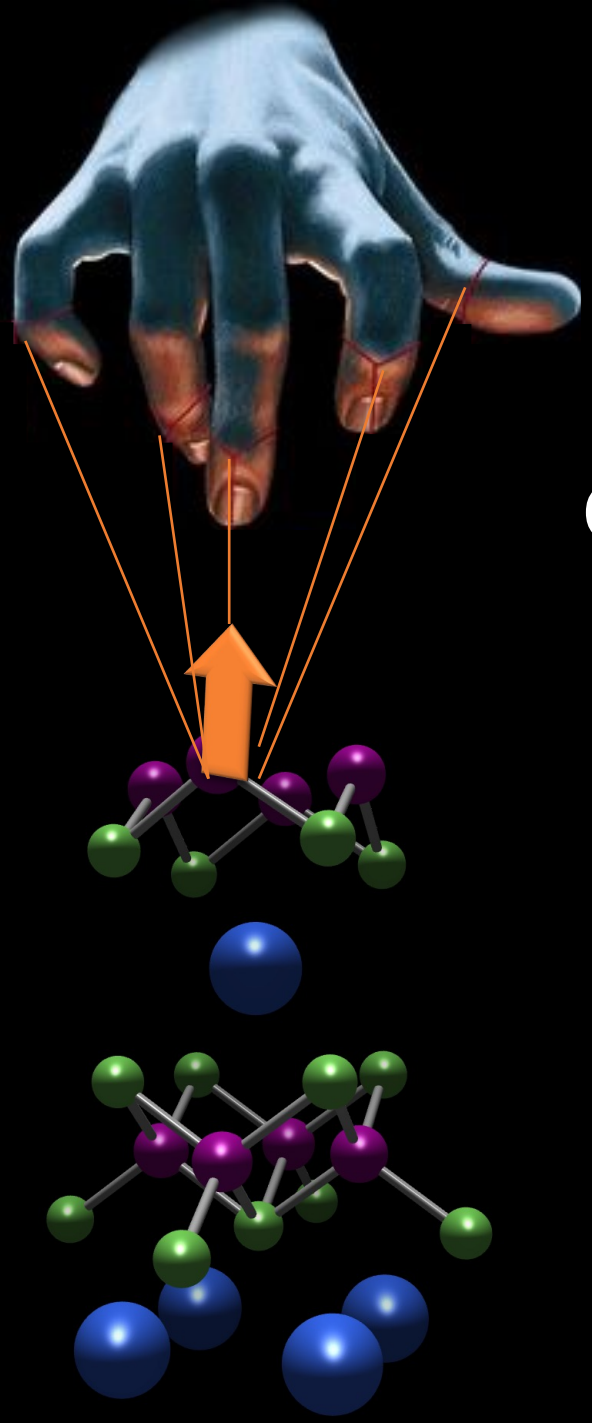
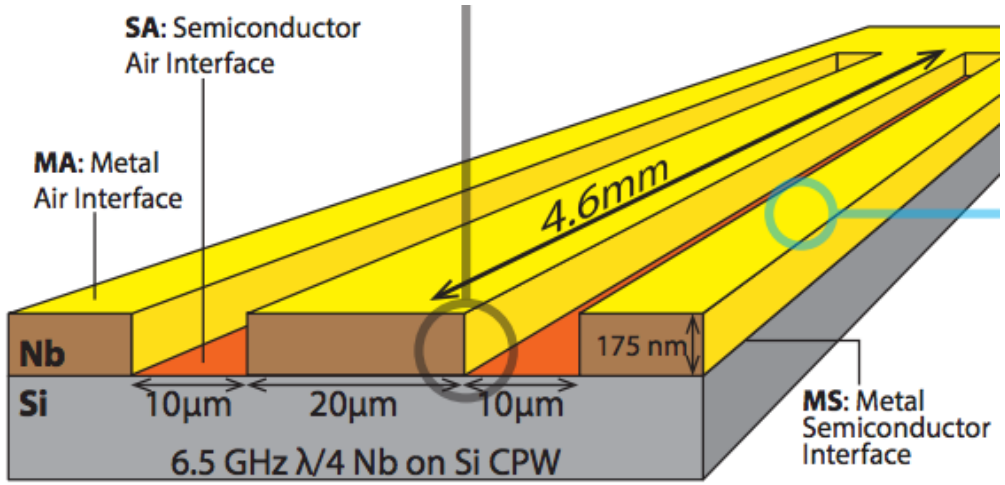


