Excited-states & QED on NISQ Devices

NARANGLAB
MATERIALS THEORY AT HARVARD

HARVARD
School of Engineering
and Applied Sciences

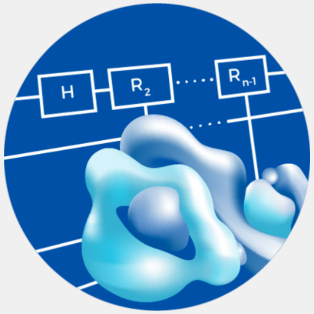
Why are we here?

OUTLINE

Excited-state Dynamics and Interaction with Molecules

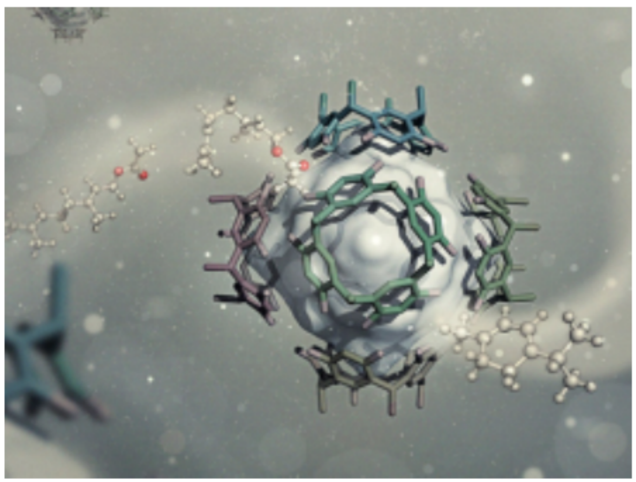
Quantum Materials and Topological Interactions

Quantum Information Science

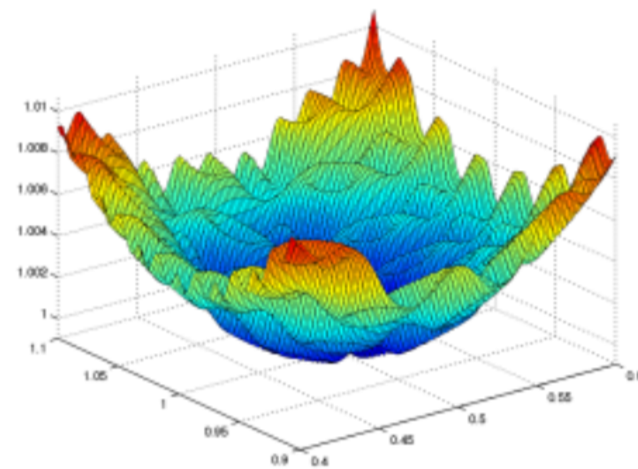


Quantum Information: Early Applications

Quantum Simulation

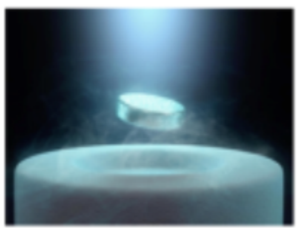


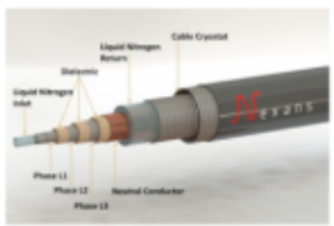
Numerical Optimization



Feynman's Application: Quantum Simulation

30% of cycles on DOE computers spent on: quantum simulation for materials, drug design, solar cells, industrial catalysts, energy



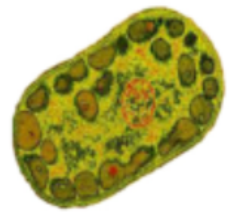


$$H = -t \sum_{\langle pq \rangle} \sum_{\sigma} (a^{\dagger}_{p,\sigma} a_{q,\sigma} + c.c.) + U \sum_{p} a^{\dagger}_{p,\uparrow} a_{p,\uparrow} a^{\dagger}_{p,\downarrow} a_{p,\downarrow}$$

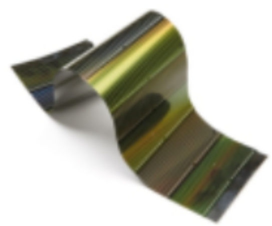
The Fermi Hubbard model: the key to high temperature superconductivity

Haber process: 2% of world energy

$N_2 + 3\,H_2 \rightarrow 2\,NH$: 500°C, 20 Mpa



Simulations of energy transport: the key to economic and efficient solar



Truism:
the macroscopic world is classical.
the microscopic world is quantum.

Goal of QIS: controllable quantum behavior in scalable systems
Why?

Classical systems cannot simulate quantum systems efficiently (a widely believed but unproven conjecture).

But to control quantum systems we must slay the dragon of decoherence …
Is this merely *really, really hard*?
Or is it *ridiculously* hard?

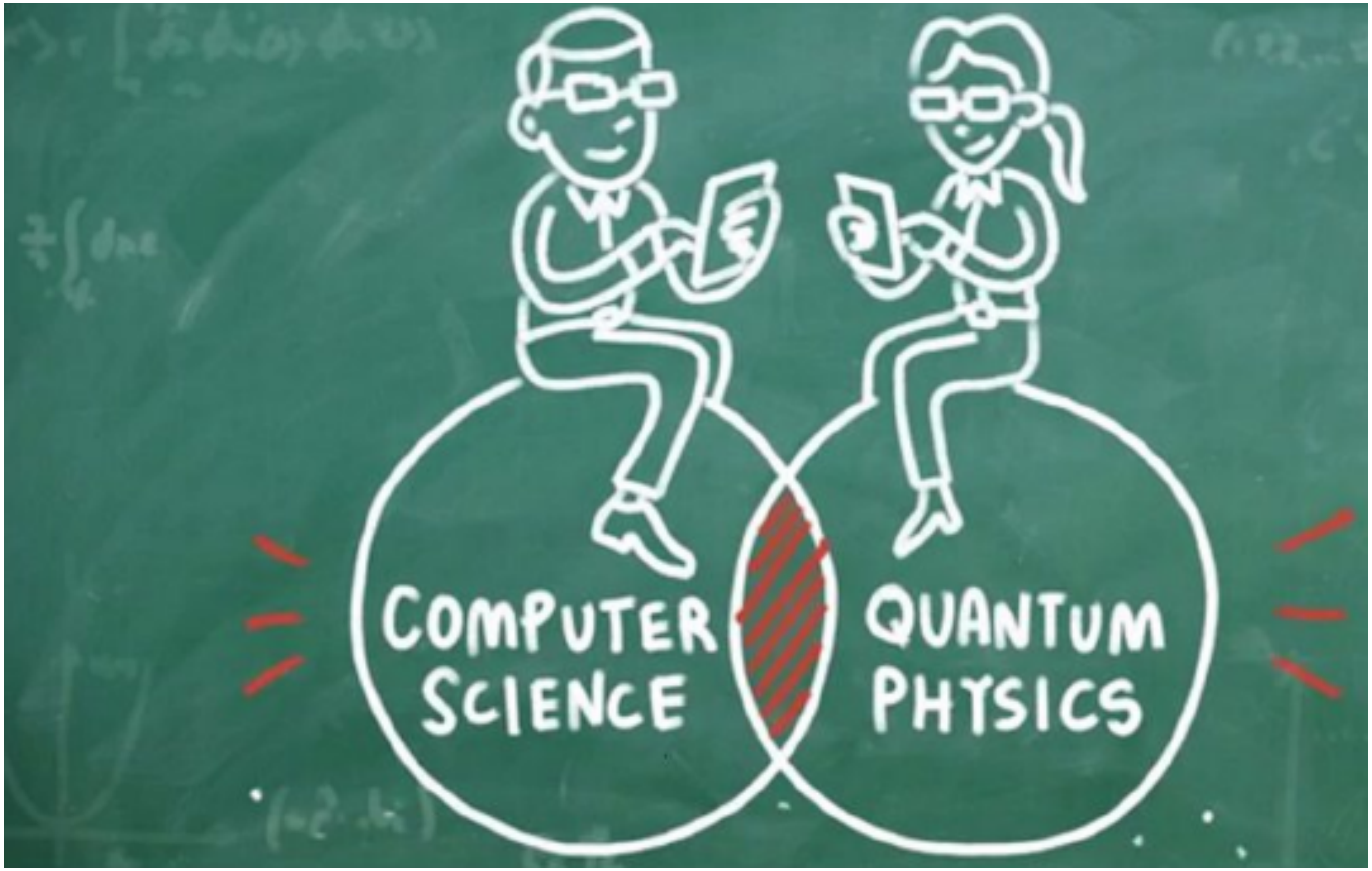
Convergence

Concern about the horizon of Moore's law scaling (running out of "room at the bottom").

Ability to control "single quantum systems" like single atoms or electron spins.

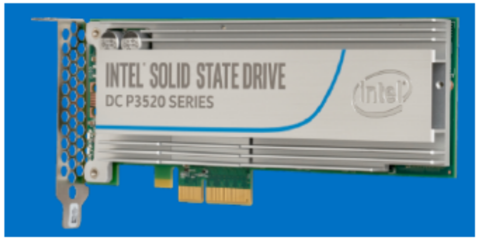
Recognition of computational power inherent in quantum mechanics.

Relevance to the security of public key cryptography.

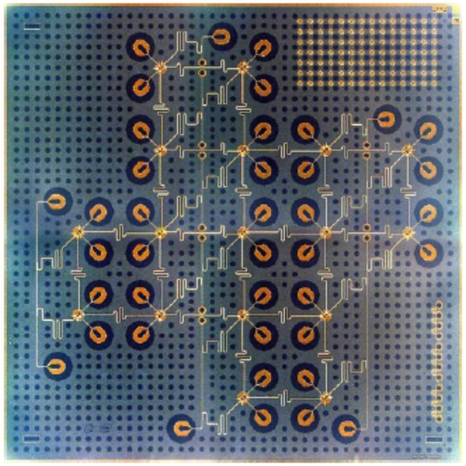

COMPUTER
SCIENCE
QUANTUM
PHYSICS

Classical vs. Quantum Hardware

Processor
- 10^9 transistors
- 10^3 pins



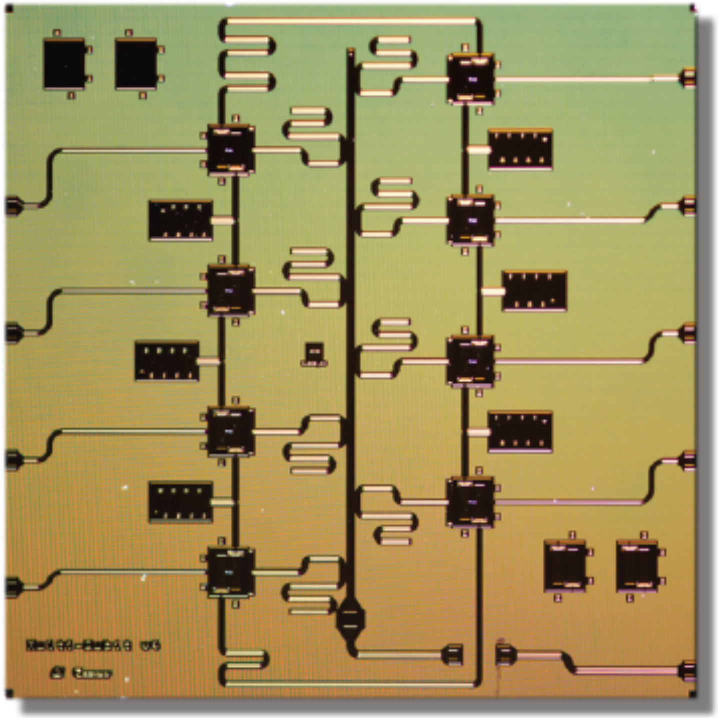
3D NAND Memory
- 10^{12} bytes
- 10^2 pins



17-Qubit Transmon Array
- 17 qubits
- 40 pins

Two approaches to quantum computer scaling
1) New paradigm for packaging and control
2) Share connections or multiplex (within the framework of Moore's Law)

Have superconducting qubits won?



