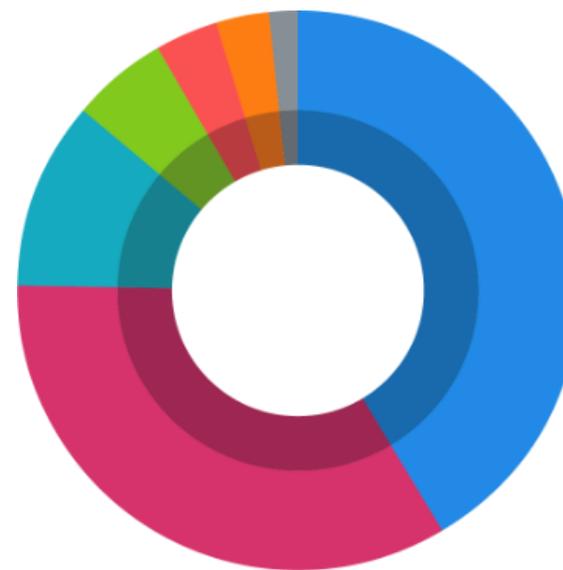
*Materials Science & Engineering Program*

# Outline

- Short introduction
- Why use quantum information science for sensors?
- Predictive quantum simulations for candidate materials
- Preliminary work with quantum control calculations

# UC Riverside (UCR)

- Official Hispanic Serving Institution
- Demographics:
- 57% first-generation students to attend college
- Designated as “*top-performing institution for African American & Latino/a students*” by The Education Trust – **1 of only 3 institutions in the nation**