Computing Needs for Quantum Materials:
Science Cases in HEP and QC

Sinéad M. Griffin
LBNL

Why we need high-accuracy quantum materials calculations for Quantum Computing

What Theorists Want



M.V.P. Altoé et al. arXiv.2012.07604 (2020)

Why we need high-accuracy quantum materials calculations for Quantum Computing

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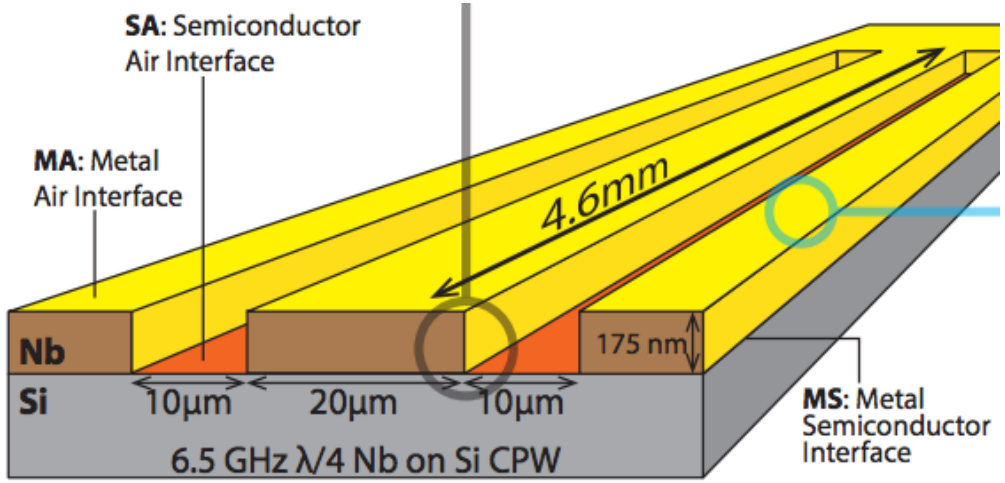
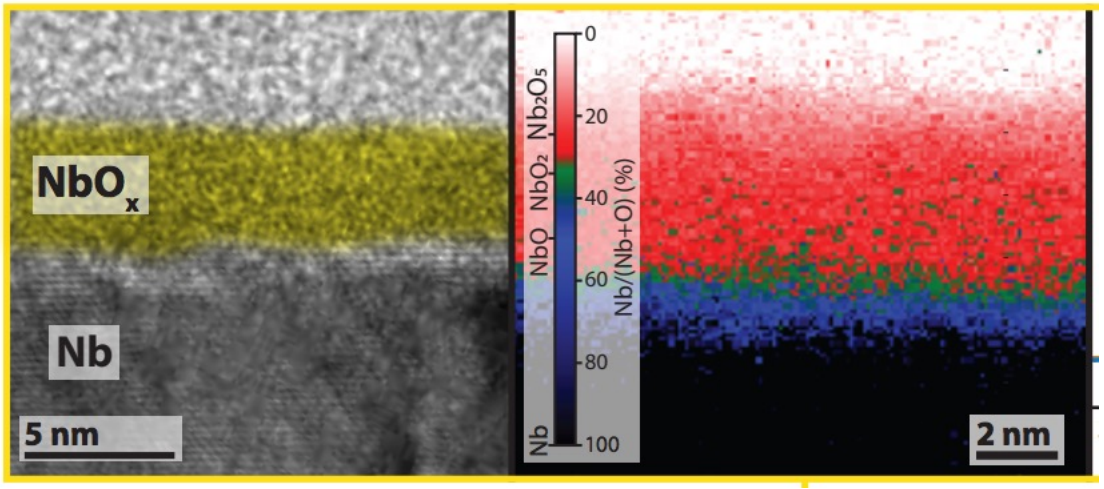


