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

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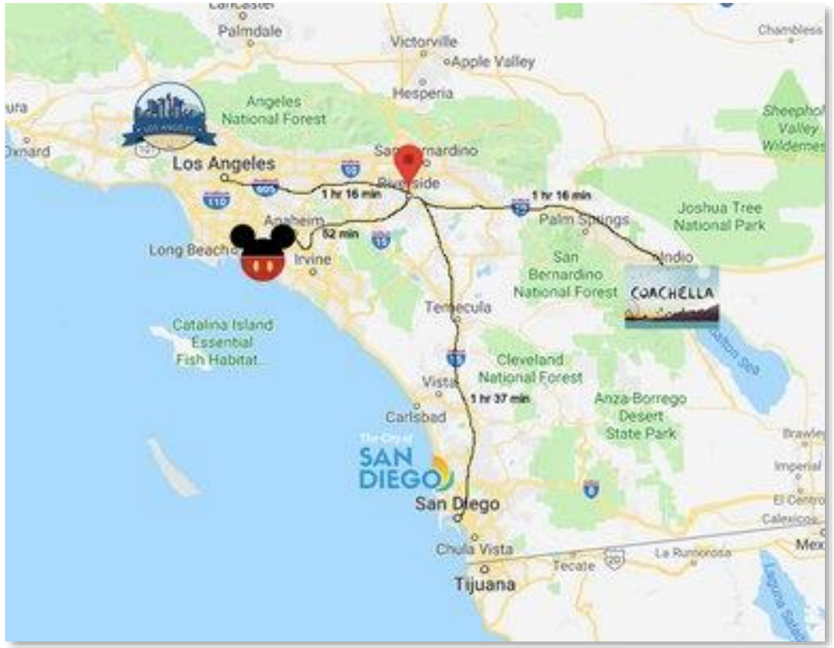
Materials Science & Engineering Program

Outline

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

Introduction

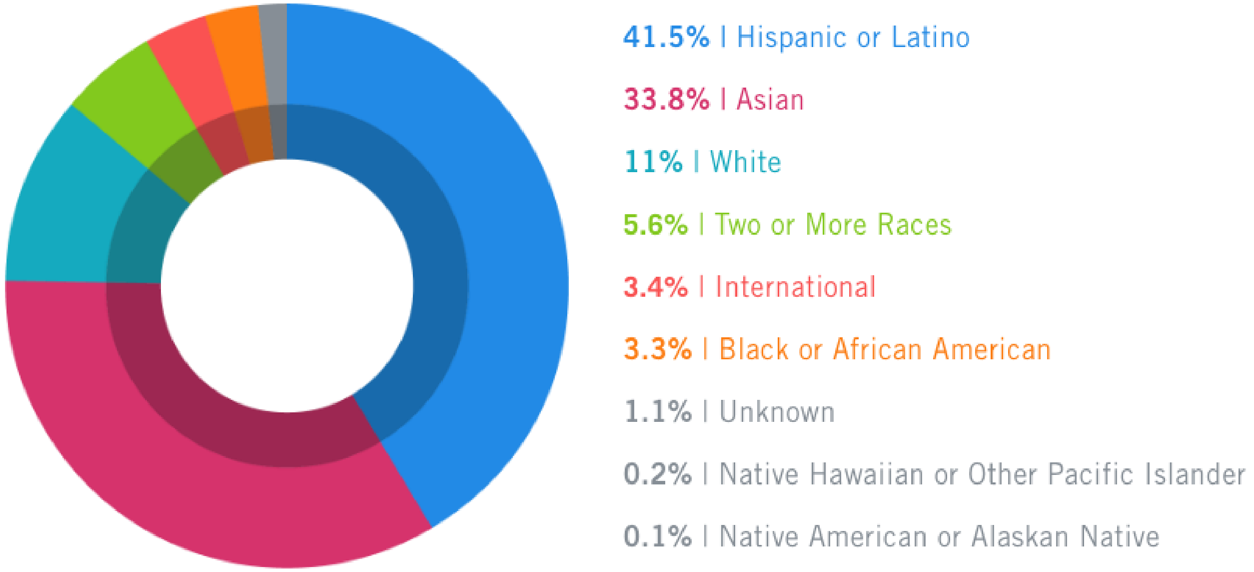
- B.S. in Physics and Chemistry – *Rice University (2001)*
- Ph.D. in Physical Chemistry – *M.I.T. (2007)*
- Staff Scientist Sandia National Labs (2007-2013)
- Associate Prof. at UC Riverside Physics/MatSci/Chemistry/ChemE (2014-now)
- Visit us (virtually) at http://www.bmwong-group.com



UC Riverside (UCR)

- Official Hispanic Serving Institution

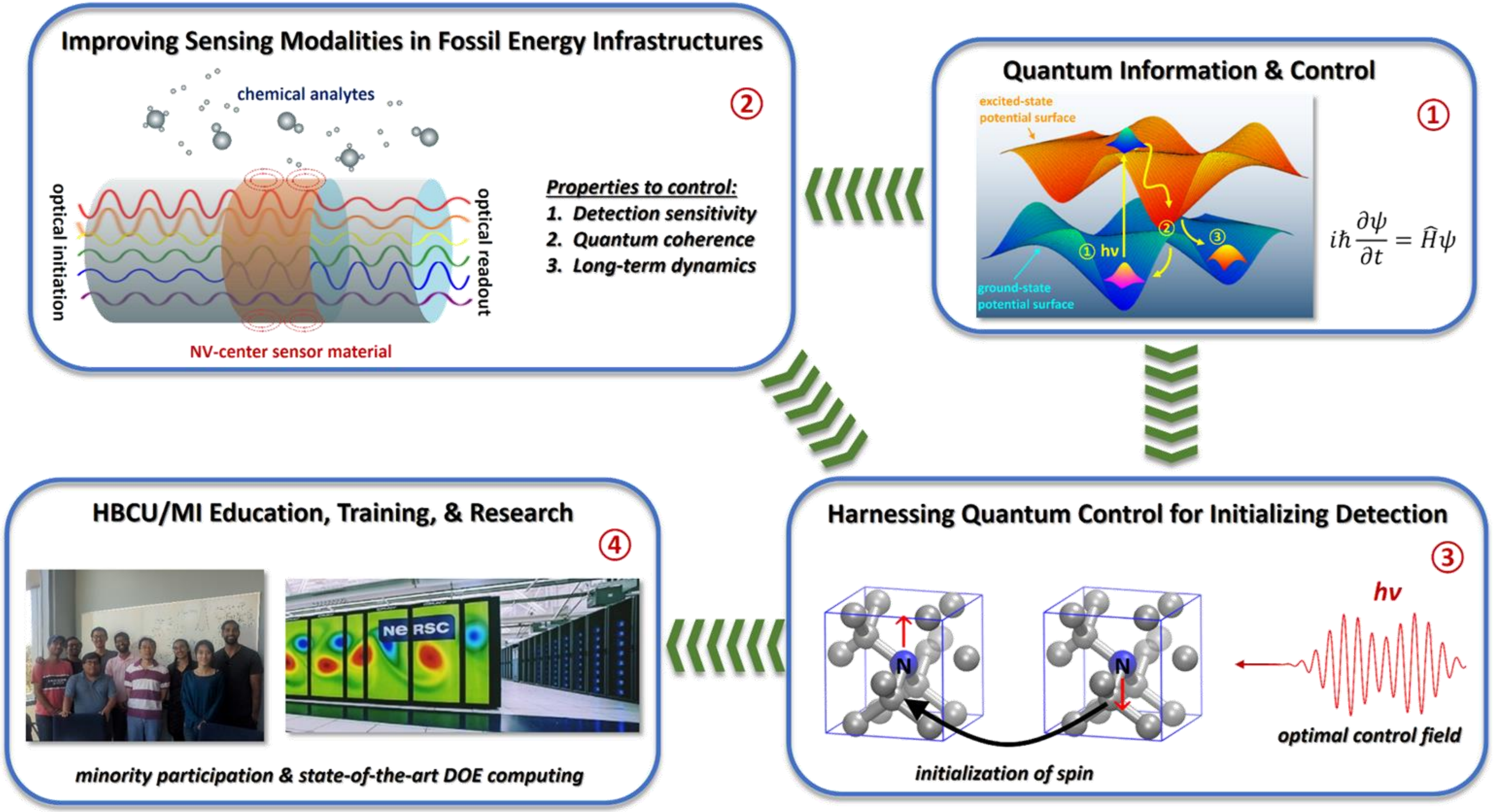
- Demographics:



- 57% first-generation students to attend college

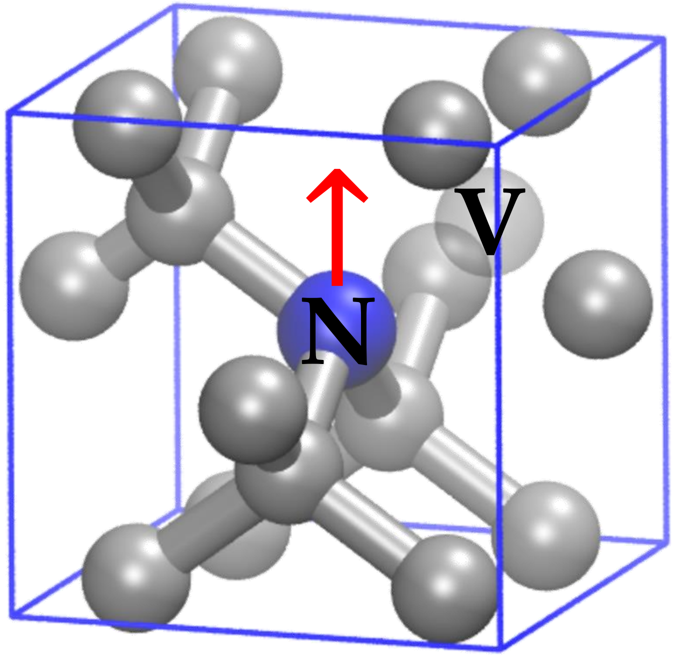
- Designated as *"top-performing institution for African American & Latino/a students"* by The Education Trust – **<u>1 of only 3 institutions in the nation</u>**

General Project Objectives



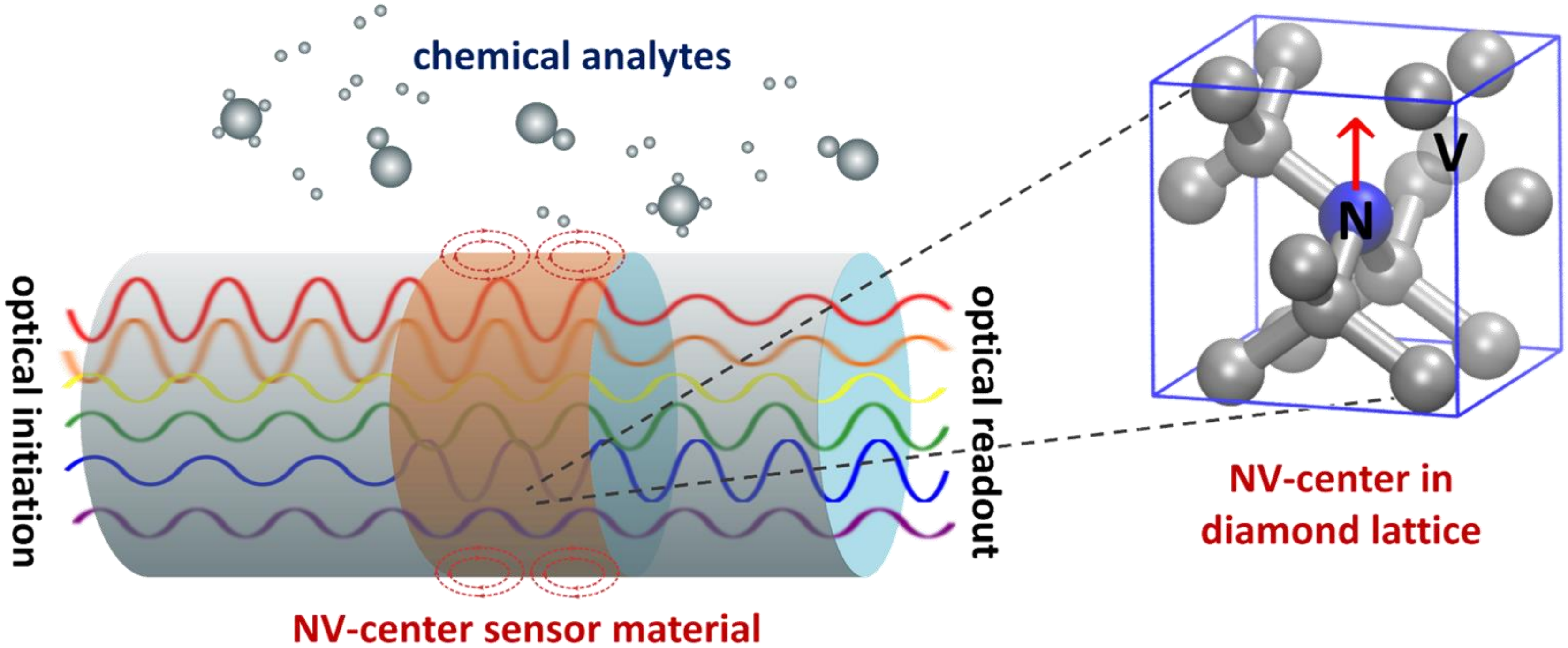
NV-Center Sensors

- 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)



DiVincenzo's Criteria

- DiVincenzo outlined 3 necessary conditions for quantum sensor
  - (1) Must have discrete resolvable energy levels separated by finite transition energy
  - (2) Must be possible to initialize sensor into well-known state and read out
  - (3) Can be coherently manipulated, leading to transitions between energy levels

DiVincenzo's Criteria (cont.)