41.5% | Hispanic or Latino

33.8% | Asian

11% | White

5.6% | Two or More Races

3.4% | International

3.3% | Black or African American

1.1% | Unknown

0.2% | Native Hawaiian or Other Pacific Islander

0.1% | Native American or Alaskan Native

# General Project Objectives

**Improving Sensing Modalities in Fossil Energy Infrastructures** ②

chemical analytes

optical initiation

optical readout

NV-center sensor material

**Properties to control:**

1. *Detection sensitivity*
2. *Quantum coherence*
3. *Long-term dynamics*

**Quantum Information & Control** ①

excited-state potential surface

ground-state potential surface

$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi$

**HBCU/MI Education, Training, & Research** ④

minority participation & state-of-the-art DOE computing

**Harnessing Quantum Control for Initializing Detection** ③

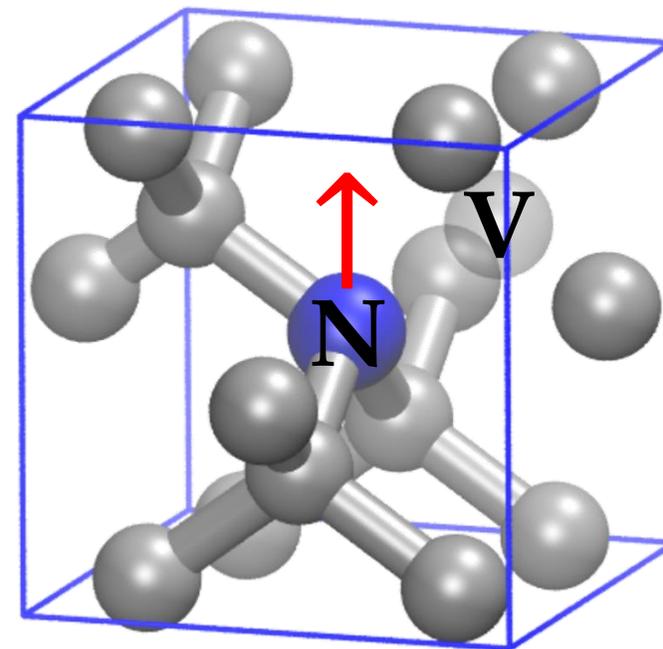
initialization of spin

optimal control field

$hv$

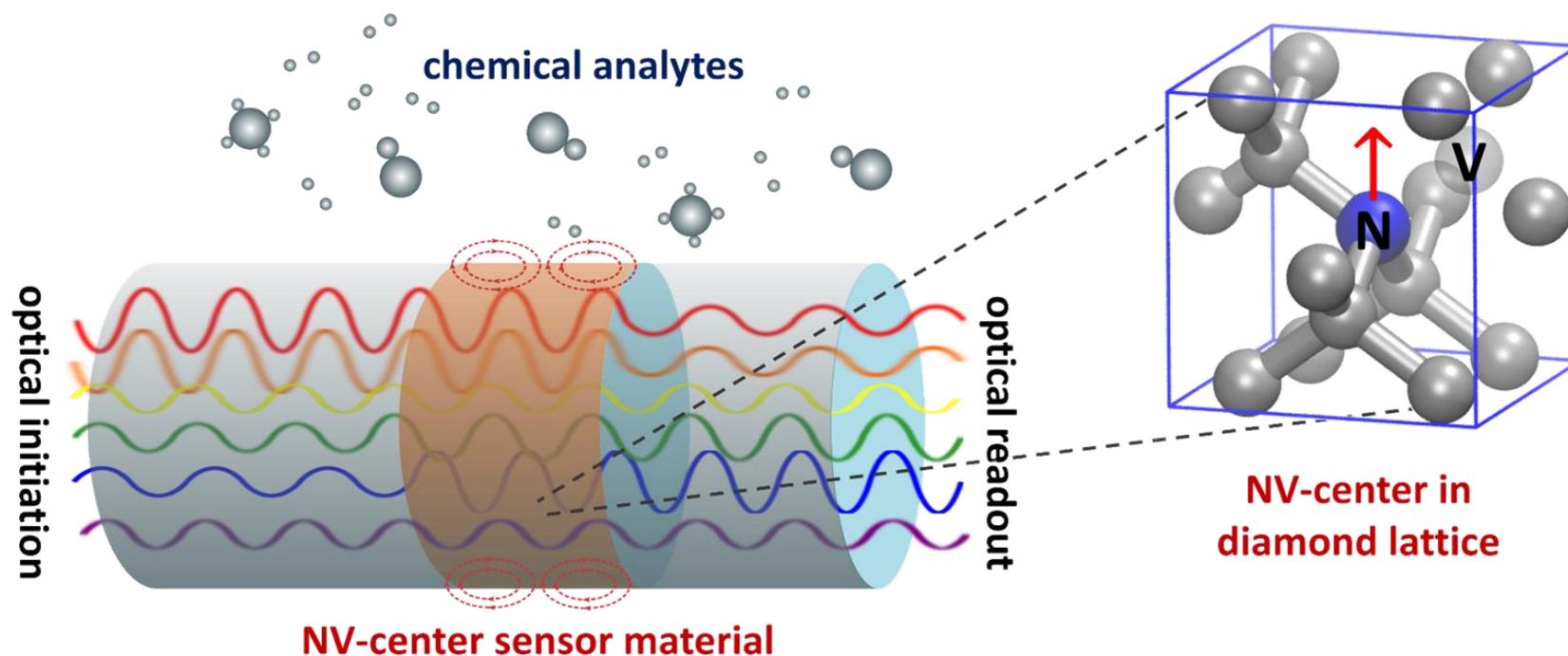
# NV-Center Sensors

- Nitrogen vacancy (NV) centers: structural point defects in bulk carbon
- Contain stable, localized electron spin that can be used as sensor
- Coherence signals can persist at 700 – 1000 K (*essential for harsh fossil energy environments*)
- Can be controlled with electromagnetic fields



# NV-Center Sensors (cont.)

- NV centers near the surface have not been thoroughly explored
  - Defects at surface can enable sensitive detection of chemical analytes in fossil energy infrastructures (discussed later)

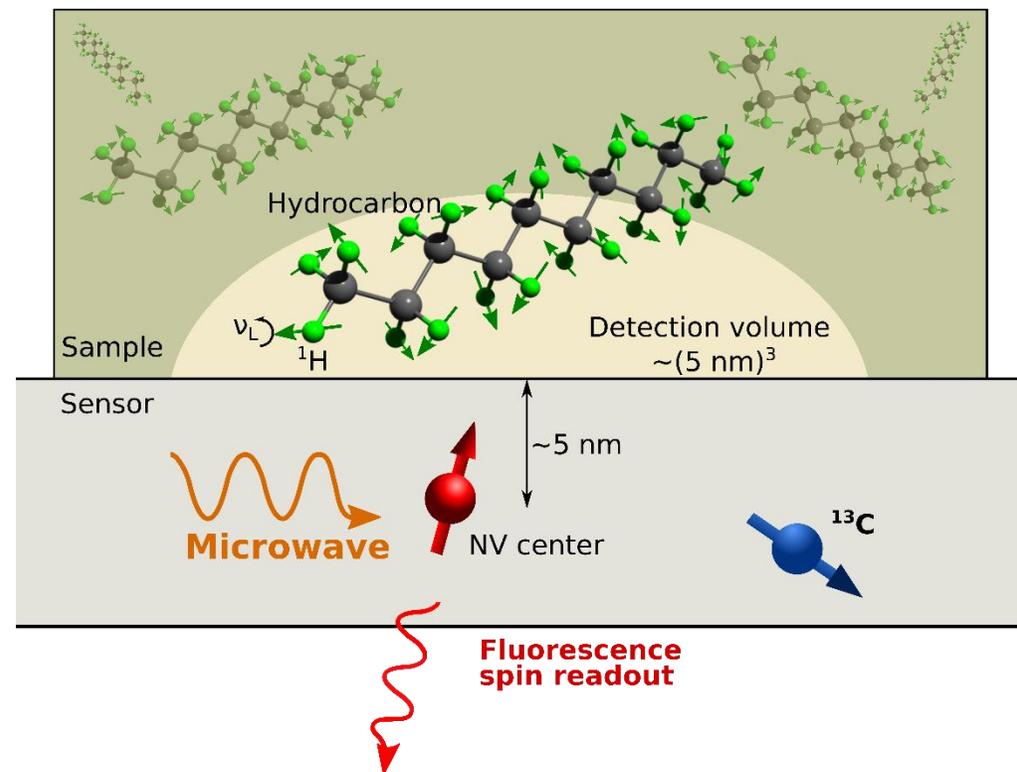


# Near-Surface NV-Centers

- Current resolution of NV-center sensors  $\sim (5 \text{ nm})^3$  (size of large protein)