What We Get

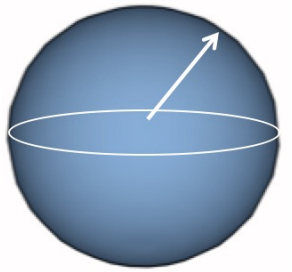


1. Real materials are messy
2. We find a Hamiltonian that is good enough to describe them (and integrate out everything else)

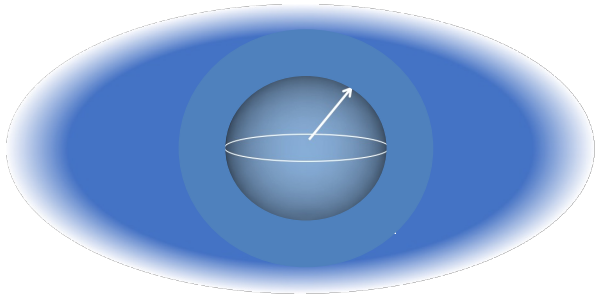
M.V.P. Altoé et al. arXiv.2012.07604 (2020)

Why we need high-accuracy quantum materials calculations for Quantum Computing

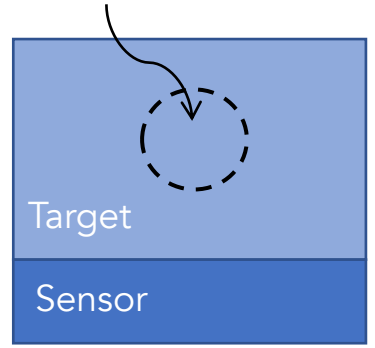
A brief success story: improving superconducting resonator quality factor x5



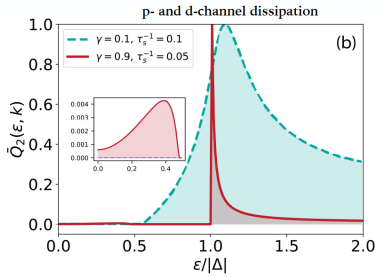
Fundamental qubit design
Material selection



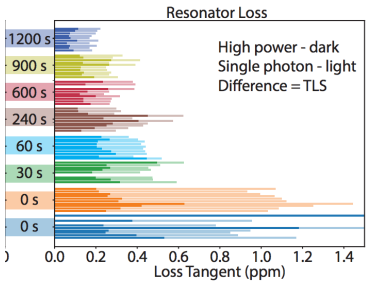
Origins of decoherence
Inhomogeneities, interfaces, defects