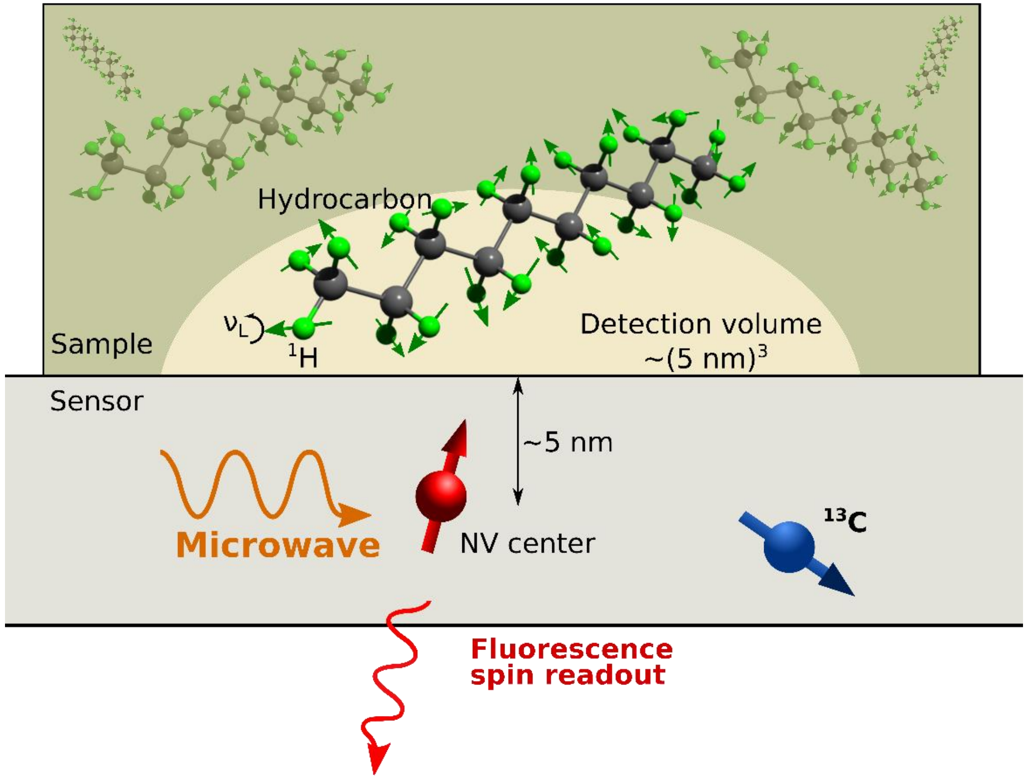
- Approaches in this project obey all 3 DiVincenzo's criteria:
  - (1) Electron spin in NV center can be excited to quantized energy states ✓
  - (2) Electrons in NV centers can be initialized with electromagnetic pulse, which can be simulated with quantum control algorithms ✓
  - (3) NV center spin state has long coherence time with added advantage of sub-nanometer spatial resolution ✓

Near-Surface NV-Centers

- Current resolution of NV-center sensors ~(5 nm)^3 (size of large protein)

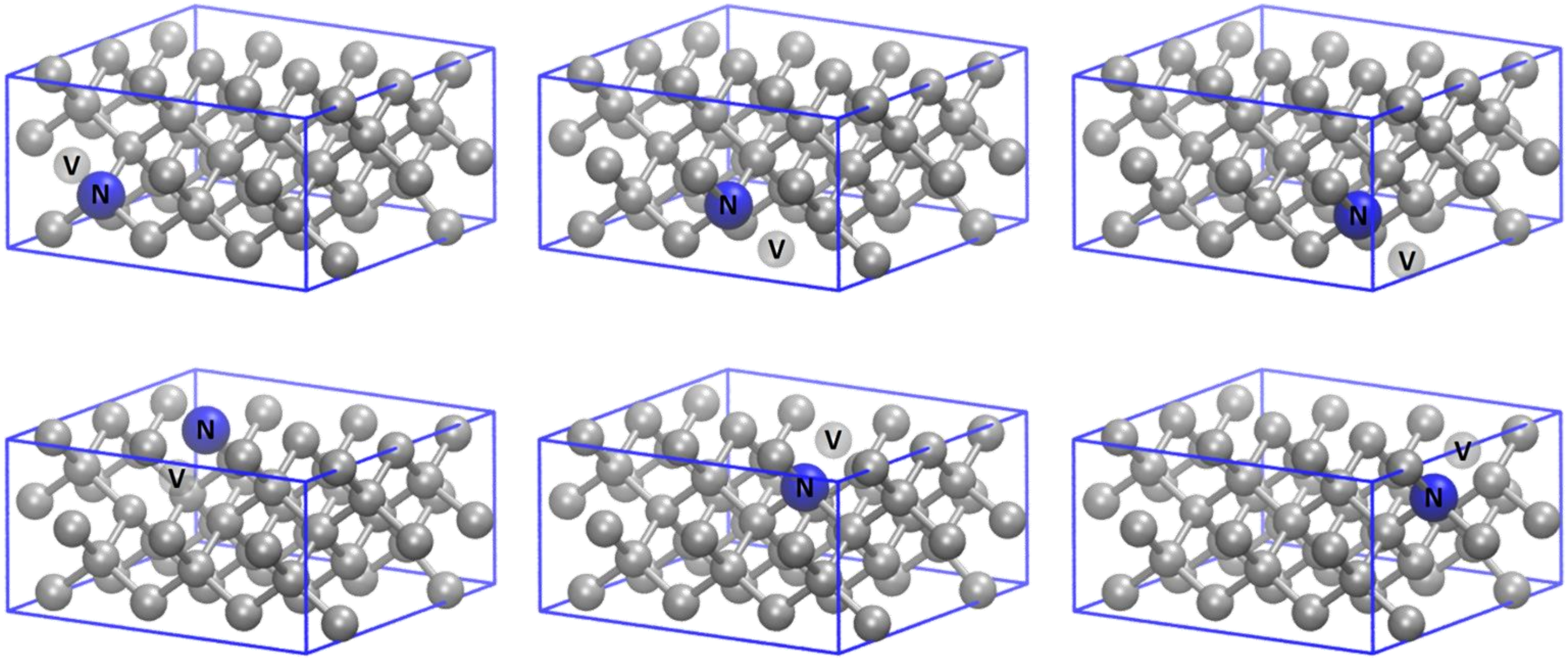
- Dipolar magnetic field $B_{\mathrm{dip}} = \frac{\mu\mu_0}{4\pi}\frac{\sqrt{3\cos^2\theta+1}}{r^3}$

  - Since $B_{\mathrm{dip}} \sim \frac{1}{r^3}$, 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



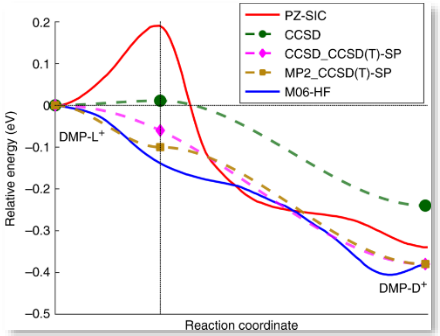
examples of NV-center configurations near top surface of lattice