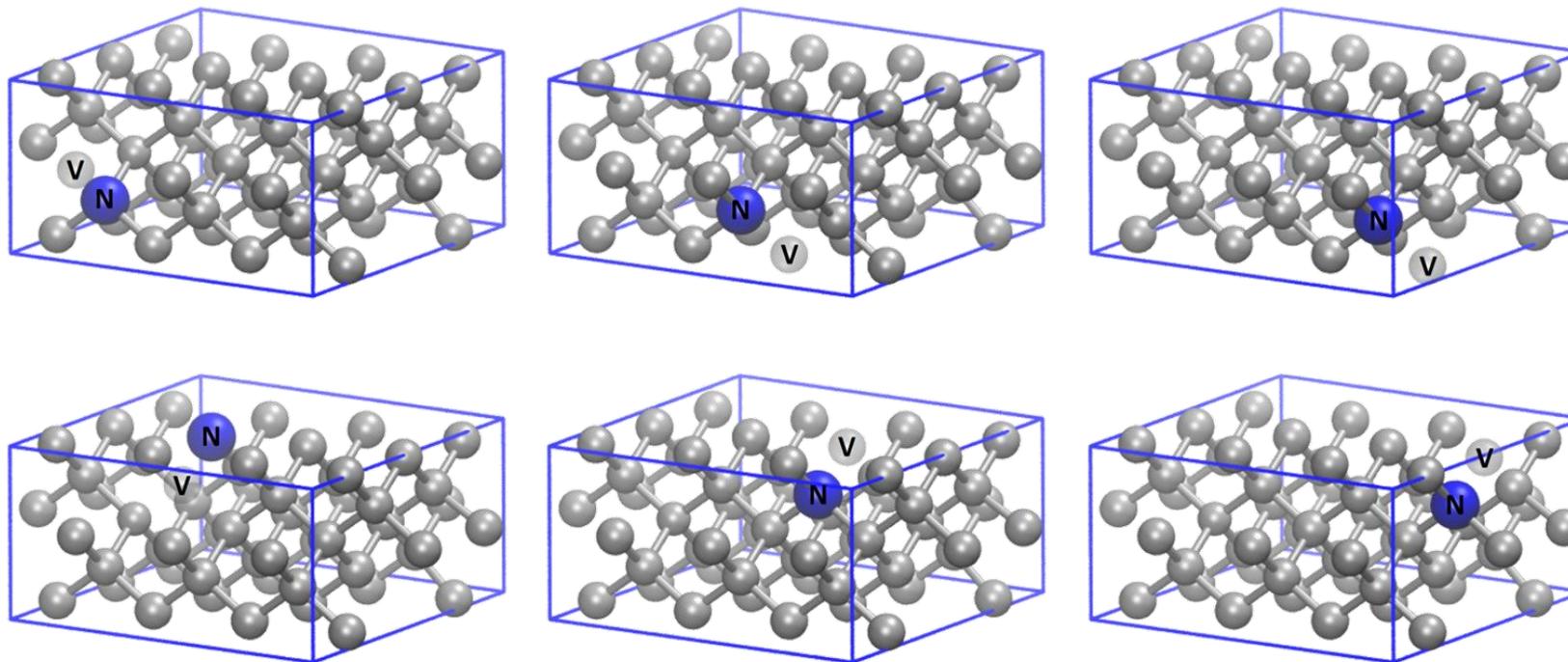
- Dipolar magnetic field  $B_{\text{dip}} = \frac{\mu\mu_0}{4\pi} \frac{\sqrt{3\cos^2\theta+1}}{r^3}$

- Since  $B_{\text{dip}} \sim \frac{1}{r^3}$ , sensitivity can be increased 3 orders of magnitude by reducing distance of NV center from surface by factor of 10