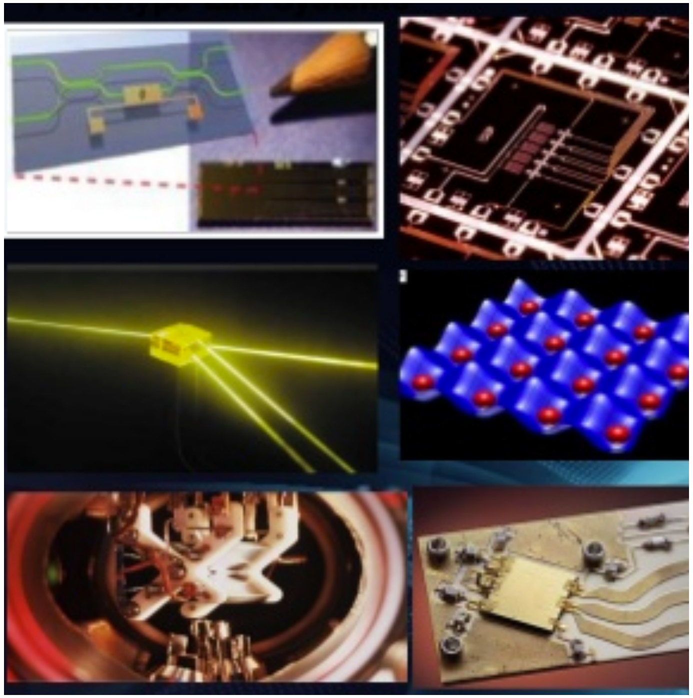
Eight superconducting qubits in a ring topology. The chip is 10mm x 10mm, with submicron Al/AlOx/Al tunnel junctions forming transmon qubits.
Photo: QNL, UC Berkeley.

Qubit Figures of Merit
- T_1 time (energy relaxation)
- T_2 time (decoherence)
- 1-2 qubit gate fidelity
- Qubit readout fidelity
- 2 qubit gate times
- Qubit number & connectivity

State-of-the-Art
- 50 -100 microsecond lifetimes
- 10-50 physical qubits
- Gate fidelities ~ 99%

Outlook
- > 100 microsecond lifetimes
- > 100 physical qubits
- Gate fidelities > 99.9%
- State readout fidelity > 99.9%
- Logical qubit operation
- Error corrected operation

Physical Platforms



- Spin-based
- Photonic
- Atom/cold atom
- Hybrid
- Others

Do they all need a dilution refrigerator?

Entering the NISQ-era

Noisy Intermediate Scale Quantum Technology (Coined by John Preskill)

50-100 qubits

Limitation: Noise in quantum gates

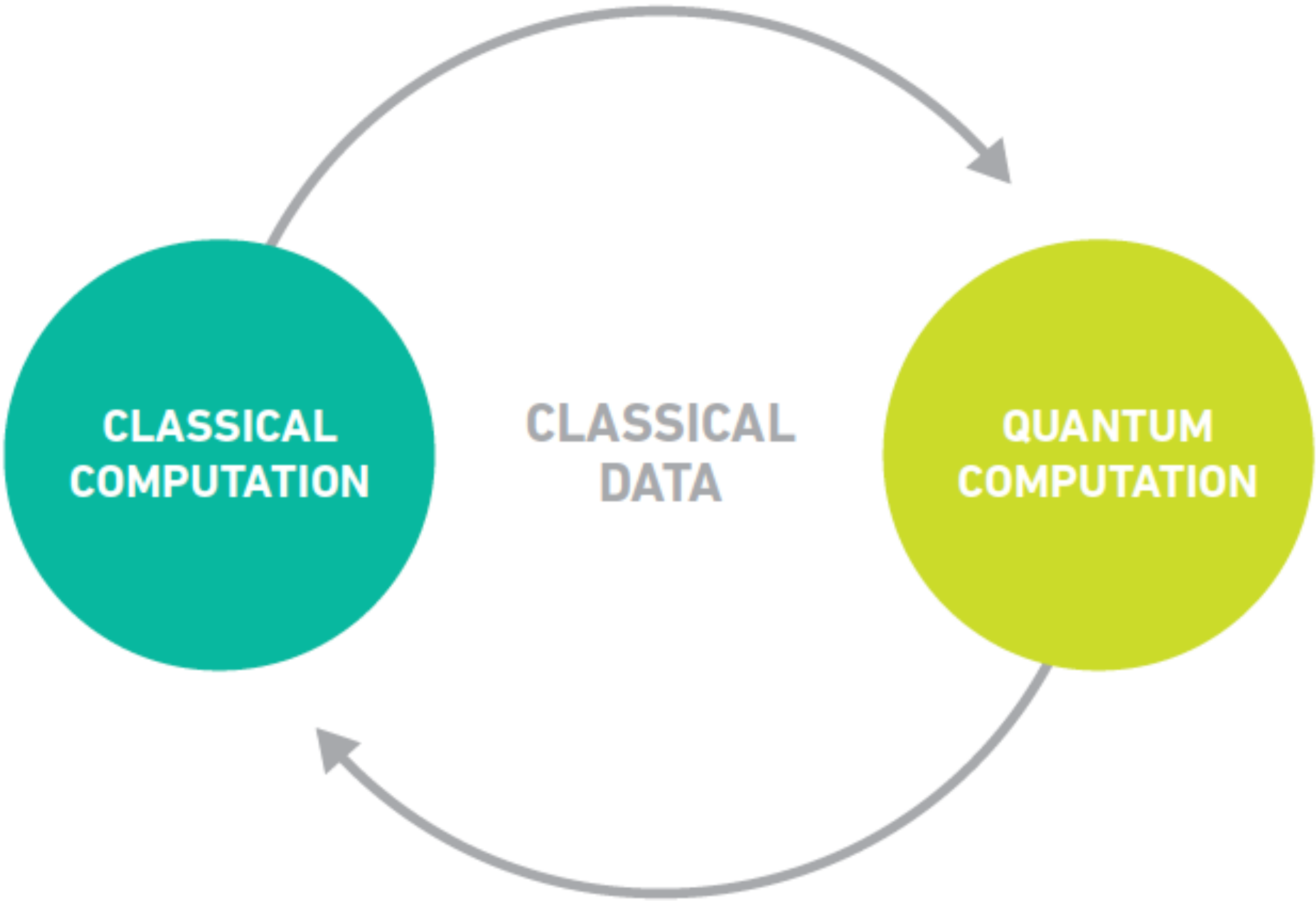
Could still profoundly impact Feynman’s app.

‘ Quantum Volume’ - IBM

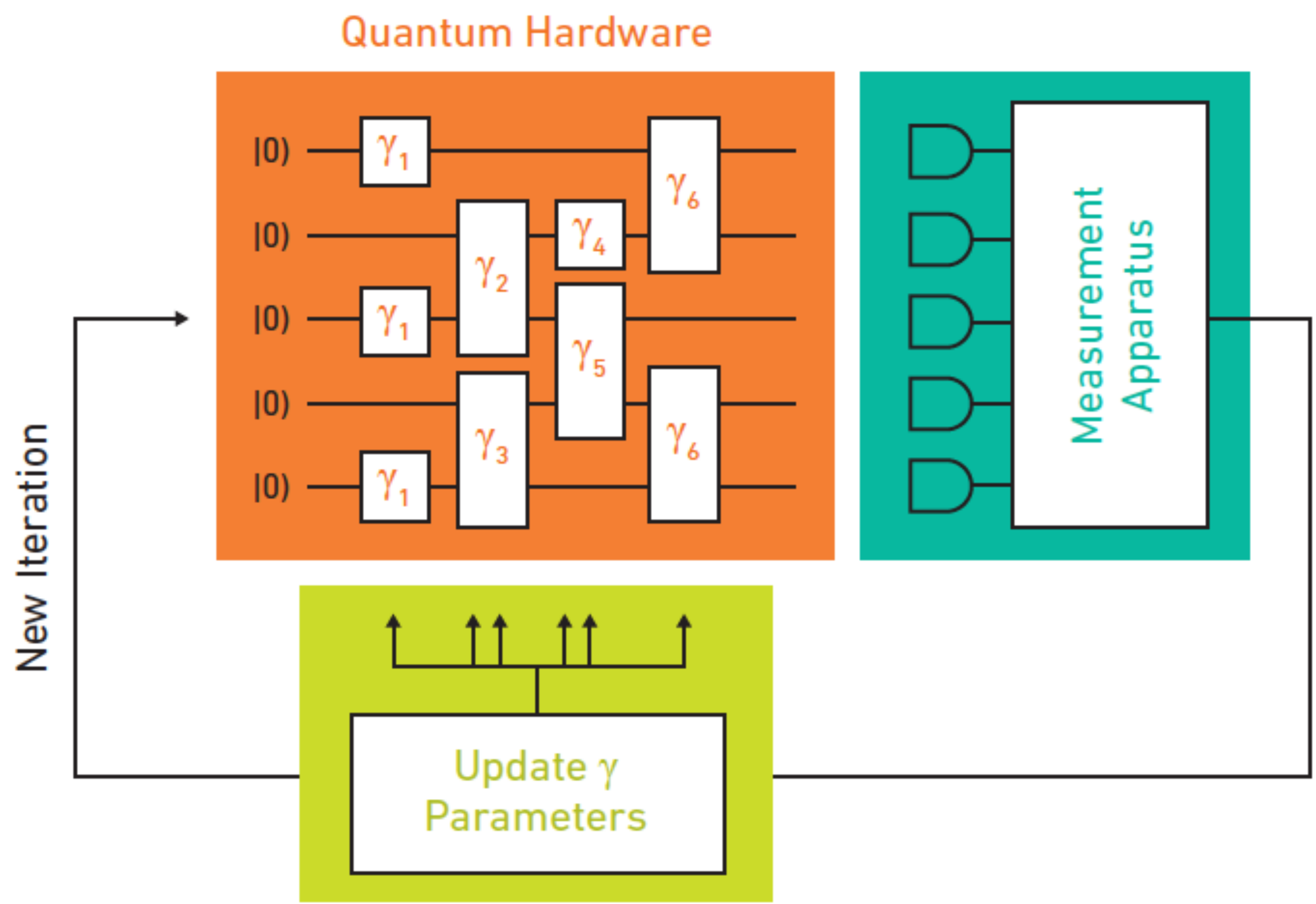
(i) Number of physical qubits N
(ii) Connectivity between qubits
(iii) Number of gates that can be applied before errors or decoherence mask the result
(iv) Available hardware gate set
(v) Number of operations that can be run in parallel

$$\tilde{V}_{\mathrm{Q}} = \min\left[N, d(N)\right]^2$$

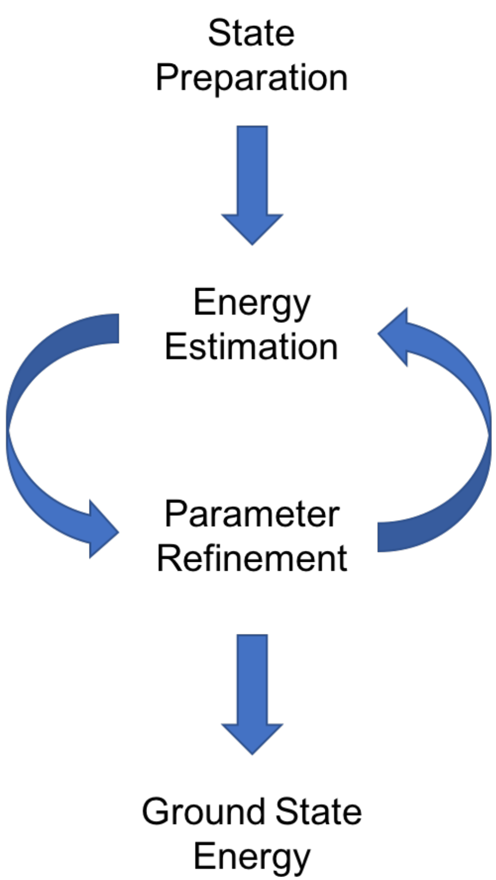
HYBRID QUANTUM-CLASSICAL SCHEME FOR COMPUTATION.