Architecture design and performance



Connect calculated performance to measurements

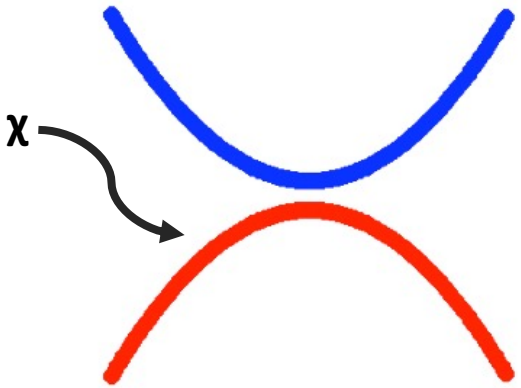


Altoé et al. PRX Quantum **3**, 020312 (2022), Sheridan et al. arXiv:2111.11684

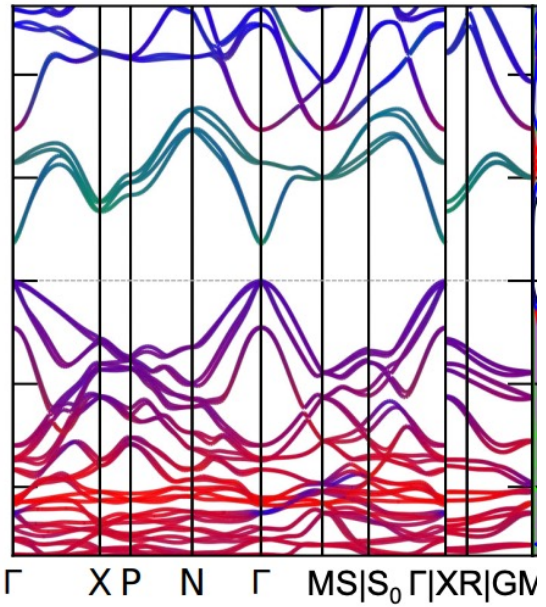
Why we need high-accuracy quantum materials calculations for High-Energy Physics

Example: Dark matter interactions with electronics in semiconductors/Dirac semimetals

Model electronic structure



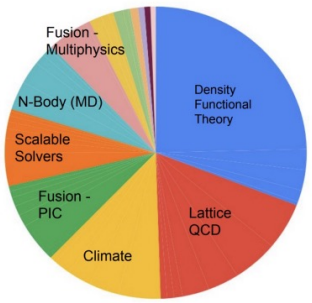
Real electronic structure



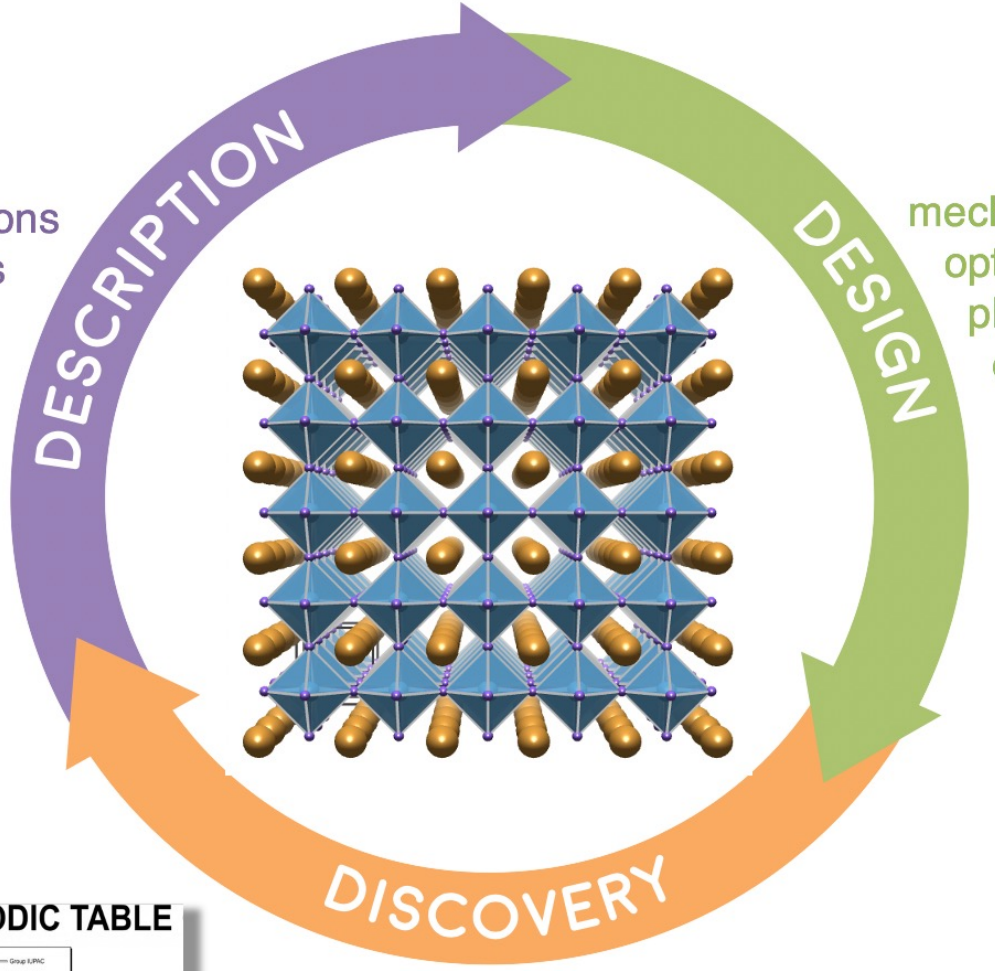
1. Real Hamiltonians are complex – can result in processes/signals not considered
2. Materials design can now optimize materials selection to maximize cross section