# Initial NV-Center Configurations

- Use DFT to down-select initial NV-center configurations

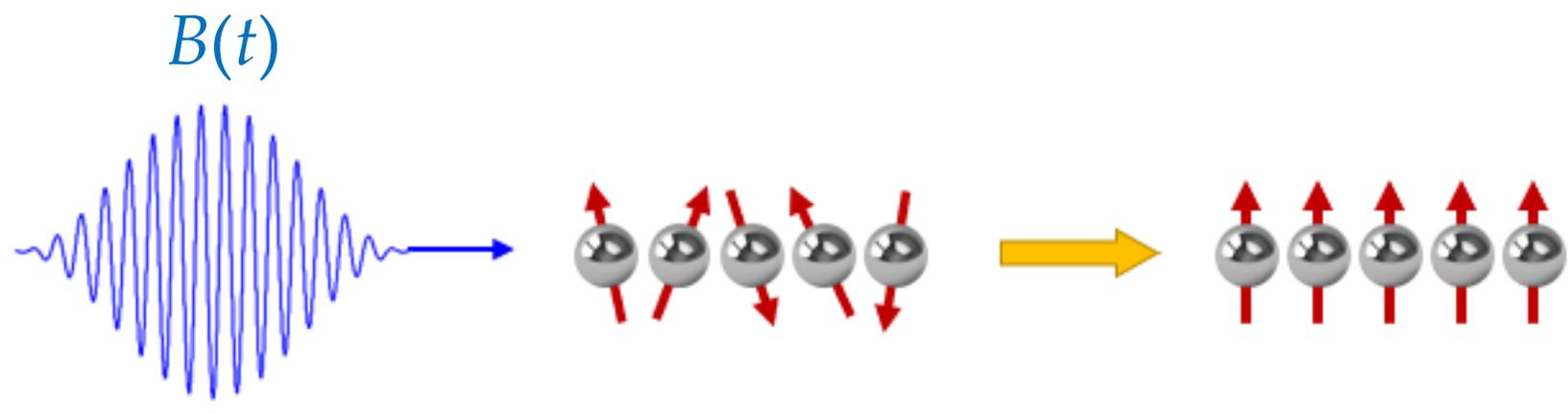


examples of NV-center configurations near top surface of lattice

- Carry out ab initio MD at various temperatures to test their stability

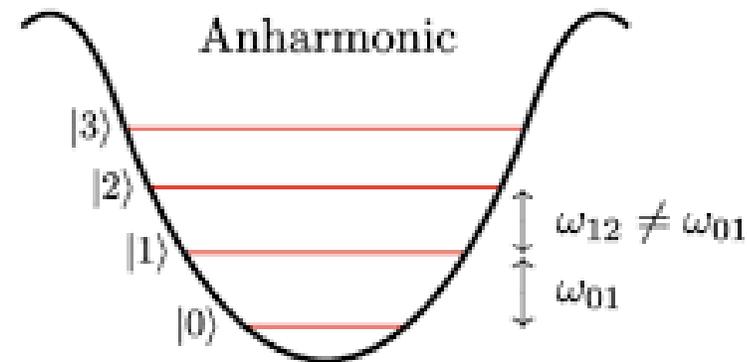
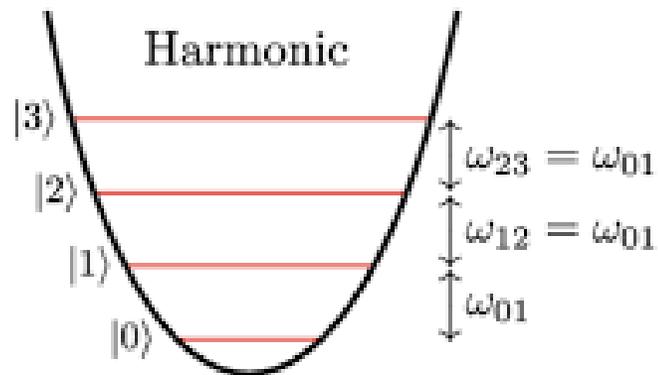
# Purpose of Project

- Efficient manipulation of large qubit systems with external magnetic fields
- Quantum gate operation
- Quantum computing