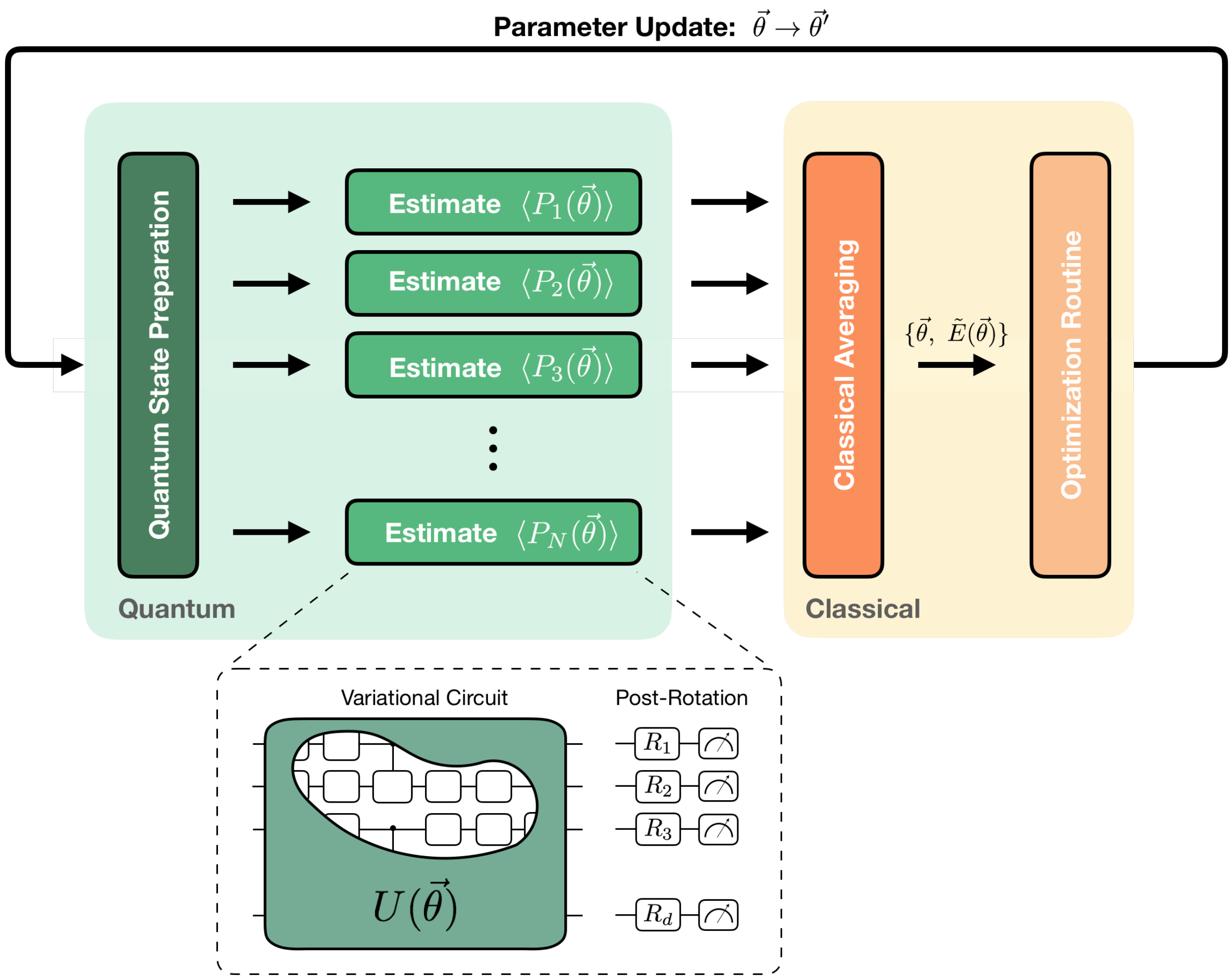


DIAGRAMMATIC REPRESENTATION OF QUANTUM/CLASSICAL HYBRID SCHEMES ENCOMPASSED BY VQE AND QAOA.



Variational Quantum Eigensolver (VQE)





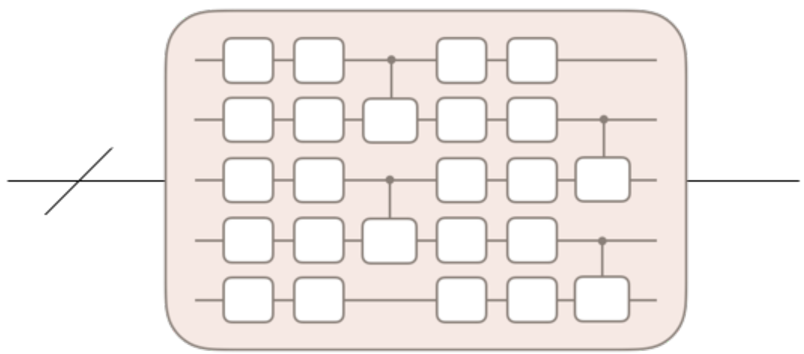
Variational Quantum Eigensolver (VQE)

State Preparation

Reference State

Parametrized Circuit

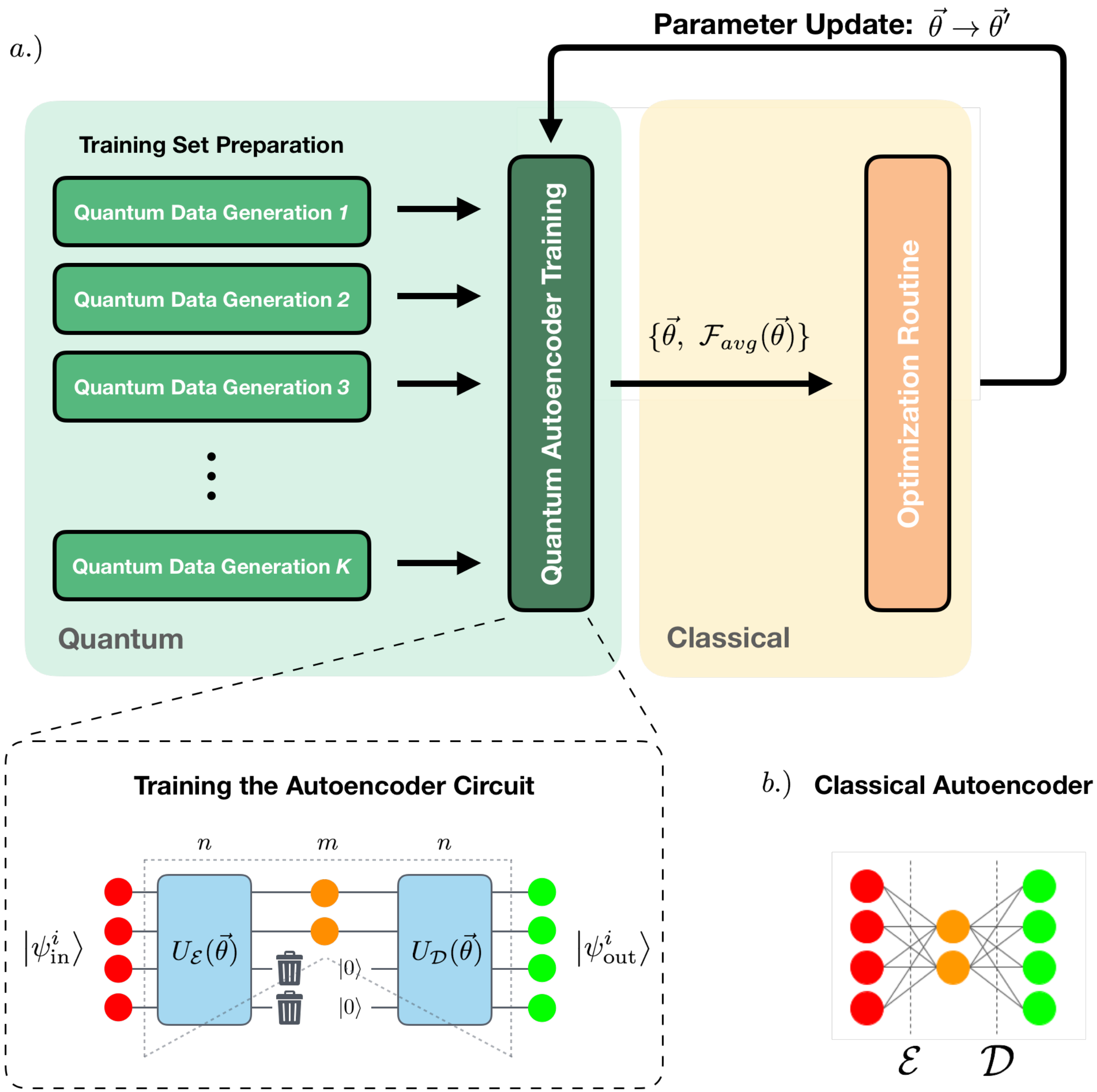
$|\Phi_0\rangle$



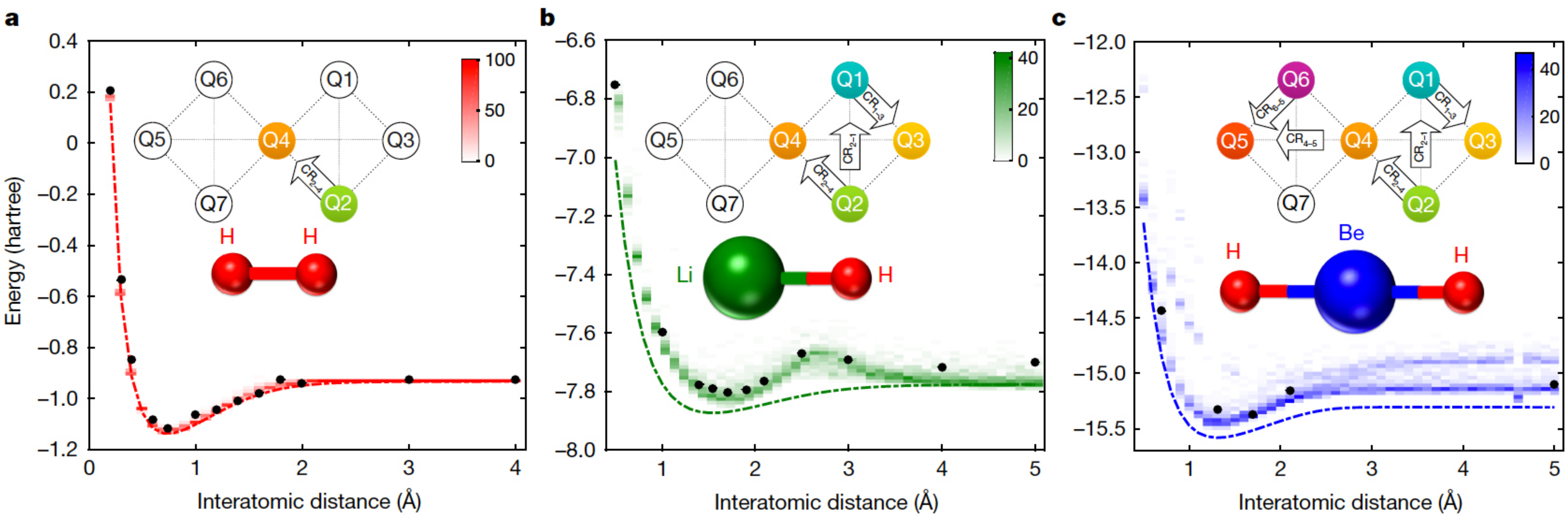
$|\Psi(\vec{\theta})\rangle$

$U(\vec{\theta})$

Quantum Autoencoder Circuit



Small Molecules on IBM Q



Abhinav Kandala, Antonio Mezzacapo, Kristan Temme, Maika Takita, Markus Brink, Jerry M. Chow, and Jay M. Gambetta. "Hardware-efficient Variational Quantum Eigensolver for Small Molecules and Quantum Magnets." *Nature.* doi:10.1038/nature23879