Essig et al. JHEP 46 (2016), Hochberg et al. PRD 97, 015004 (2018), Inzani et al., PRR 3, 013069 (2021), Griffin et al. PRD **104**, 095015 (2021)

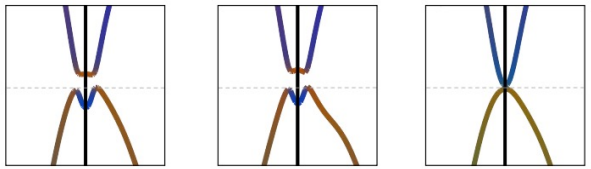
The Landscape of Quantum Materials Theory & Calculations

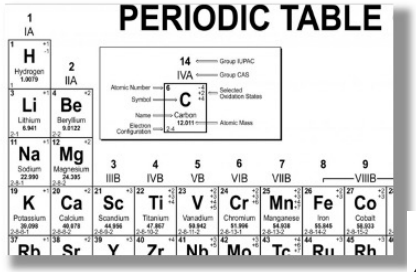


simulations
theoretical models



mechanisms
optimizing functionality
physical/chemistry
engineering





experimental guides
high-throughput

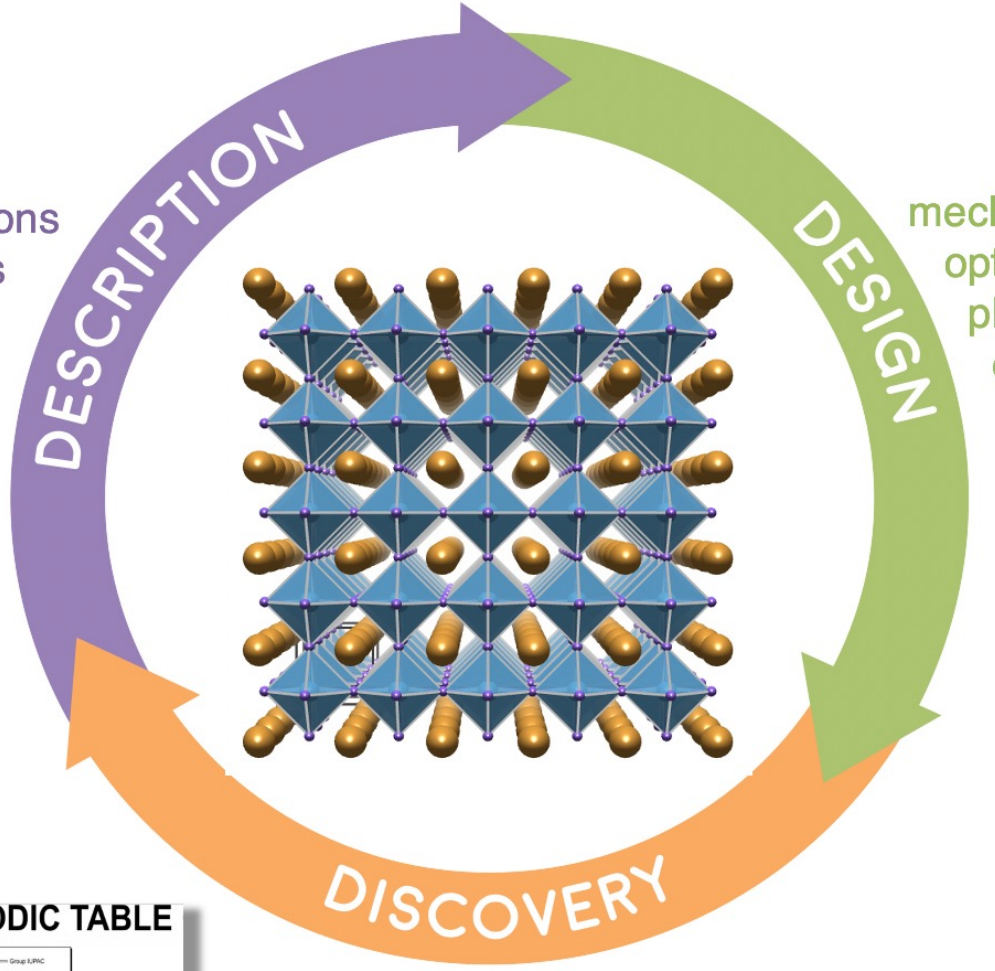