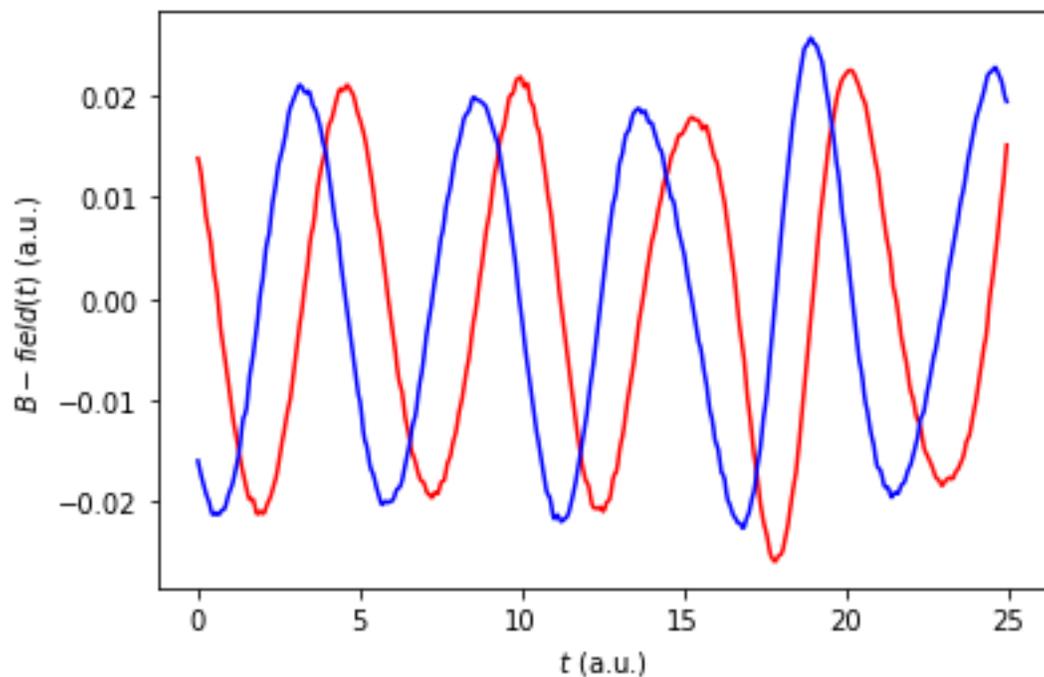


# Hamiltonian of Multi-Qubit System

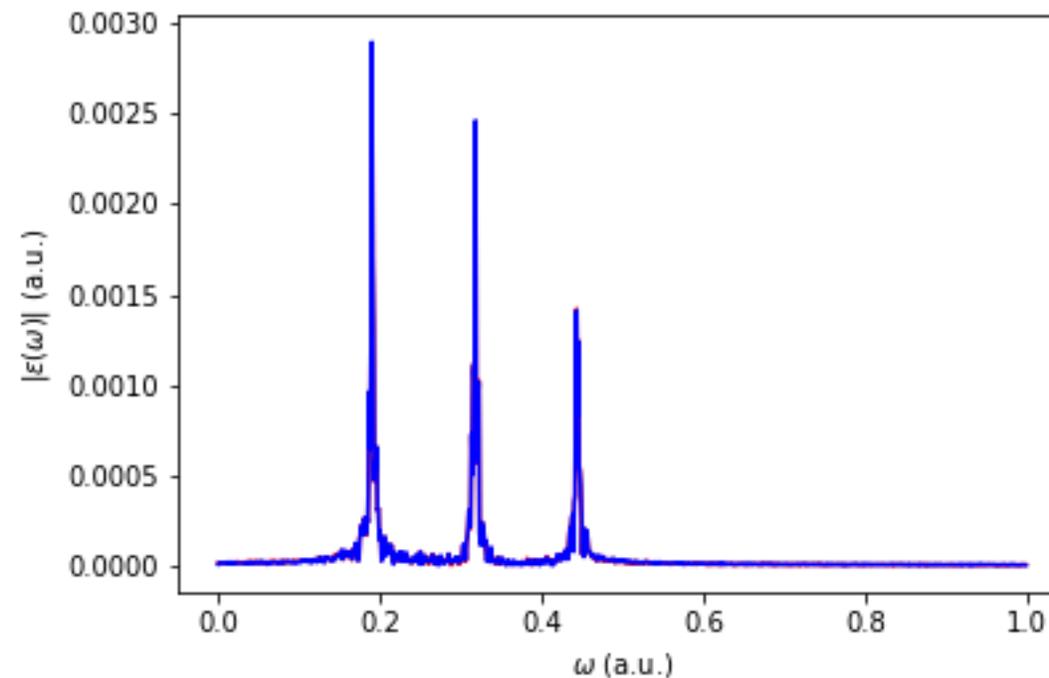
- $H = H_0 + H_c$
- $H_0 = -\left(\sum_i \sigma_z^i\right) \cdot B_z + c_{\text{coupling}}\left(\sum_i \sigma_z^i \sigma_z^{i+1}\right)$
- $H_c = \left(\sum_i \sigma_x^i\right) \cdot B_x(t) + \left(\sum_i \sigma_y^i\right) \cdot B_y(t)$