Qubit Allocation

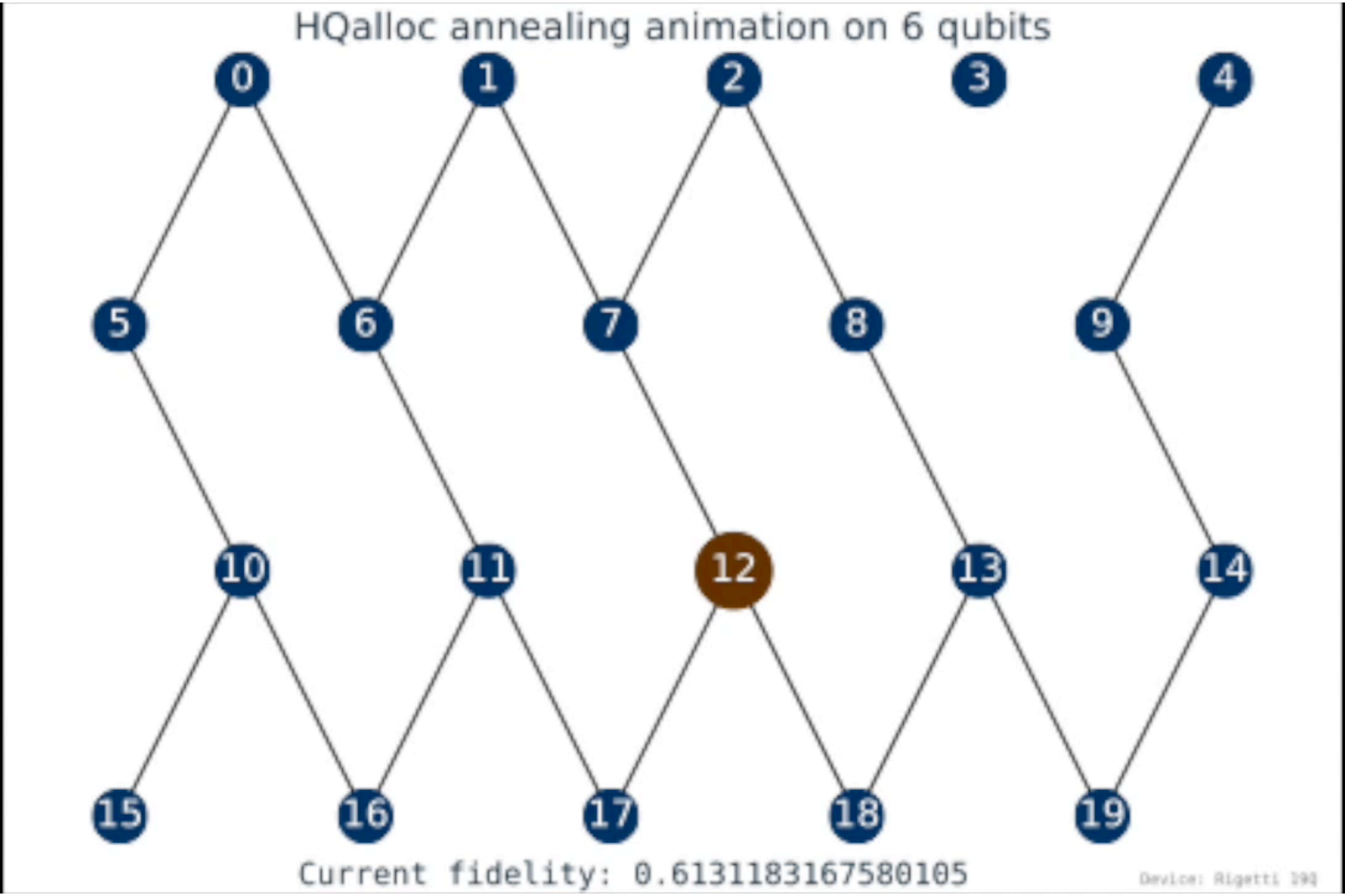
QAlloc

Solving the Qubit Allocation problem is essential to making quantum computation faster and more reliable.

My group has developed two algorithms:

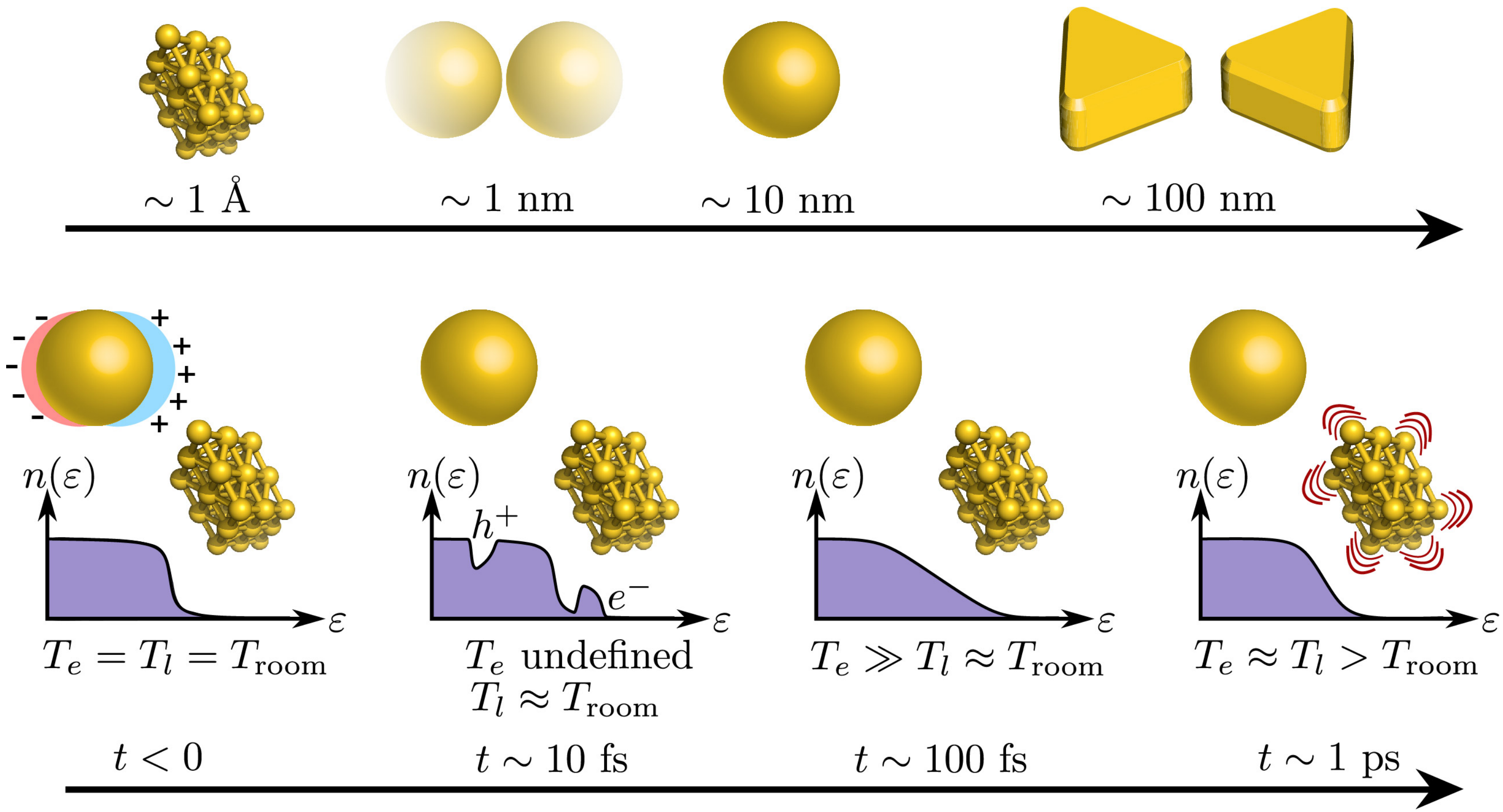
1. An exact solution to this NP-complete problem that has the ability to allocate circuits with arbitrary control flow (something that is not generally well supported with current compilers)

2. A randomized solution returning an allocation close to the optimal in few iterations.

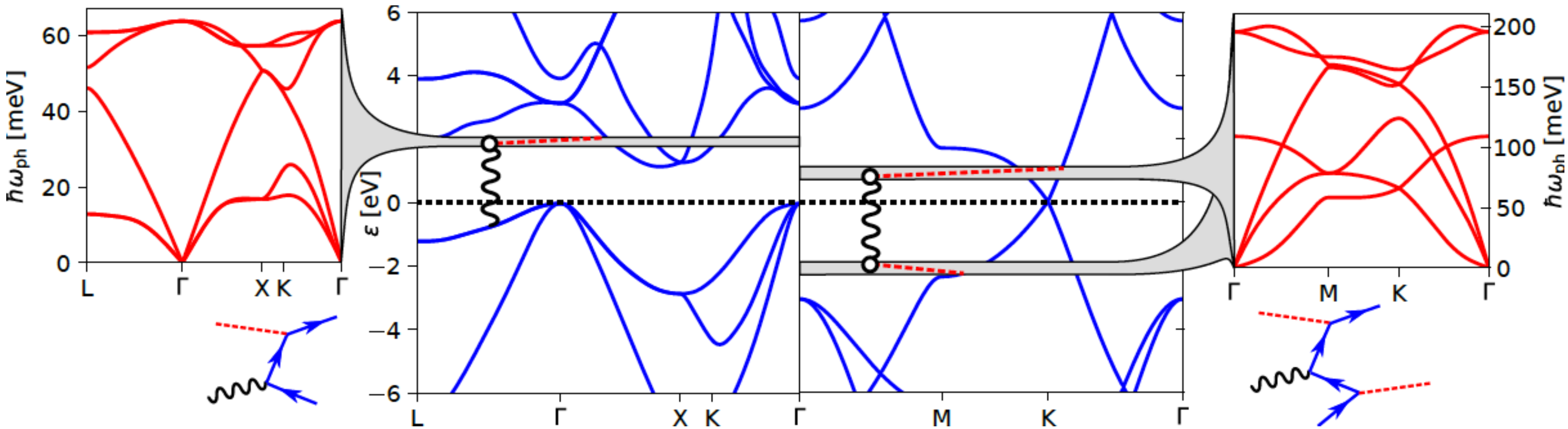

HQalloc annealing animation on 6 qubits
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
Current fidelity: 0.6131183167580105

Problems of Interest

Ultrafast and fast time-scales in excited-state photonics

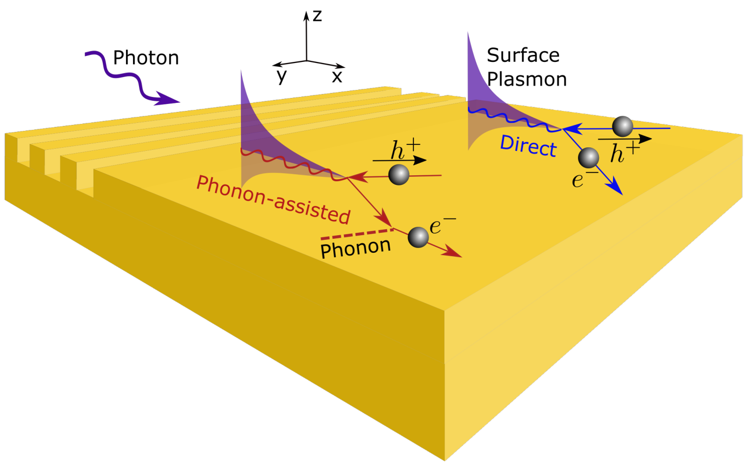


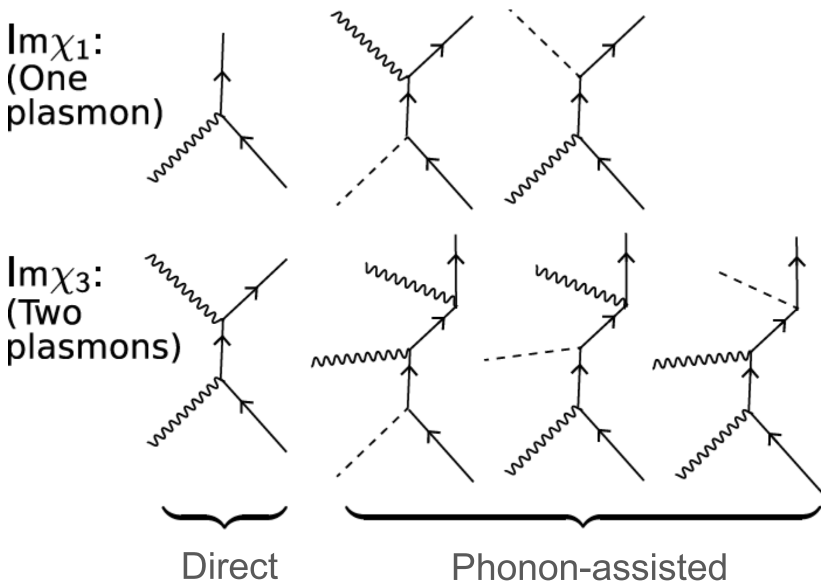
Why are electron-phonon interactions a challenge?