MATERIALS PROJECT

The Landscape of Quantum Materials Theory & Calculations

Expansion of classical calculations to larger and more complex systems

Application of QC to many-body systems e.g. strongly-correlated materials

simulations
theoretical models



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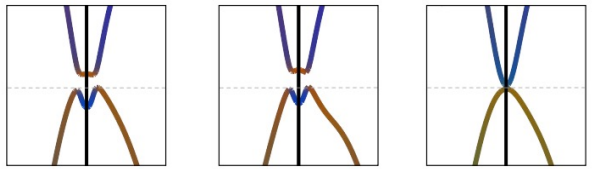

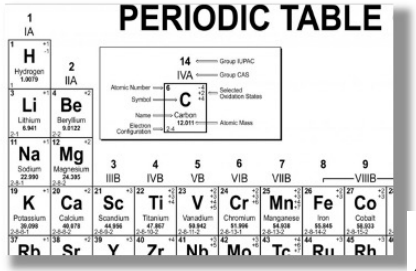

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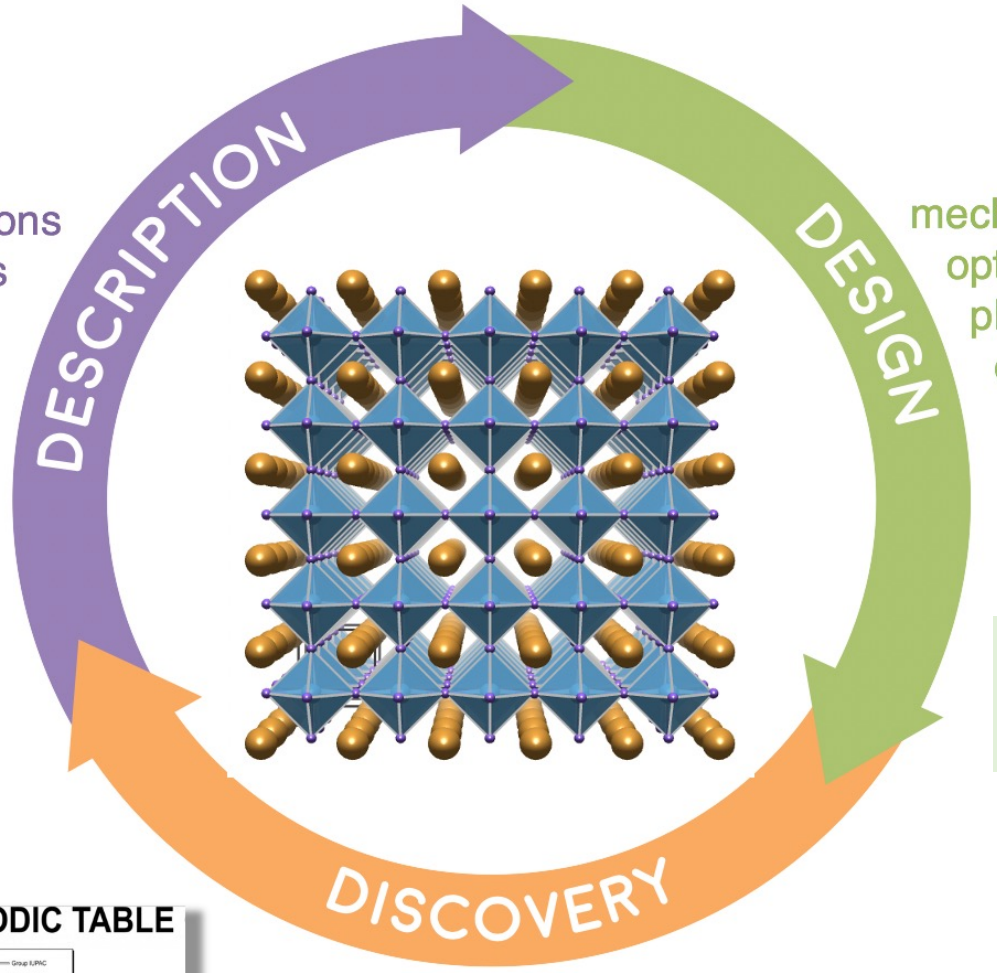