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

Ground vs. Excited-State QM

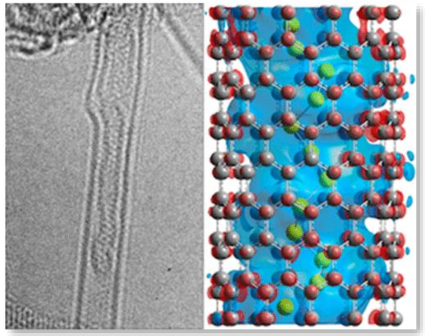
- Ground-state QM can do this:

Potential Energy Surfaces



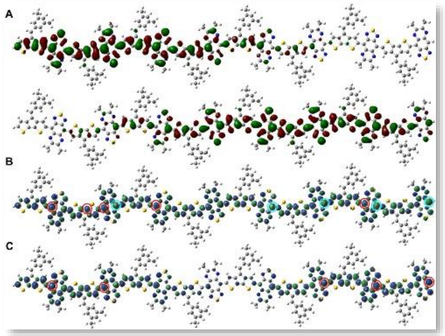
Z. Ali & B. Wong, *Nature Comm.* **9**, 4733 (2018)

Structural Properties



J. Guo & B. Wong, *ACS Nano* **12**, 9775 (2018)

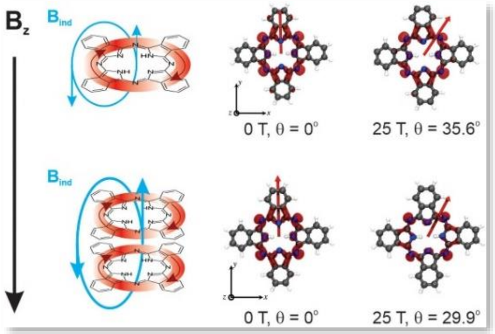
Electronic Properties



B. Wong & J. Azoulay, *Science Advances* **5**, eaav2336 (2019)

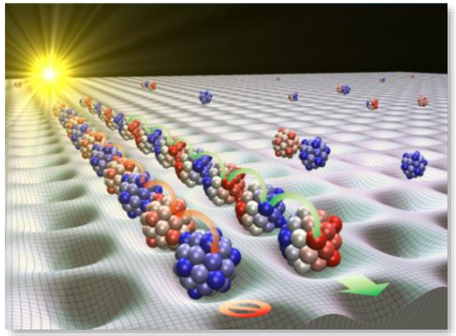
- Ground-state QM *cannot do this:*

Electronic Excited States



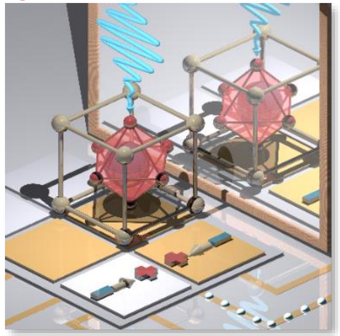
B. Wong & G. Scholes, *PNAS* **117**, 11289 (2020)

Real-Time Electron Evolution



N. Ilawe & B. Wong, *J. Mat. Chem. C* **6**, 5857 (2018)

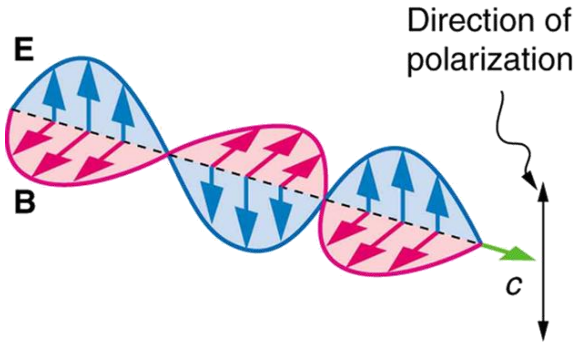
Light-Matter Interactions



C. Lian & B. Wong, *J. Phys. Chem. Lett.* **7**, 4340 (2019)

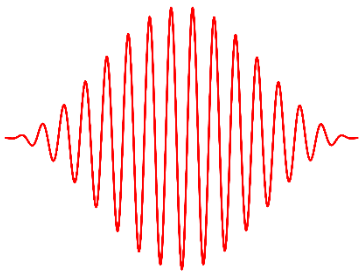
Excited-State QM for Dynamics

- (1) NV-center configurations down-selected with DFT
- (2) Excited-state QM will probe *real-time* interactions between NV centers & EM fields to understand sensor mechanisms
- Electromagnetic radiation (i.e., light) has two components
  - Magnetic field (**B**)
  - Electric field (**E**)

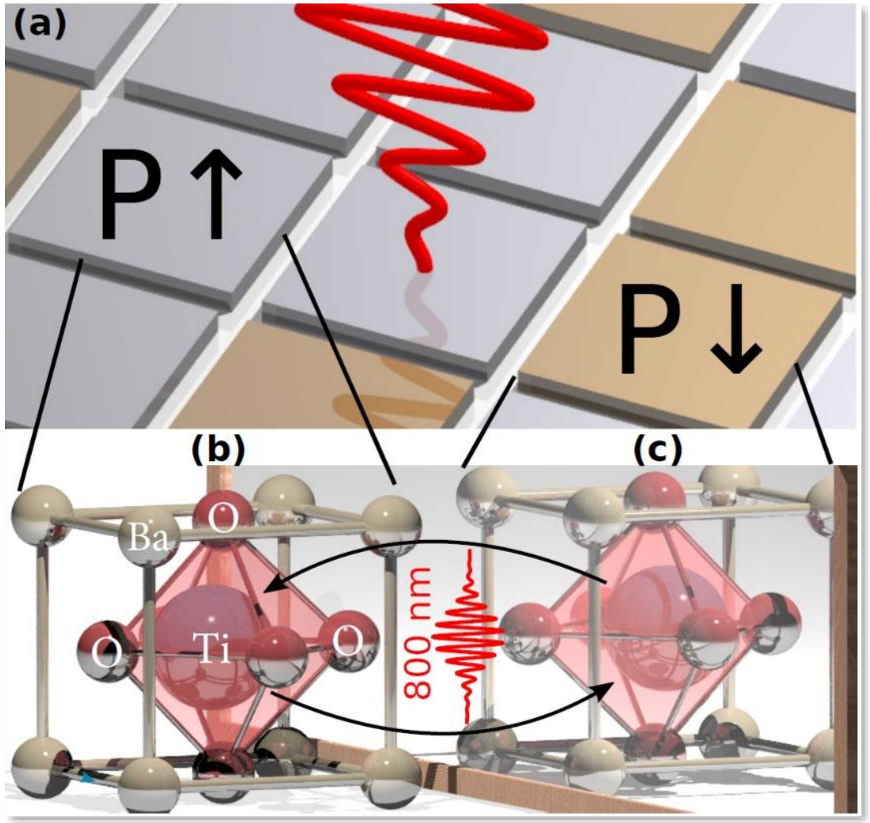


Related Work on Excited State QM

- Can we *control polarization* switching with optical pulses?
- Excellent application of our periodic RT-TDDFT approach
- Focus on $BaTiO_3$ as prototypical example
- Applied laser pulse:

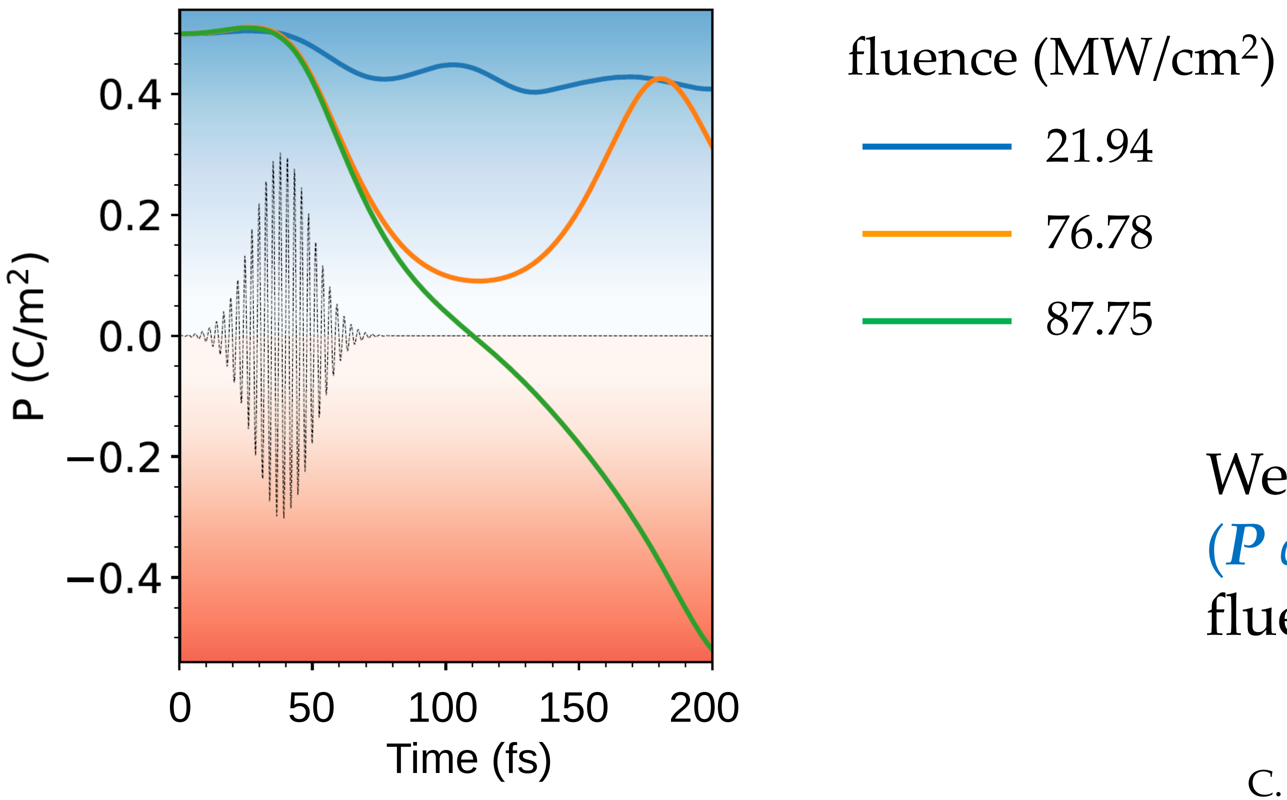


$$\mathbf{E}(t) = \mathbf{E}_0 \cos(\omega t) \exp\left[-\frac{(t-t_0)^2}{2\sigma^2}\right]$$



Polarization Switching

- With $\rho(t)$ converged, ionic movement approximated via Hellmann-Feynman forces using Ehrenfest Dynamics

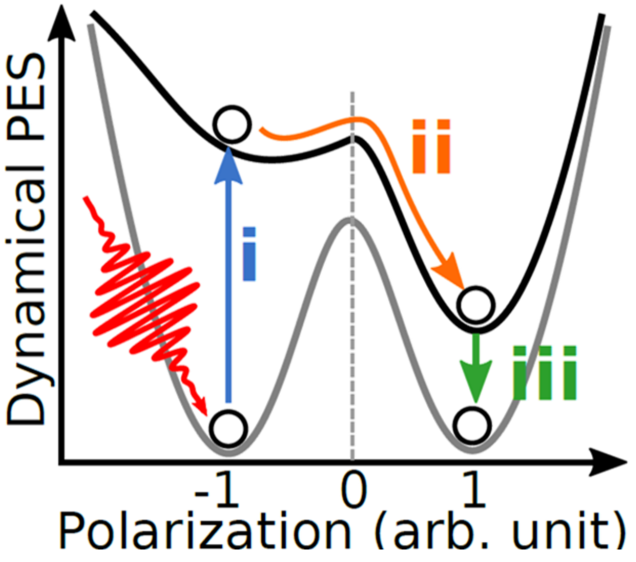


We achieve polarization switching (***P** changes sign*) when fluence = 87.75 MW/cm^2

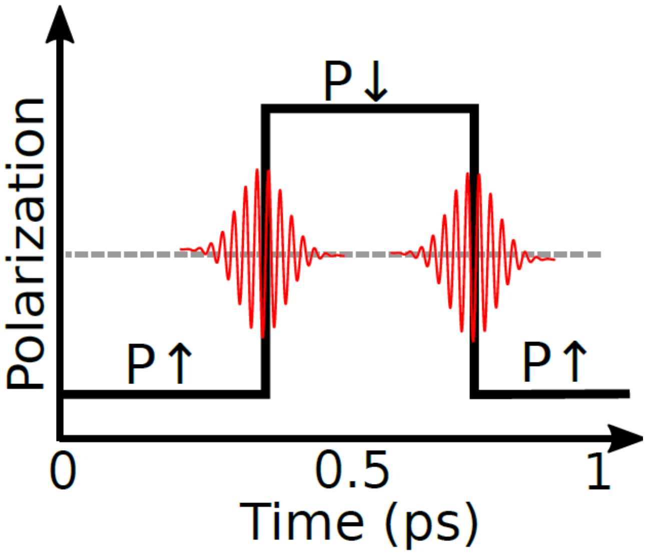
C. Lian & B. Wong, *J. Phys.Chem. Lett.* **10**, 3402 (2019)

Ferroelectric Summary

- Simplified take-home message:



laser-tune PES to change polarization



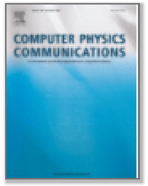
laser can reversibly switch polarization back!