# Optimal B-fields and Power Spectrum



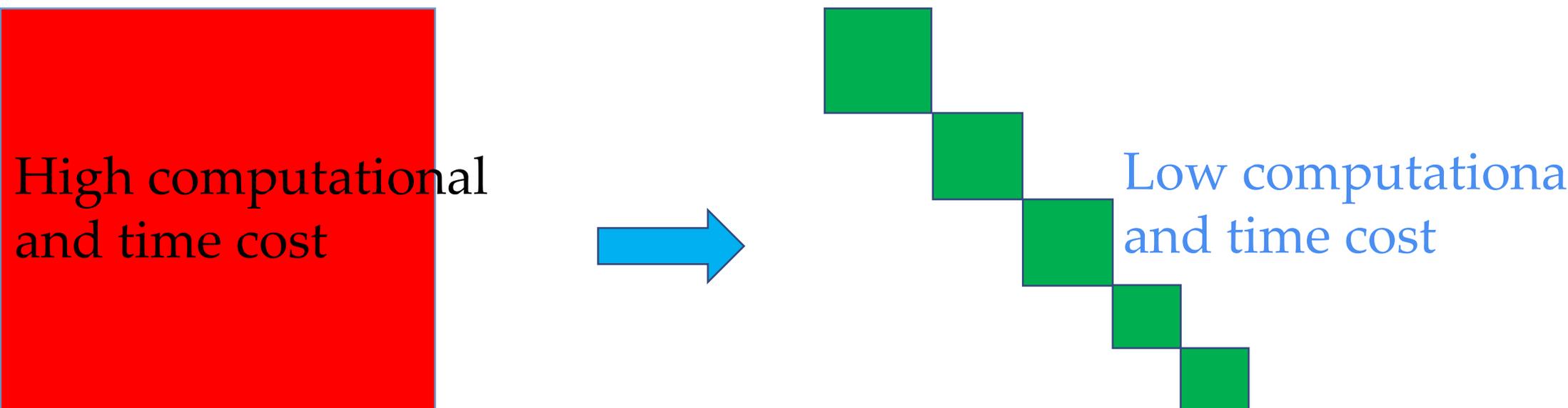
$B(t)$  vs.  $t$



$\varepsilon(\omega)$  vs.  $\omega$

# Symmetry-based Hamiltonian Decomposition

- Size of Hamiltonian increases as  $2^n$
- Decompose Hamiltonian matrix with symmetry of finite groups
- Developed for with-coupling and no-coupling cases



High computational  
and time cost



Low computational  
and time cost

# Symmetry-based Hamiltonian Decomposition

- $H_0 = -(\sum_i \sigma_z^i) \cdot B_z + c_{\text{coupling}}(\sum_i \sigma_z^i \sigma_z^{i+1})$
- $H_c = (\sum_i \sigma_x^i) \cdot B_x(t) + (\sum_i \sigma_y^i) \cdot B_y(t)$
- $\sum_i \sigma_z^i, \sum_i \sigma_x^i, \sum_i \sigma_y^i$  has  $S_n$  (permutation group) symmetry
- $\sum_i \sigma_z^i \sigma_z^{i+1}$  has  $D_n$  (dihedral group) symmetry
  
- Size of Hamiltonian decreases from  $2^n$  to  $O(n)$  or  $O(2^n/n)$

# Symmetry-based Hamiltonian Decomposition

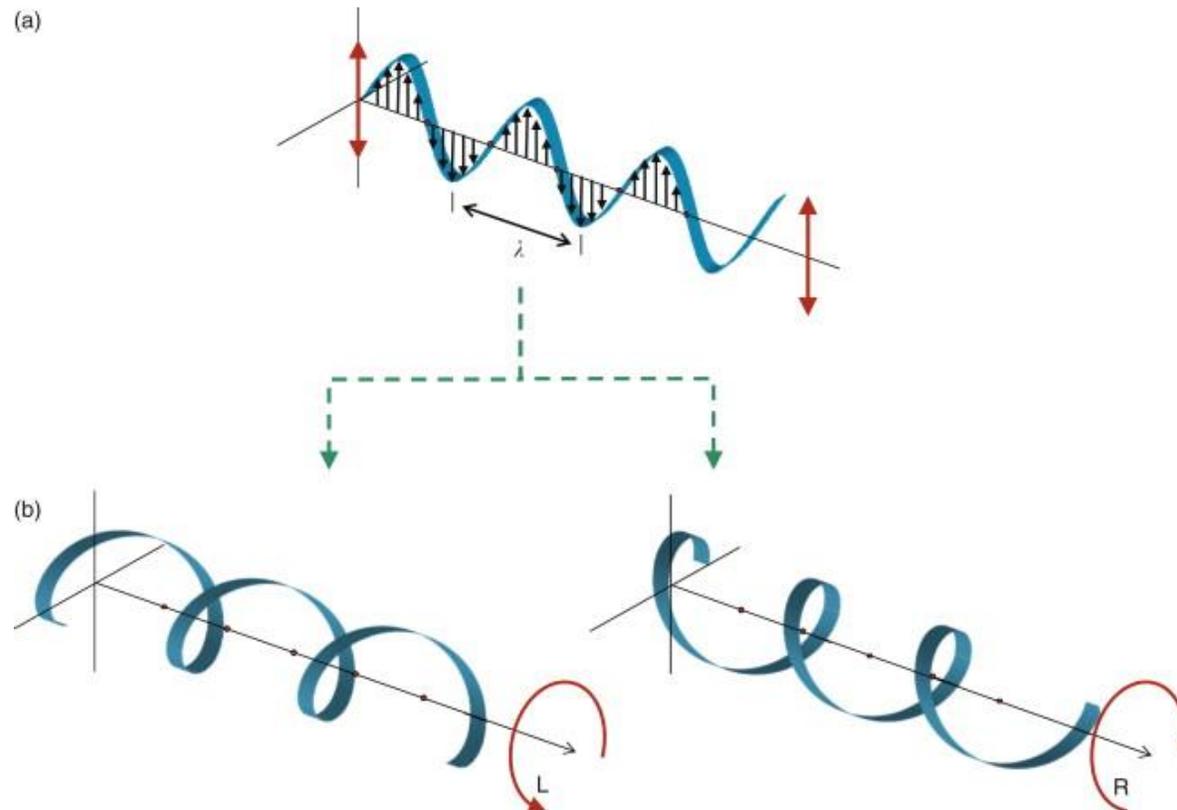
Number of qubits $n$	Size of Hamiltonian		
	Original $2^n$	$S_n$ decomposition $O(n)$	$D_n$ decomposition $O(2^n/n)$
3	8	4	4
4	16	5	6
5	32	6	8
6	64	7	13
7	128	8	18
8	256	9	30
9	512	10	46
10	1024	11	78
11	2048	12	126
12	4096	13	224
13	8192	14	380
14	16384	15	687