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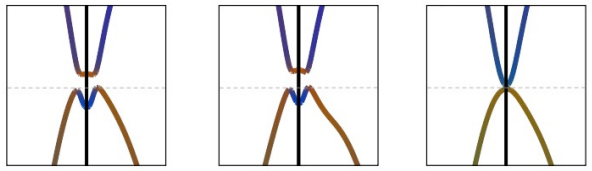
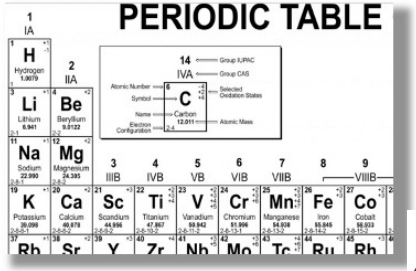


Expertise from solid-state physics and chemistry specifically focused on HEP and QC challenges



experimental guides
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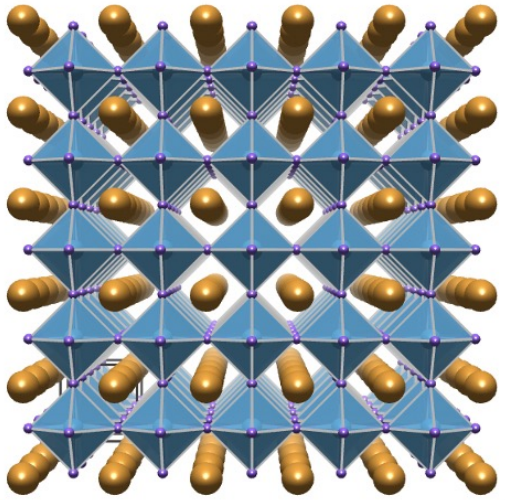
DESCRIPTION

DESIGN

DISCOVERY



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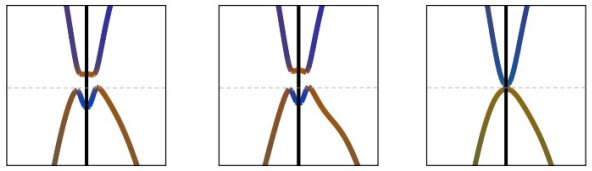

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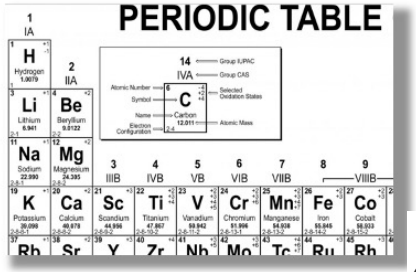


experimental guides
high-throughput

MATERIALS PROJECT

Materials informatics and databases for accelerated discovery and inverse design

Quantum Materials Needs for Discovery in HEP & QC

Improved classical and quantum calculations – methodology & codes

Classical calculations:

- Scaling to larger and more complex systems (real interfaces, defects, etc.)
- Methodology for correlated and entangled systems

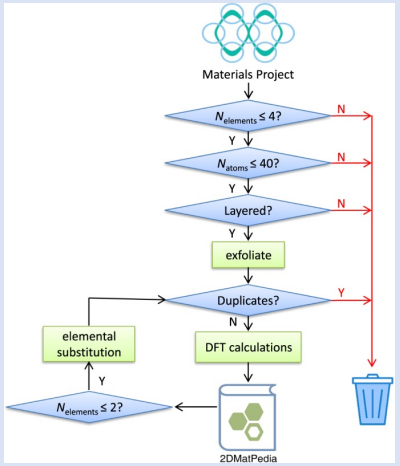
Quantum calculations:

- Benchmarks of model Hamiltonians of interest for QC readiness
- Incorporation of QC embedding methods into classical calculations (e.g. defect/atom/molecule in extended system)

Databases for open-source resources, high-throughput searches & ML

Open data and codes

- Interoperable data combining experiment and calculations
- Open-source codes
- Application and development of machine learning
- Inverse design

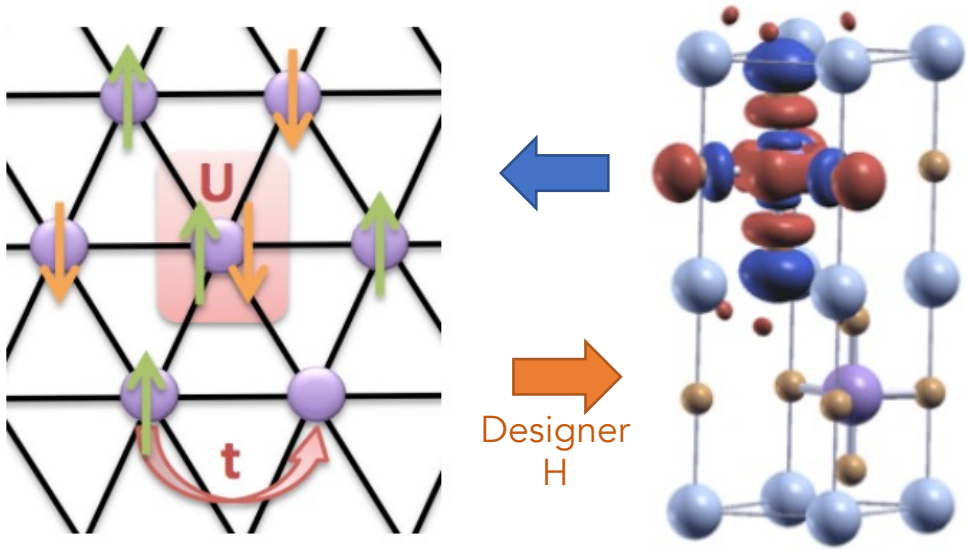


Targeted programs focused on quantum materials for HEP and QC

HEP-specific materials theory

- Understanding and predictions of experimental signatures and quantification of decoherence processes.
- Designer Hamiltonians and incorporation of state-of-the-art methods in solid-state physics for inverse design of HEP-relevant systems
- Design of HEP-specific hardware and materials

Non-controversial hot-takes



1. Materials-specific calculations are needed for next-generation detectors and experiments and for QC

2. Methodology for systems discovery from solid-state physics, chemistry and materials science can accelerate hardware improvements in HEP and QC

3. Facilitate using contemporary discoveries in quantum materials (e.g. topological and entangled systems) for applications in HEP/QC

QUANTUM SYSTEMS ACCELERATOR
Catalyzing the Quantum Ecosystem

MOLECULAR FOUNDRY
MSD Materials Sciences Division

BERKELEY LAB
Lawrence Berkeley National Laboratory

QuantISED