C. Lian & B. Wong, *J. Phys.Chem. Lett.* **10**, 3402 (2019)

Optimal Control Fields

- Excited-state QM is an initial value problem
- Can we ask the inverse question: "Can we construct fields that *enable desired behavior in NV center?*"

Computer Physics Communications
Volume 258, January 2021, 107541



NIC-CAGE: An open-source software package for predicting optimal control fields in photo-excited chemical systems ☆, ☆☆

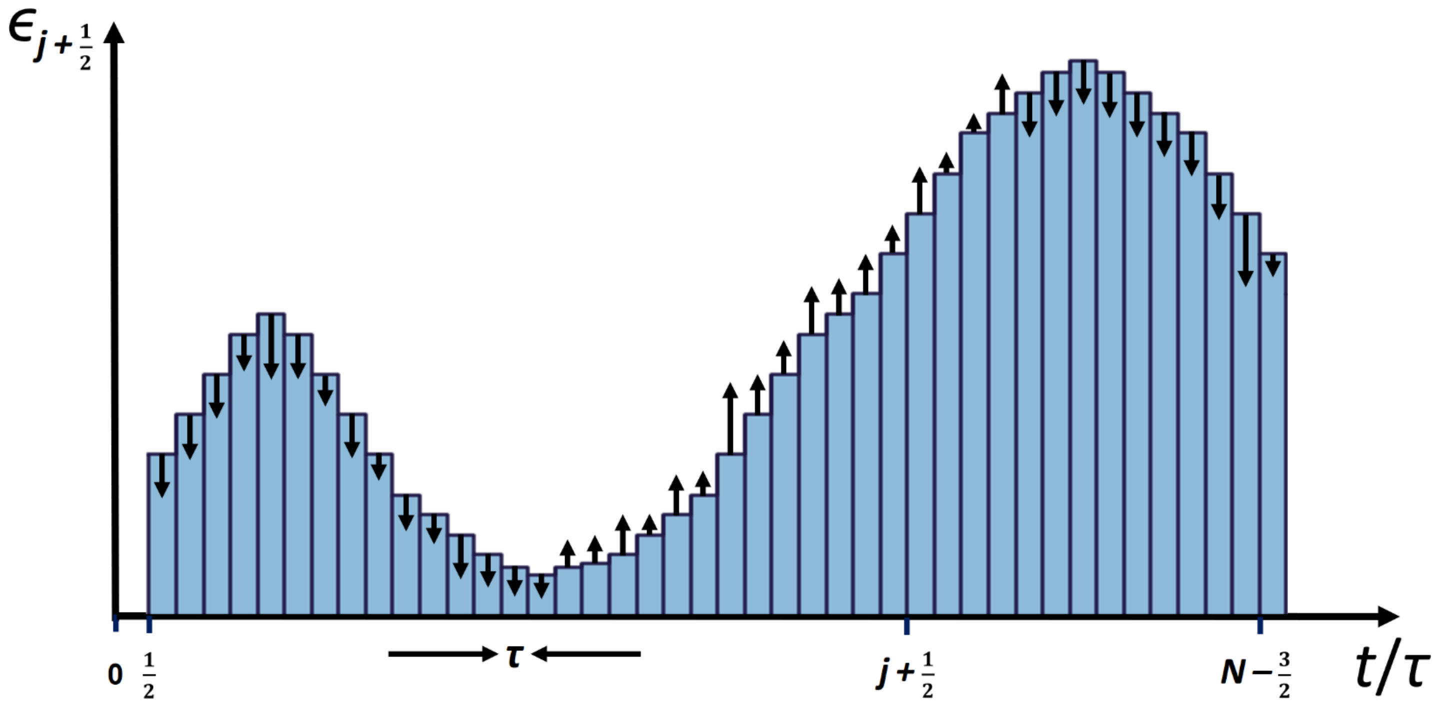
Akber Raza [a, 1], Chengkuan Hong [b, 1], Xian Wang [c], Anshuman Kumar [d], Christian R. Shelton [b], Bryan M. Wong [a, c, d, e, f]

NIC-CAGE: Novel Implementation of Constrained Calculations for Automated Generation of Excitations

A. Raza. C. Hong, X. Wang, A. Kumar, C. R. Shelton, B. M. Wong, *Comput. Phys. Commun.* **258**, 107541 (2021)

NIC-CAGE Program

- Calculates fields that enables transition to desired final state $|\psi_f\rangle$
- Uses scheme from GRAdient Pulse Engineering (GRAPE) algorithm



temporal shape of $E(t)$

vertical arrows = gradients indicating how amplitude changes to maximize transition probability

NIC-CAGE Program (cont.)

- Propagate TDSE to get final state $\psi_{N-1}(x, t = T)$ and maximize $\boldsymbol{J}$:

$$\boldsymbol{J}[\psi_{N-1}, \boldsymbol{\epsilon}] = \left|\langle\psi_f|\psi_{N-1}\rangle\right|^2 - \int_0^T \alpha \cdot \boldsymbol{\epsilon}(t)^2 dt$$

← **fluence penalty**

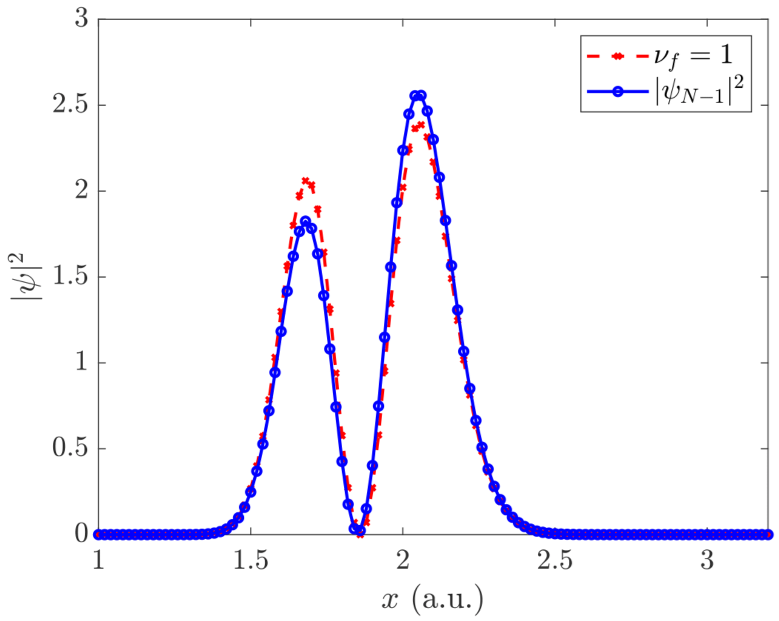
- NIC-CAGE provides *new analytic derivatives* of $\boldsymbol{J}[\psi_{N-1}, \boldsymbol{\epsilon}]$:

$$\frac{d\boldsymbol{J}}{d\epsilon_{j+1/2}} \propto \left(\prod_{k=j+1} \boldsymbol{\mathcal{H}}_{+,k}^{-1} \cdot \boldsymbol{\mathcal{H}}_{-,k}\right) \cdot \boldsymbol{\mathcal{H}}_{+,j}^{-1} \cdot [\boldsymbol{\mu} \odot (\boldsymbol{\psi}_{j+1} + \boldsymbol{\psi}_j)] \quad \text{with} \quad \boldsymbol{\mathcal{H}}_{\pm,n} = \mathbb{I} \pm \boldsymbol{\mathcal{H}}\left[x, \left(n + \frac{1}{2}\right)\tau\right]$$