# Linear Unitary Operator

- Exponential propagator
- $\exp \left[ i\tau H \left( t + \frac{\tau}{2} \right) \right] \psi(t + \tau) = \psi(t)$
- Linear unitary propagator from NIC-CAGE: Novel Implementation of Constrained Calculations for Automated Generation of Excitations
- $\left[ I + \frac{i\tau}{2} H \left( t + \frac{\tau}{2} \right) \right] \psi(t + \tau) = \left[ I - \frac{i\tau}{2} H \left( t + \frac{\tau}{2} \right) \right] \psi(t)$
- Analytical form of the gradient  $\frac{dP}{dB}$  for back-propagation

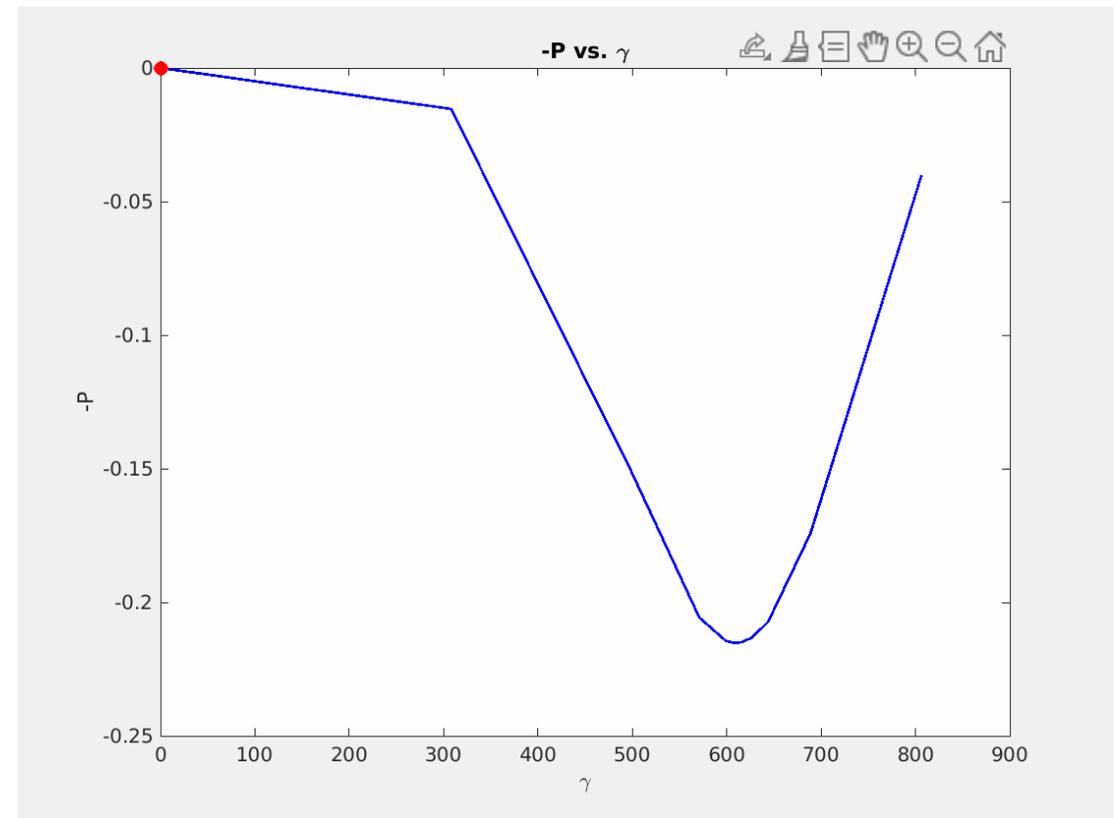
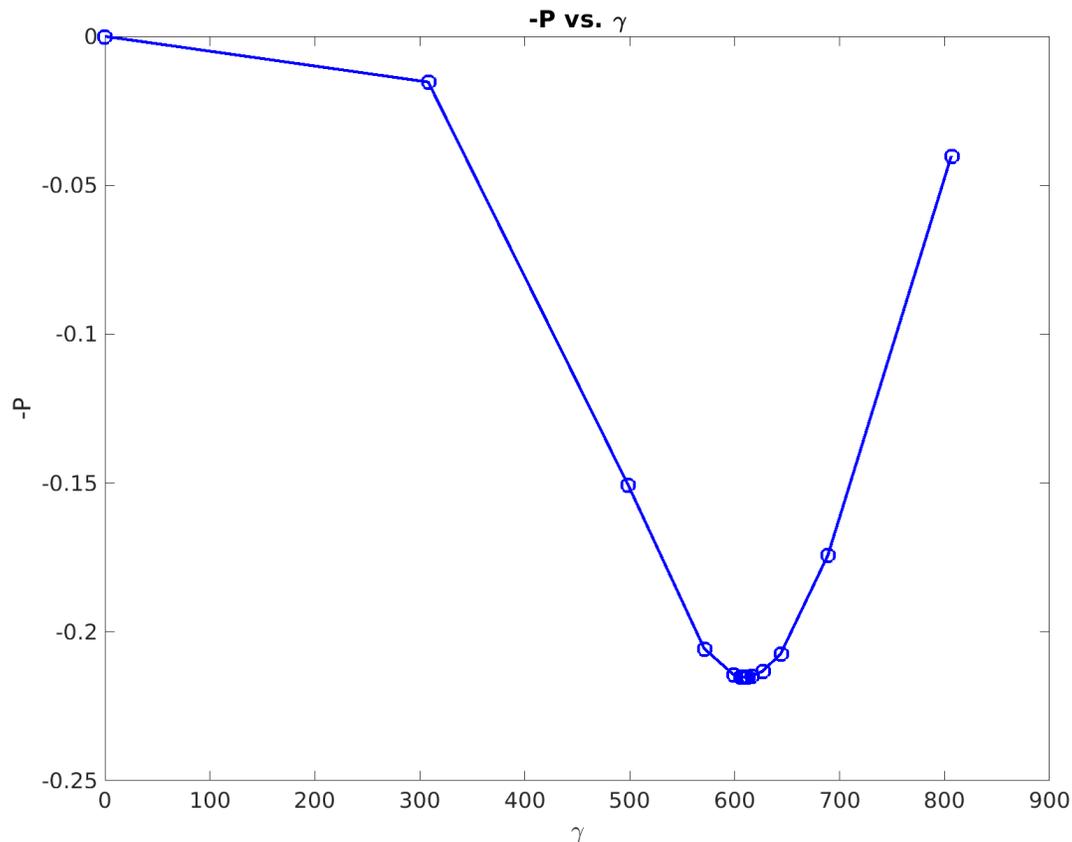
# Technical Improvements