- Energy mismatch
- Frohlich-type Hamiltonians (linear displacement); Debye-Waller factor
- Non-adiabatic phonons

Interband, phonon-assisted intraband and nonlinear transitions

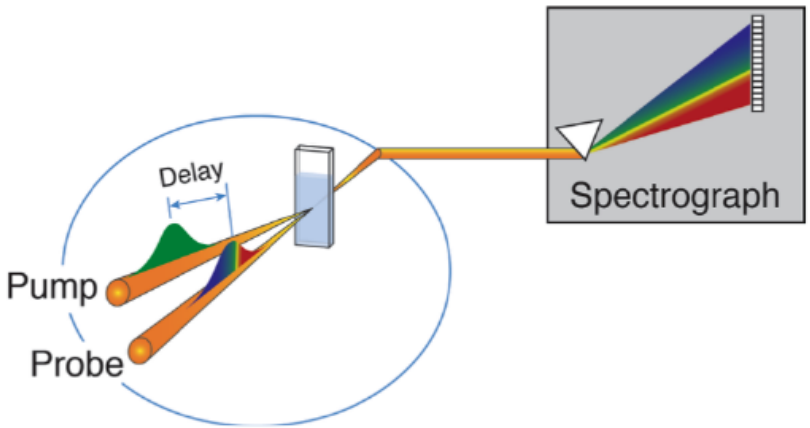


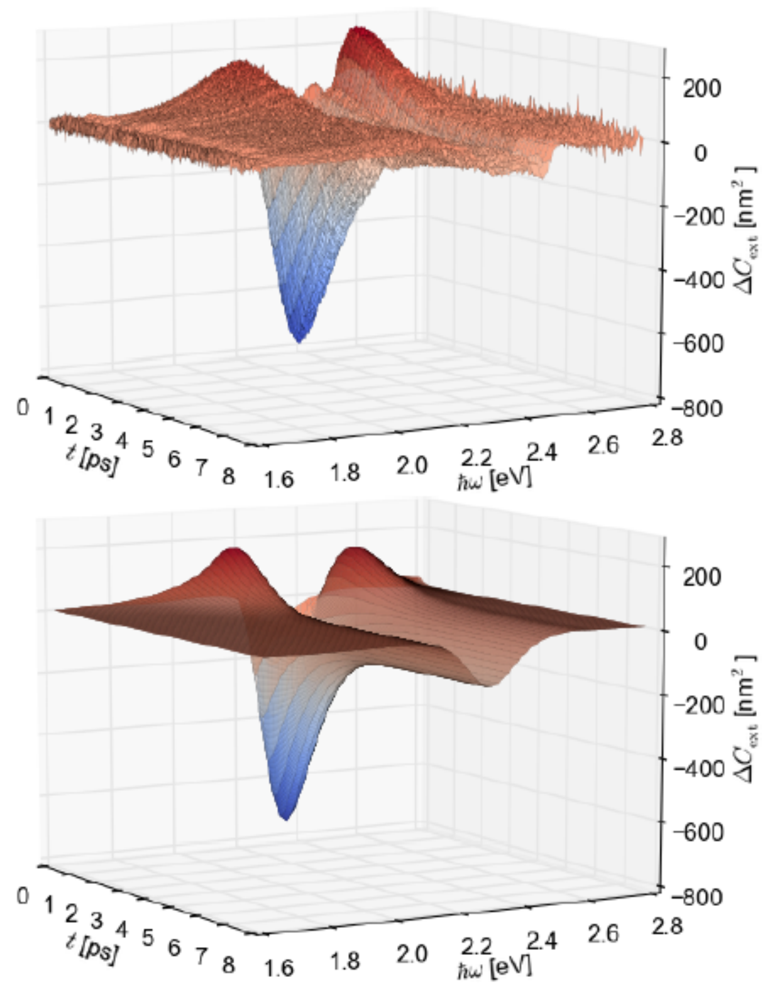


- Quantitative predictions of microscopic mechanisms & comparisons with experimental linewidth
- Predicting nonlinear signatures of nonequilibrium carriers

Narang et al, *Nature Communications* 5, 5788 (**2014**)
Brown, Narang, et al, *ACS Nano* (**2015**)
Narang, et al*, Journal of Phys. Chem. C* (**2016**)
Fitzgerald, Narang, et. al Proc. Of IEEE (**2016**)

Quantitative understanding of ultrafast dynamics

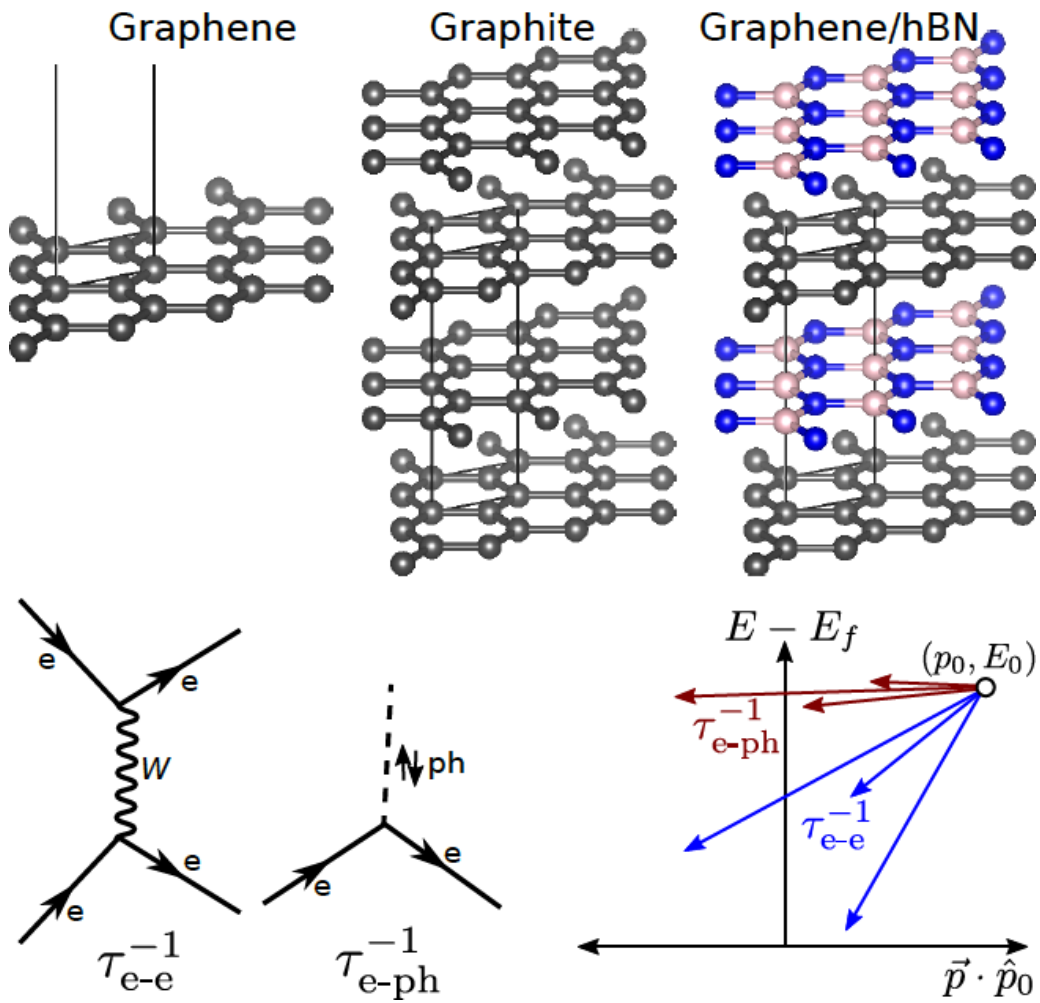




- Measure material response at femtosecond to nanosecond timescales
- Carrier generation + relaxation + optical response => quantitative predictions from first principles

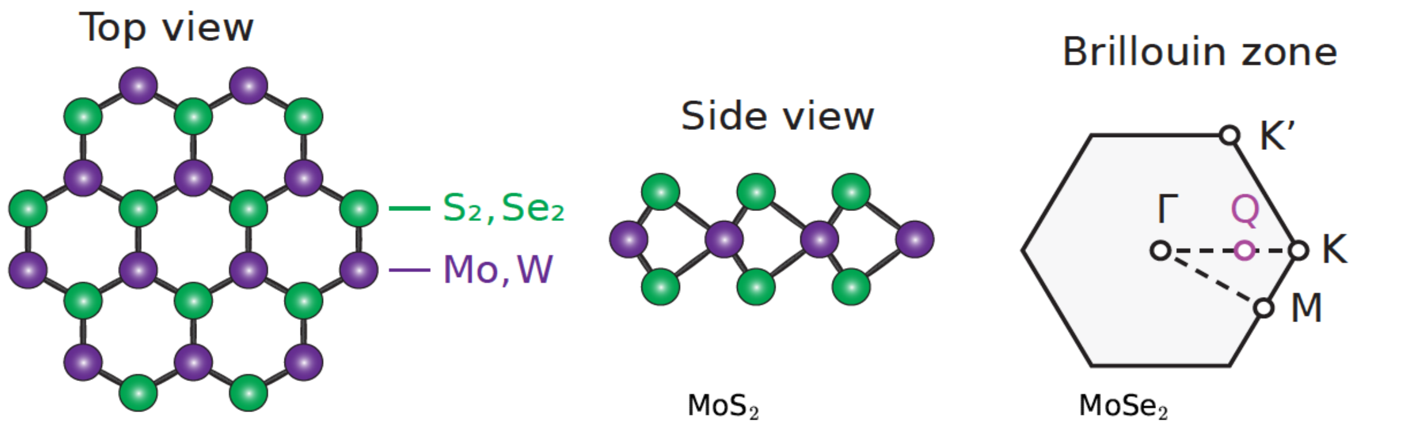
Brown, Narang et. al., *Phys. Rev. B.* (**2016**)
Brown, Narang et. al., *Phys. Rev. Lett.* (**2017**)