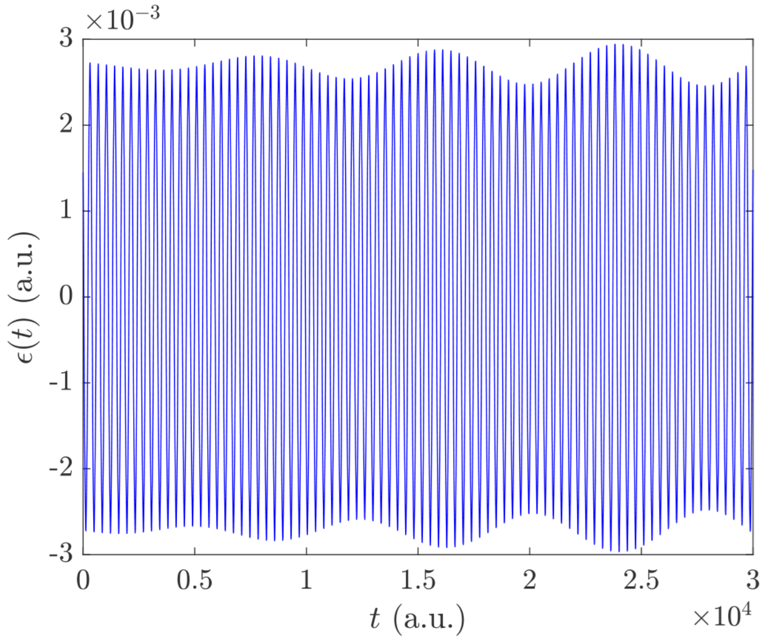
- Take-home message: **no matrix exponentials!**
  → Much faster than Octopus and QuTiP software packages

NIC-CAGE Examples

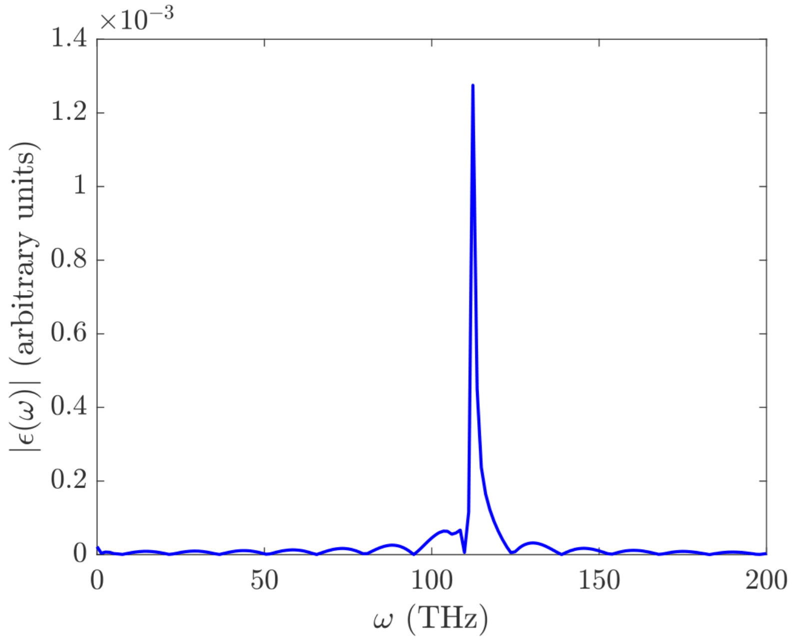
- Single anharmonic potential well



$\nu = 0 \rightarrow \nu = 1$



"optimized" electric field



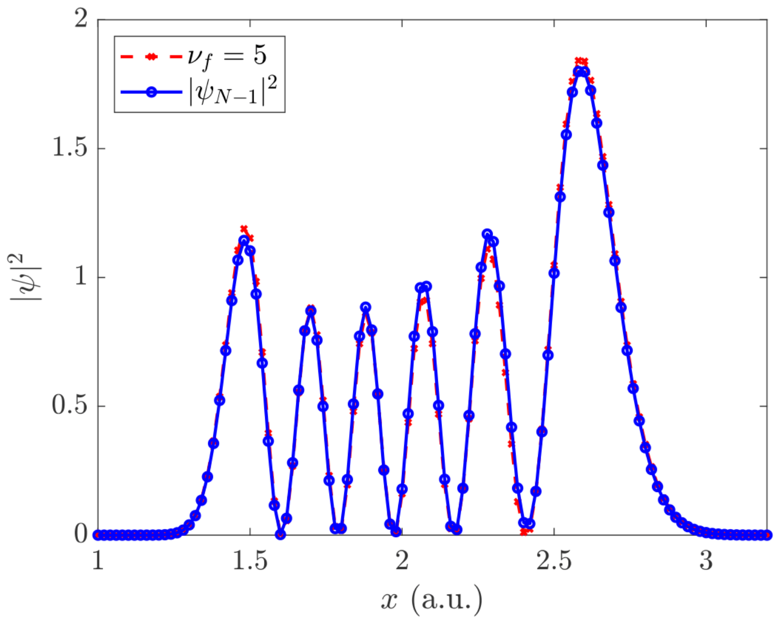
power spectrum

red: target $|\psi_1^2|$
blue: NIC-CAGE propagation

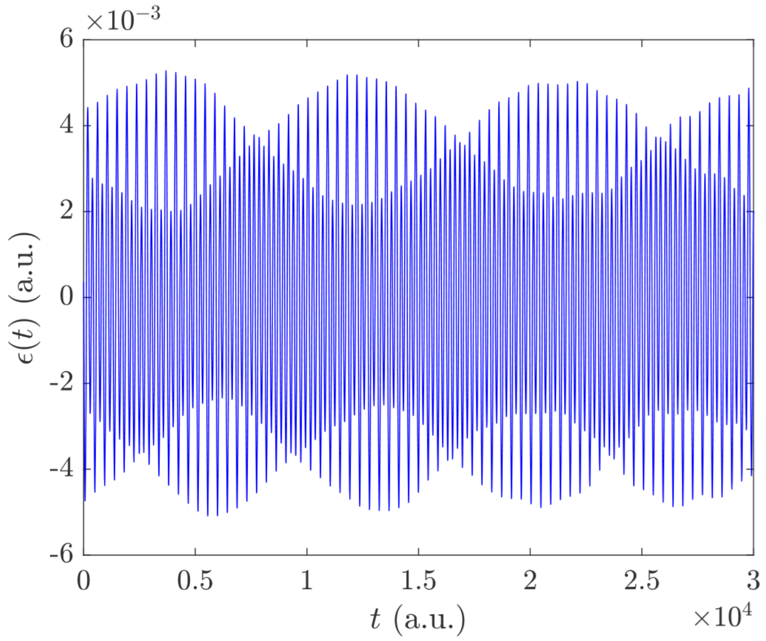
A. Raza & B. Wong, *Comput. Phys. Commun.* **258**, 107541 (2021)

NIC-CAGE Examples (cont.)