- B-fields in x- and y- direction, polarization



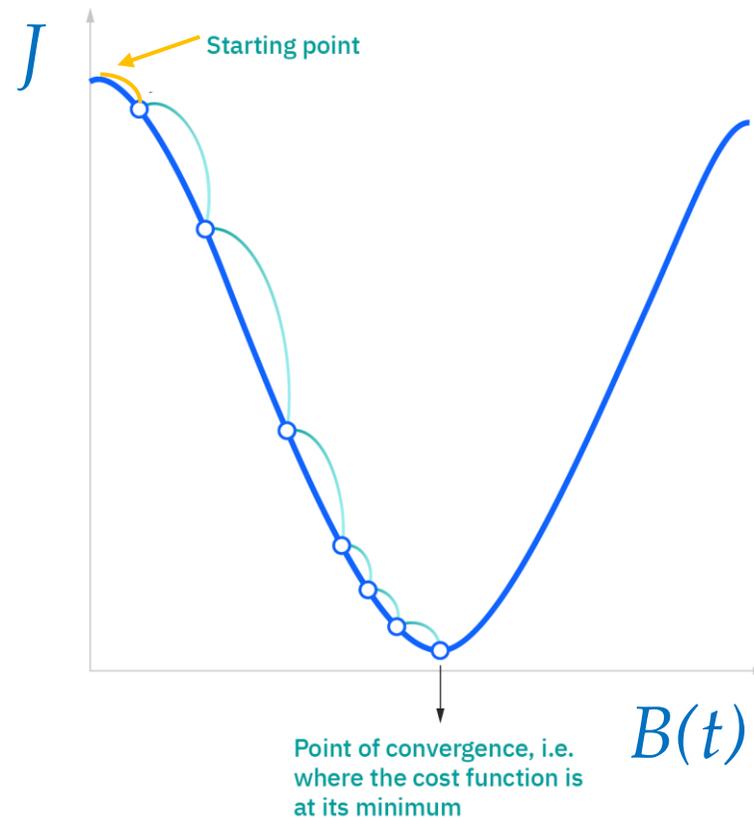
# Technical Improvements

- Golden section search, more robust & faster



# Technical Improvements

- Heuristic amplified gradient



# Conclusion & Acknowledgements

- Predictive quantum simulations provide rational guidance for constructing quantum sensors for fossil energy infrastructures
- Quantum information science *almost perfect application for sensors & interaction with external fields*



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