Ultrafast dynamics in 2D heterostructures

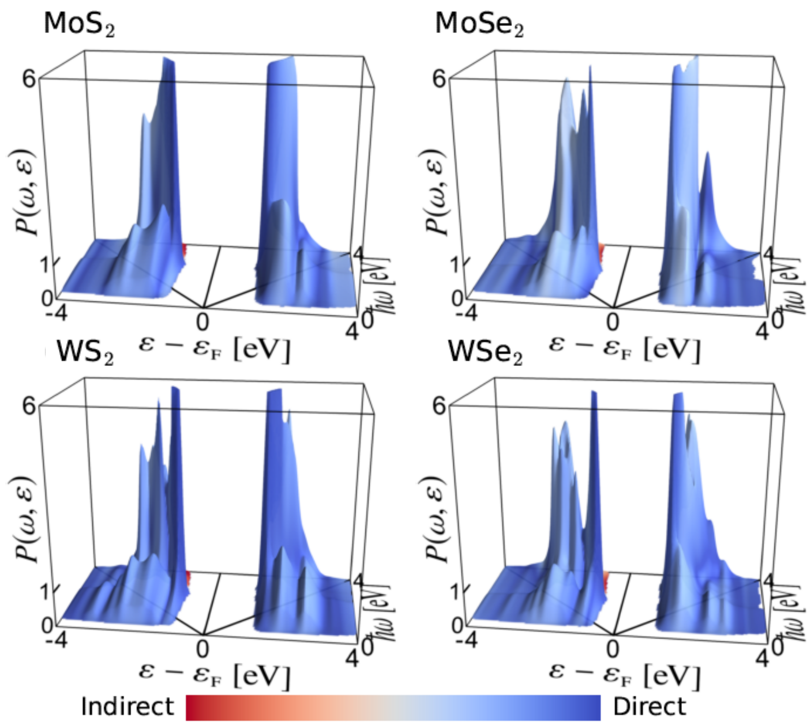


Narang, et al, *Advanced Optical Materials* (**2017**)
Papadakis, Narang, et al, *ACS Photonics* (**2017**)
Shirodkar, Narang, Soljacic, Kaxiras, et. al, Phys. Rev. B (**2018**)

Photonics in van der Waals Heterostructures

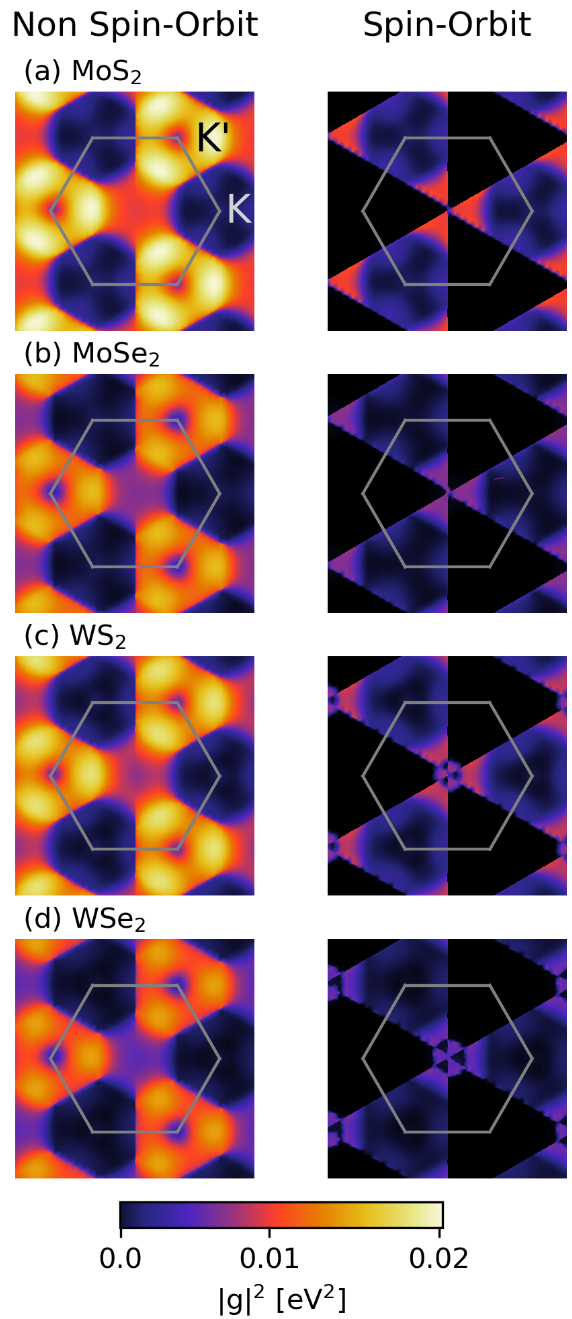


- Collective excitations of many flavors
- Non-equilibrium features e.g. generation and relaxation of excited carriers challenging to map out experimentally
- Role of valley symmetry and broken symmetry



Ciccarino, et al, *Nano Letters* (**2018**) – Recently Accepted

Dynamics & Spin Valley Locking in TMDCs

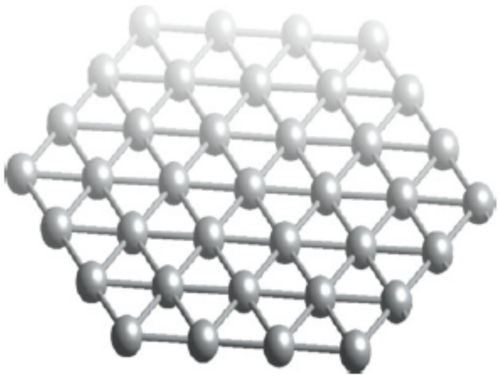


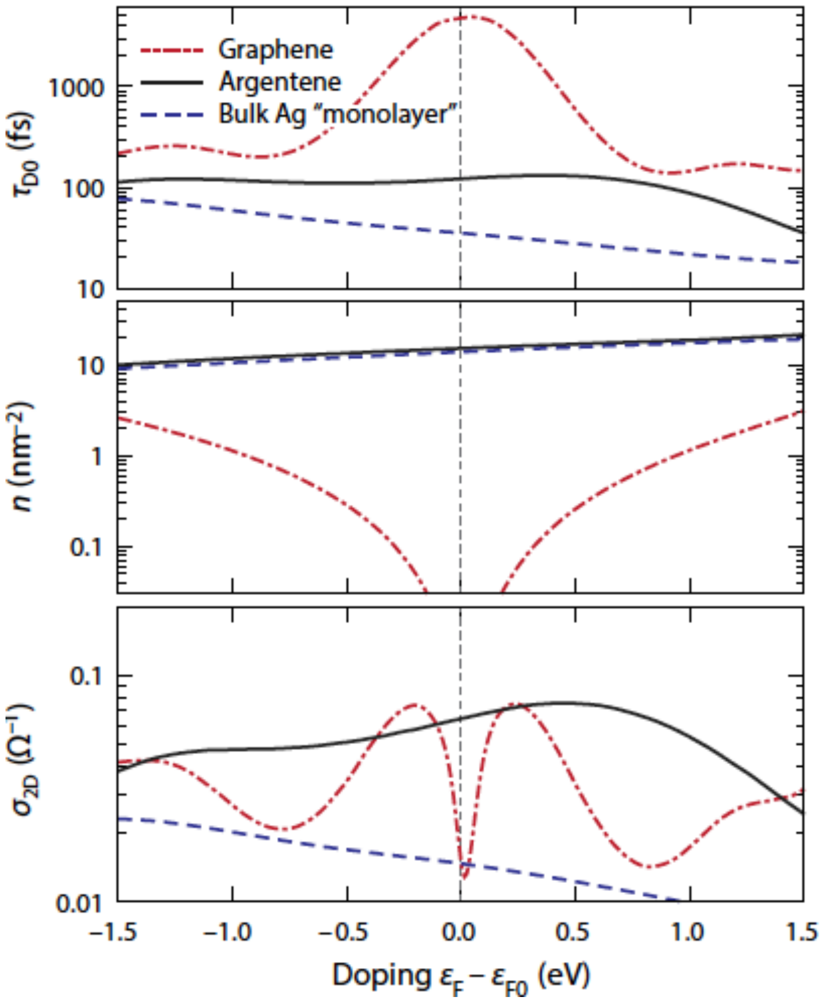
- Asymmetry between contributions from el-el vs el-ph when spin-orbit interactions are considered

- Long, el-ph driven lifetimes near the Fermi-level, important for photonic applications

Ciccarino, et al, *Nano Letters* (**2018**) – Recently Accepted

2D Metals: *Argentene*



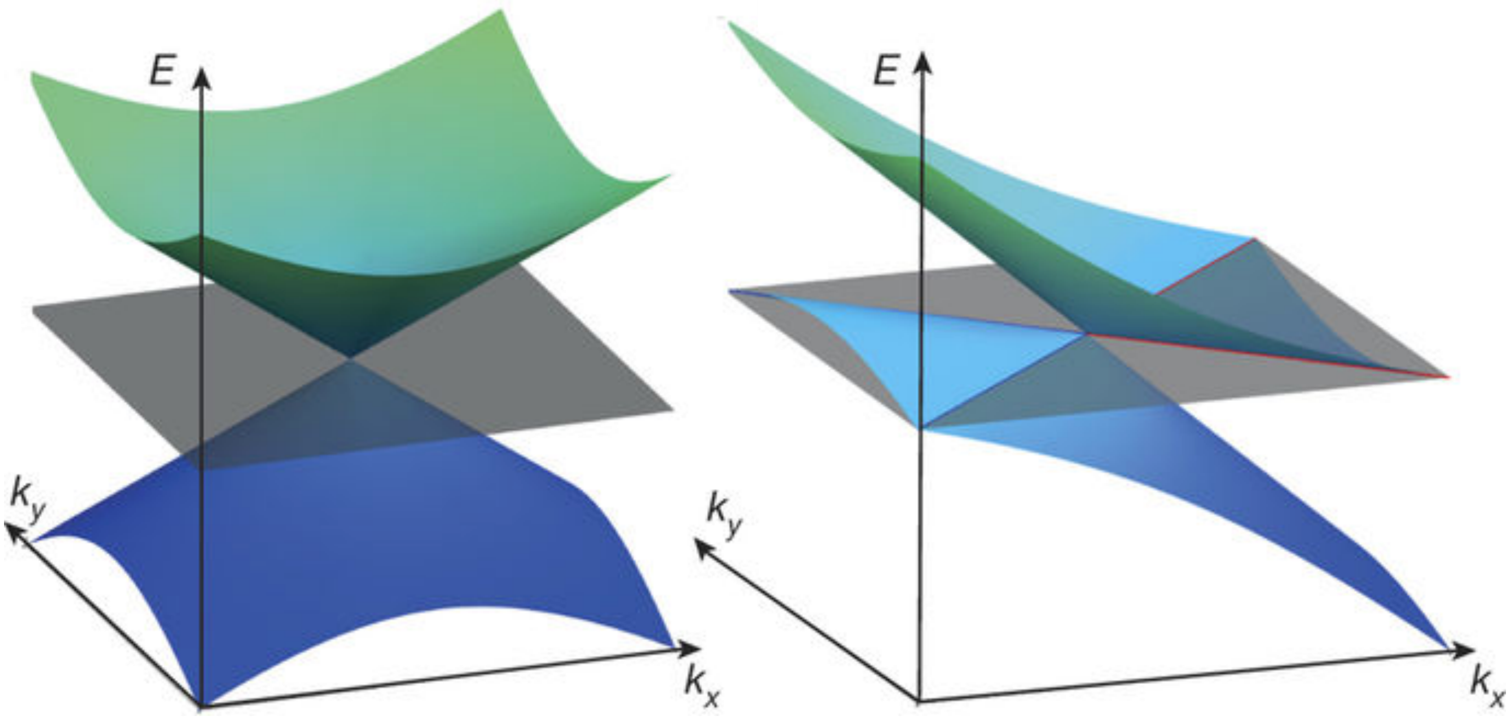


- Predicted stability and barrier on vdW substrates
- Explicit calculations of time dynamics vs. jellium/model calculations