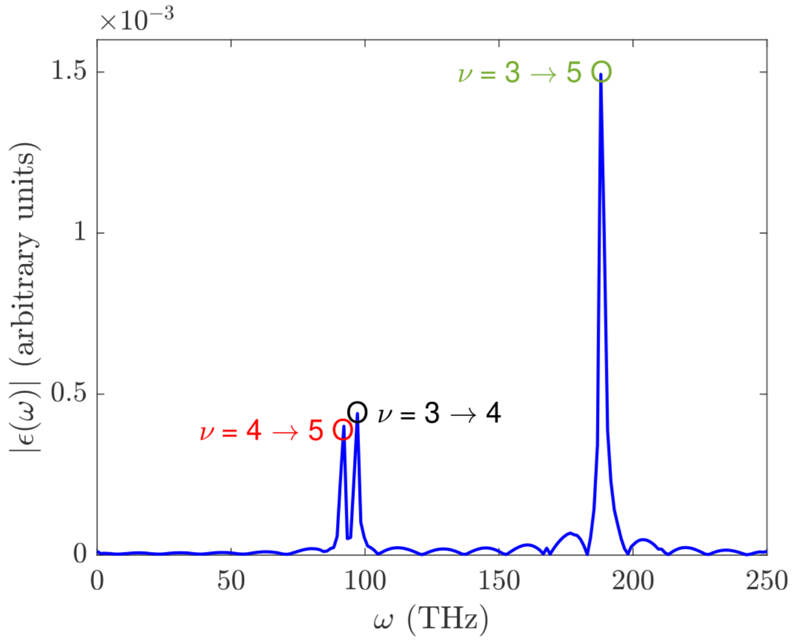
- Single anharmonic potential well



$\nu = 0 \rightarrow \nu = 5$



"optimized" electric field



power spectrum

red: target $|\psi_5^2|$
blue: NIC-CAGE propagation

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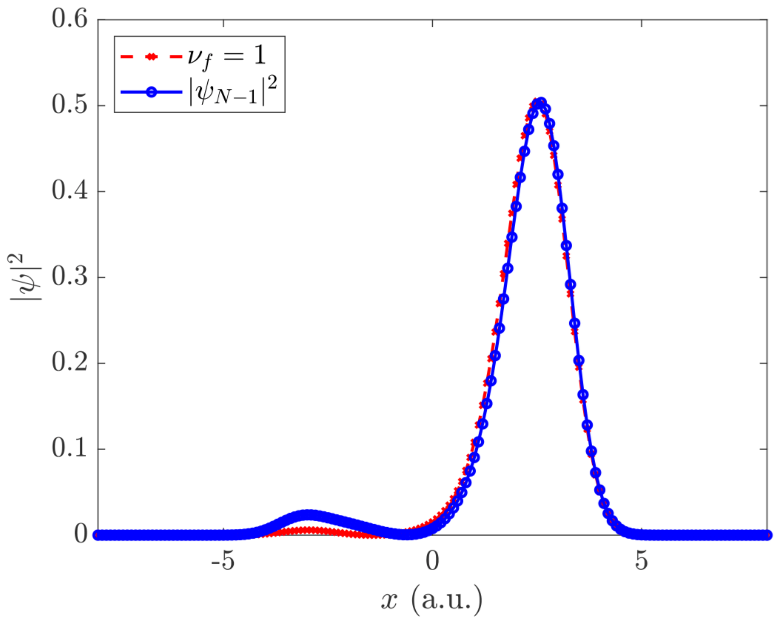
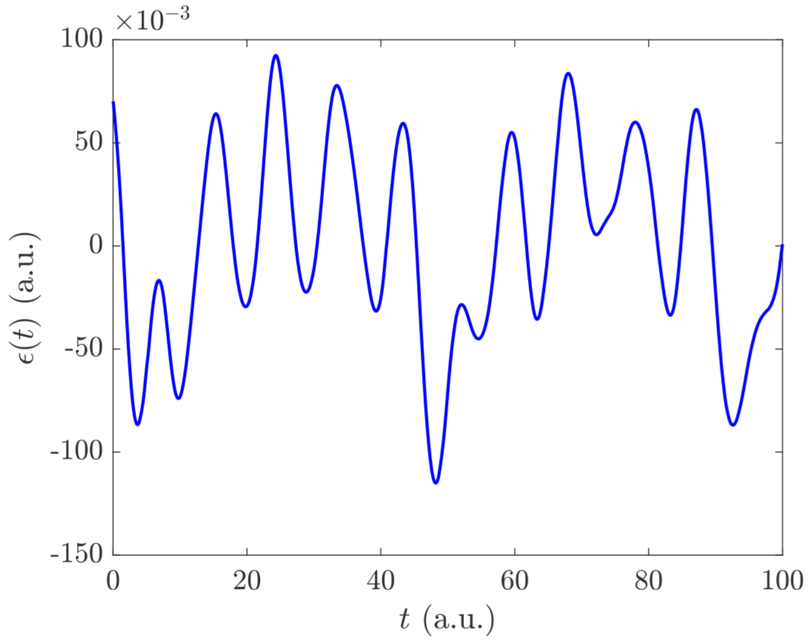
NIC-CAGE Examples (cont.)

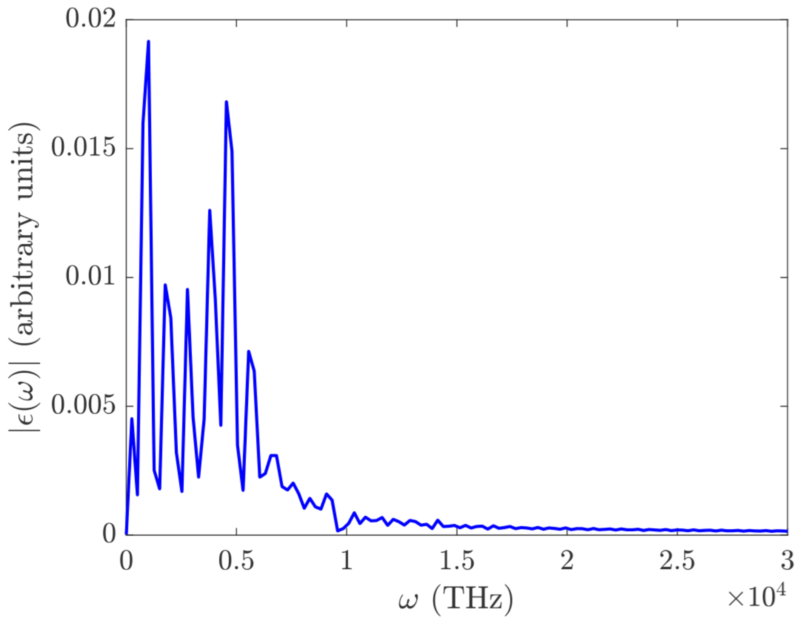
- Anharmonic double-well potential *(restricted propagation time)*



$\nu = 0 \rightarrow \nu = 1$



"optimized" electric field



power spectrum

red: target $|\psi_1^2|$
blue: NIC-CAGE propagation

A. Raza & B. Wong, *Comput. Phys. Commun.* **258**, 107541 (2021)

Conclusion & Acknowledgements

- Predictive quantum simulations provide rational guidance for constructing quantum sensors for fossil energy infrastructures
- Quantum information science *almost perfect application of excited-state quantum calculations*
- Supported by UCR/HBCU DE-FE0031896

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