Narang, et al, arXiv preprint arXiv:1806.02672(**2018**) – in review

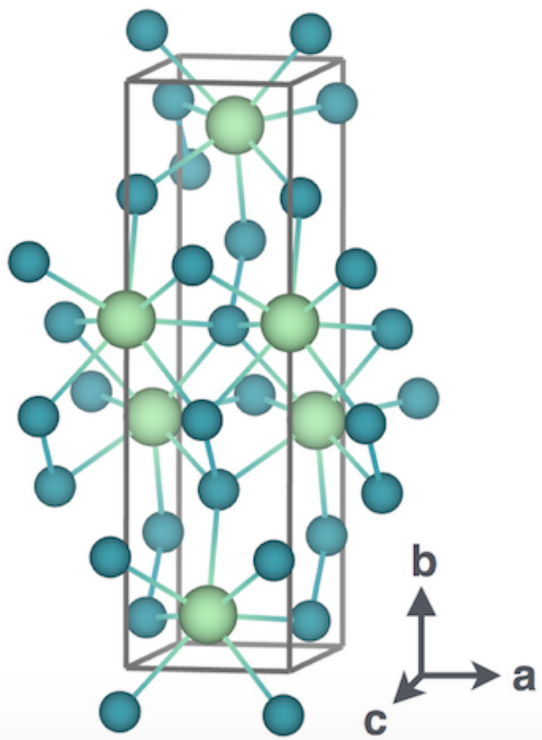
Quantum Materials: Type II Weyl Semimetals

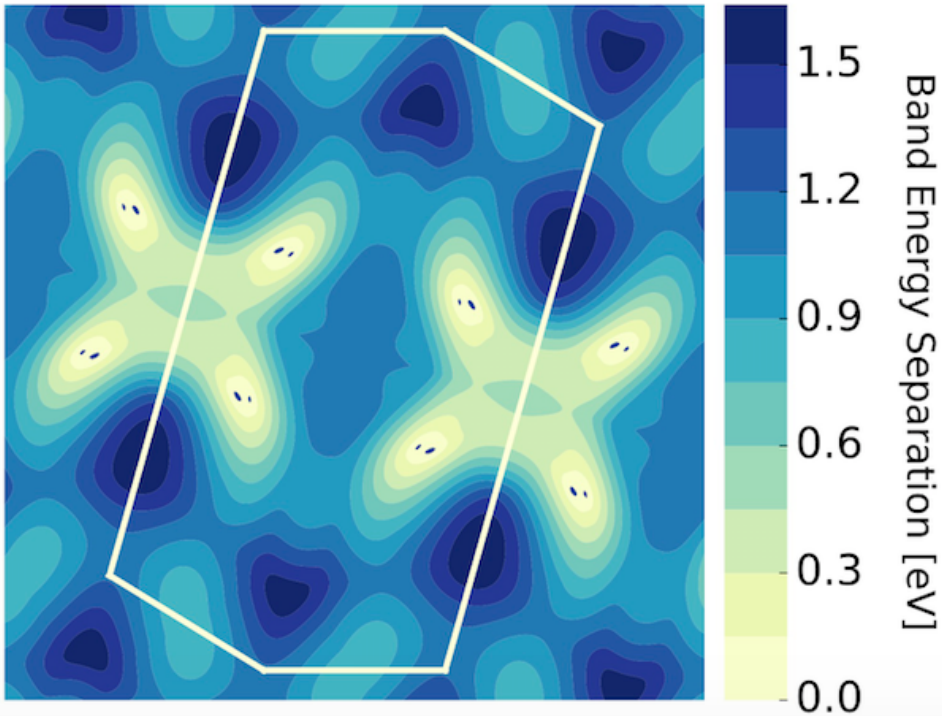
Understanding Type II Weyl Semimetals



Specifically, WP_2 : Anisotropy

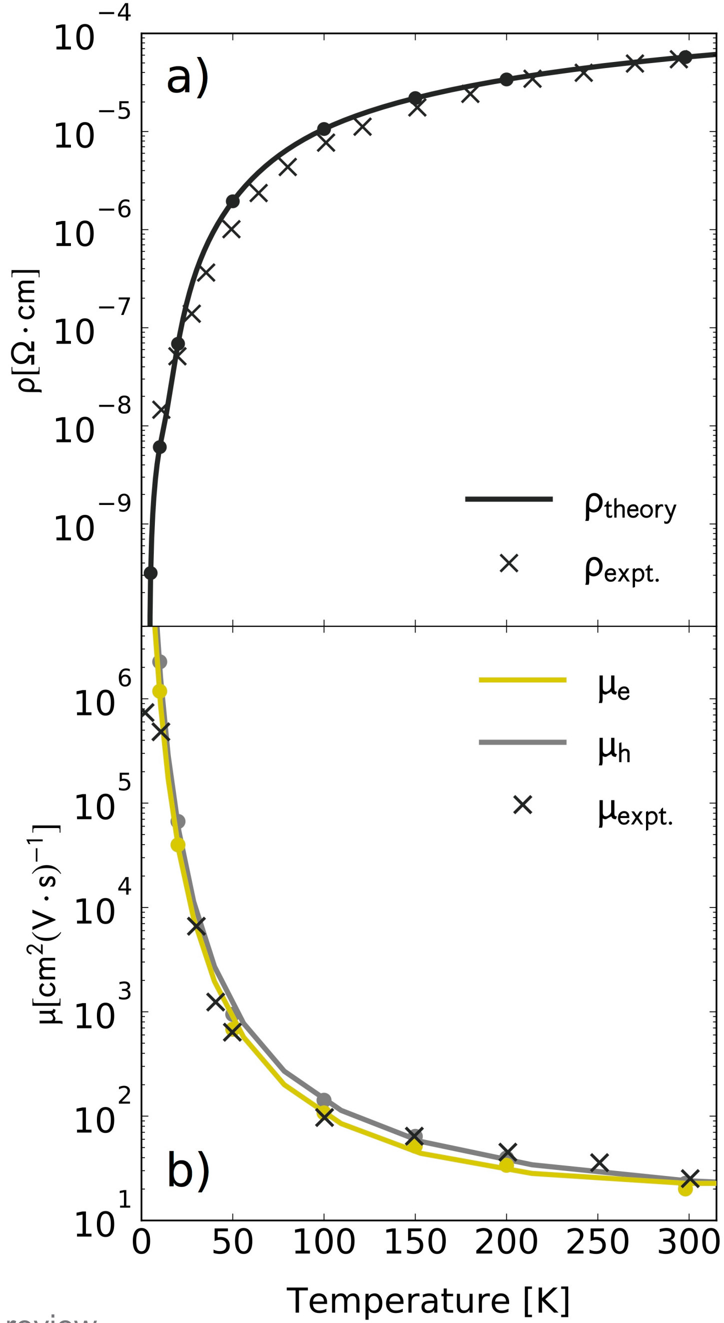
- Type II Weyl semimetal
- Orthorhombic/$Cmc2_1$
- Recently reported hydrodynamic flow (2017)
- Transport anisotropy allows us to study 2D electron flow



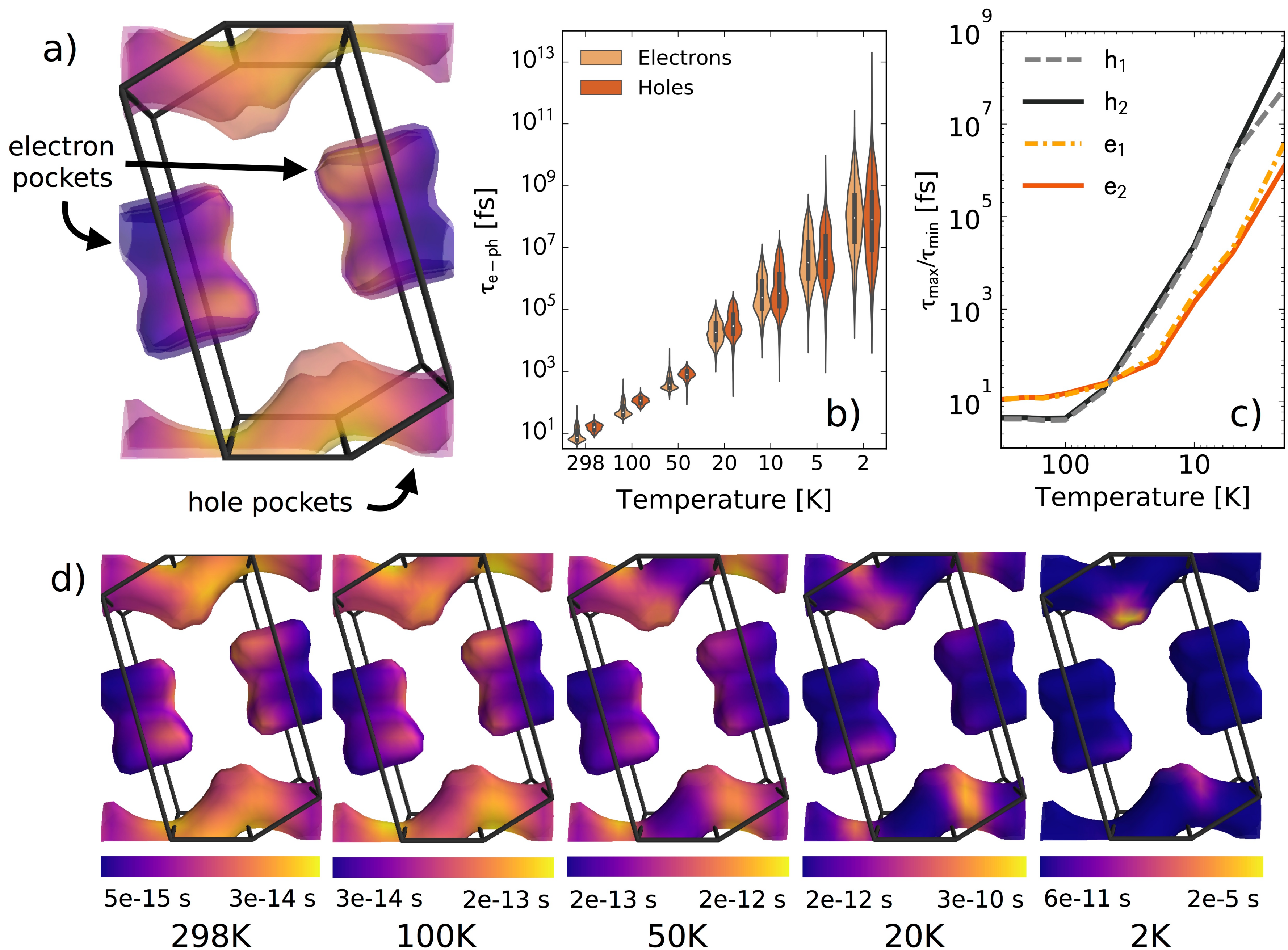


Coulter, et al, arXiv preprint arXiv:1804.06310(**2018**) – in review

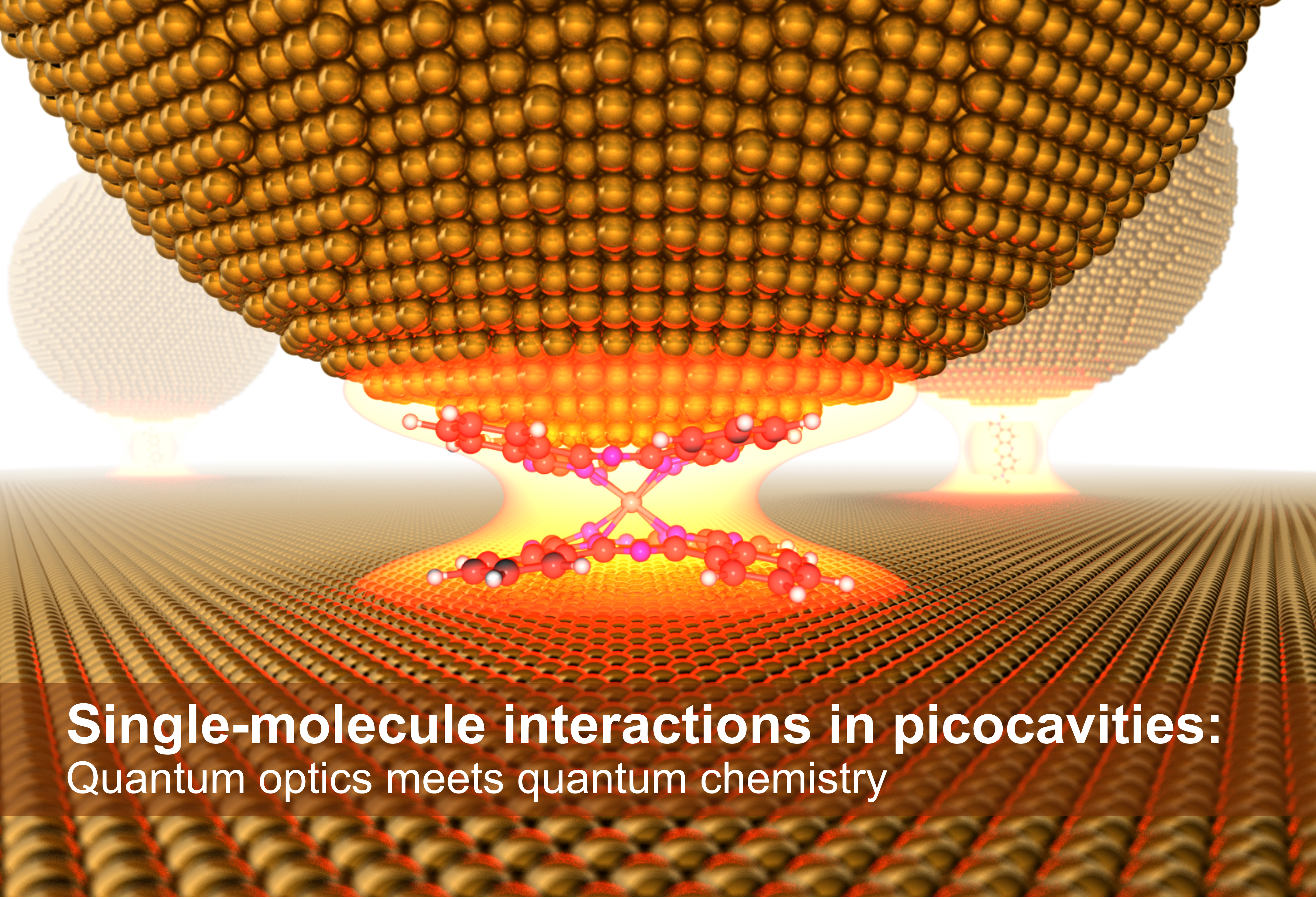
Parameter-free Quantum Transport



Coulter, et al, arXiv preprint arXiv:1804.06310(**2018**) – in review



Coulter, et al, arXiv preprint arXiv:1804.06310(**2018**) – in review

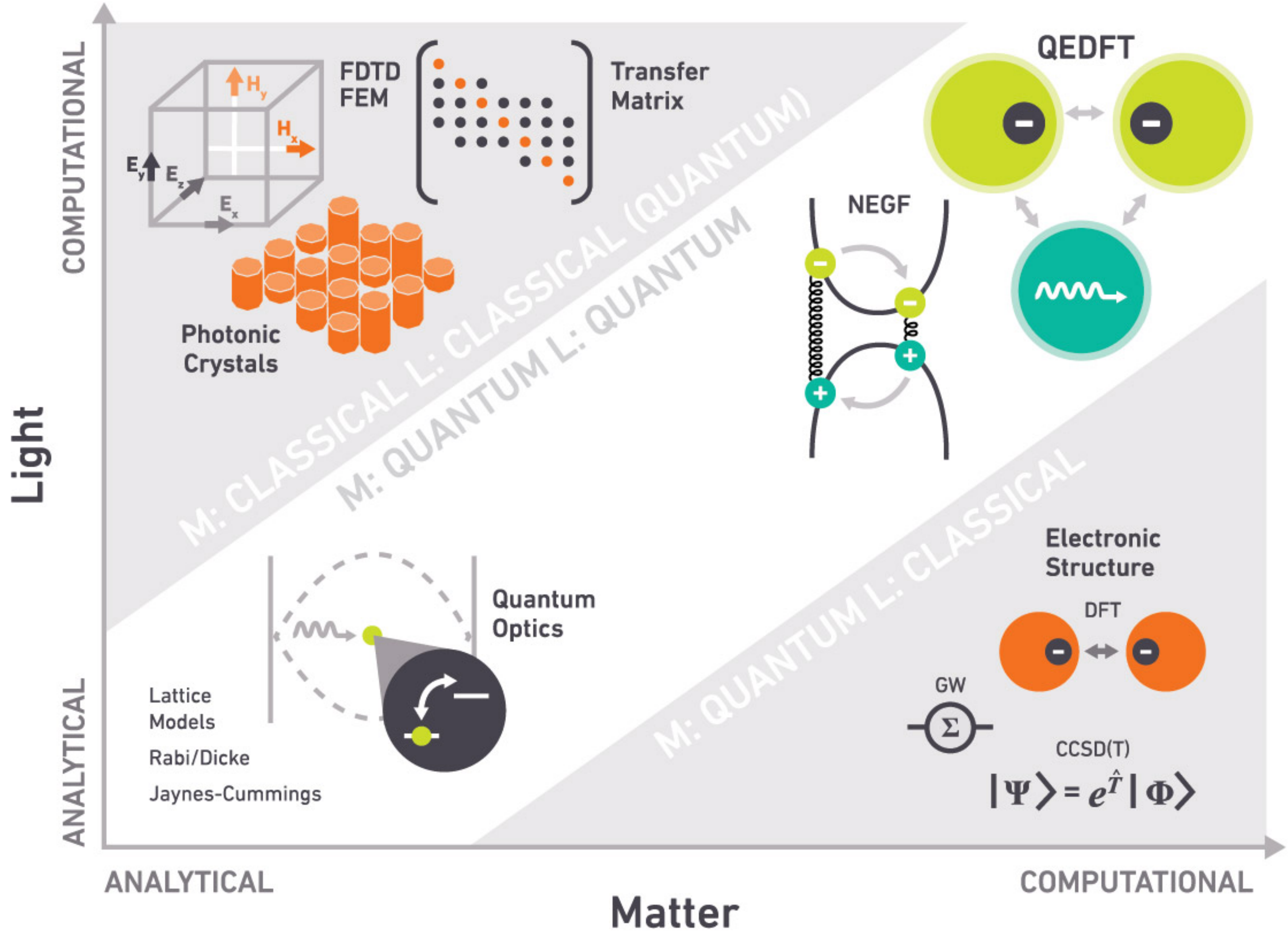


Single-molecule interactions in picocavities:

Quantum optics meets quantum chemistry

In collaboration with Prof. Jeremy Baumberg, Upcoming in *Nature Communications;* Mertens, Narang, Baumberg, *Nanoletters* (**2017**)
Cortes, Narang et. al. arXiv:1607.05657 (**2016**), *Nature Communications* (**2017**)

QED + Electronic structure + QIS?



Flick, Rivera and Narang (**2018**) accepted to *Nanophotonics*
Flick and Narang, arXiv preprint arXiv:1804.06295 (**2018**) – accepted to *Phys. Rev. Lett.*

Conclusions & Outlook

Why QIS and opportunities in the NISQ-era

Quantum Materials at the Atomic-scale

QED + matter + QIS

What's next?

NARANGLAB
MATERIALS THEORY AT HARVARD

HARVARD
School of Engineering
and Applied Sciences

Team and Funding

NARANGLAB
MATERIALS THEORY AT HARVARD

LEAD PI NARANG

DR. JOHANNES FLICK

DFG Prize Postdoctoral Fellow

JENNIFER COULTER

Department of Energy CSG Fellow

NICHOLAS RIVERA

Department of Energy CSG Fellow, MIT School of Science Fellow

CHRISTOPHER CICCARINO

Harvard Chemical Physics

GEORGE VARNAVIDES

MIT DMSE (co-advised)

FUNDING AND SUPPORT

Harvard University Center for the Environment

HARVARD UNIVERSITY CENTER FOR THE ENVIRONMENT

Lead of graduate consortium on energy and environment, funded for quantum catalysis studies.

CIQM CENTER for INTEGRATED QUANTUM MATERIALS
Quantum Information Science and Technology

QUANTUM MATERIALS

Part of NSF-funded center

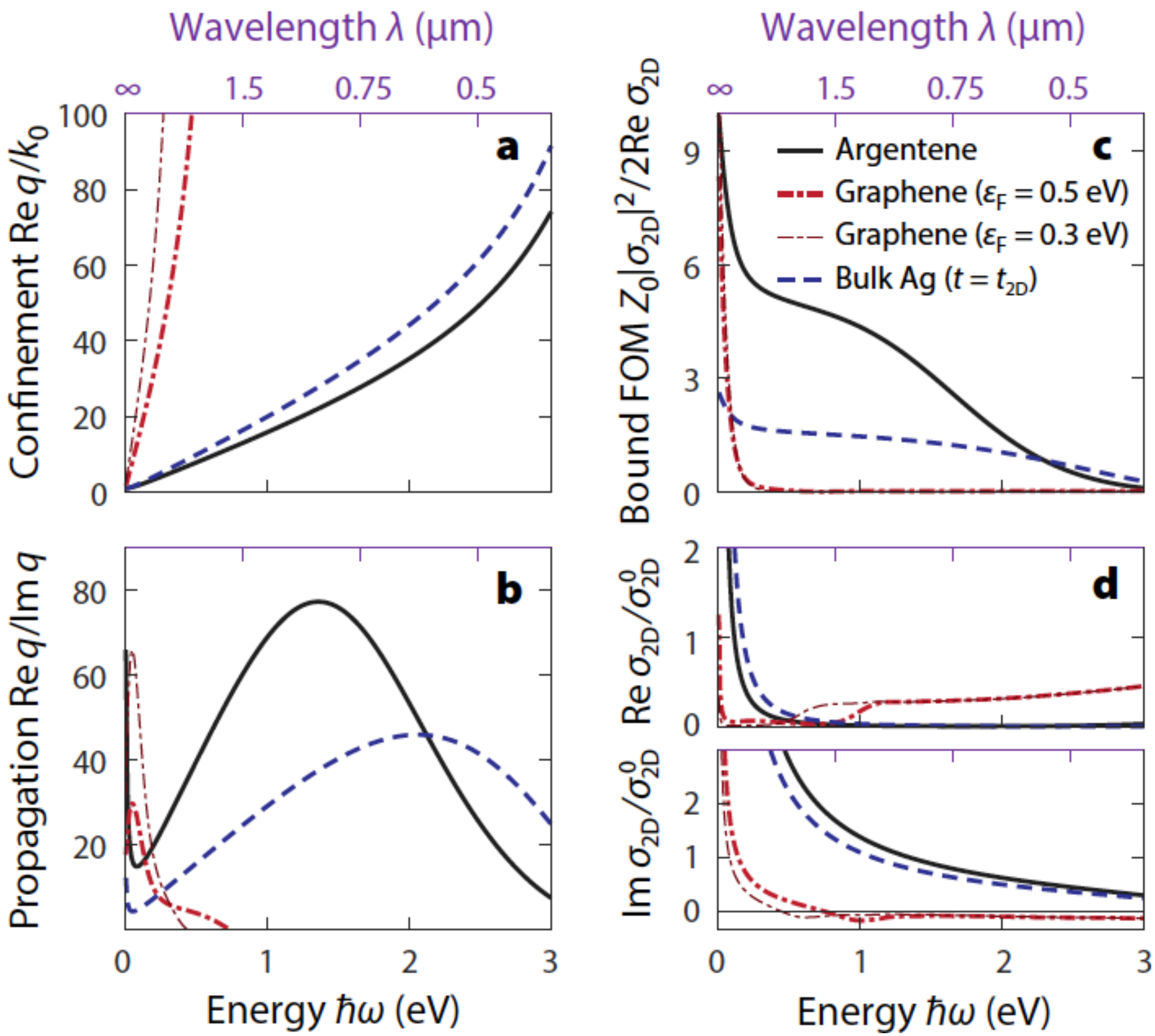
DEPARTMENT OF DEFENSE UNITED STATES OF AMERICA

NEW QUANTUM EMITTERS FOR QUANTUM INFORMATION SCIENCE

Co-PI on MURI

Additional Slides -

Photonic Figures of Merit: *Argentene*



Narang, et al, arXiv preprint arXiv:1806.02672(**2018**) – in review