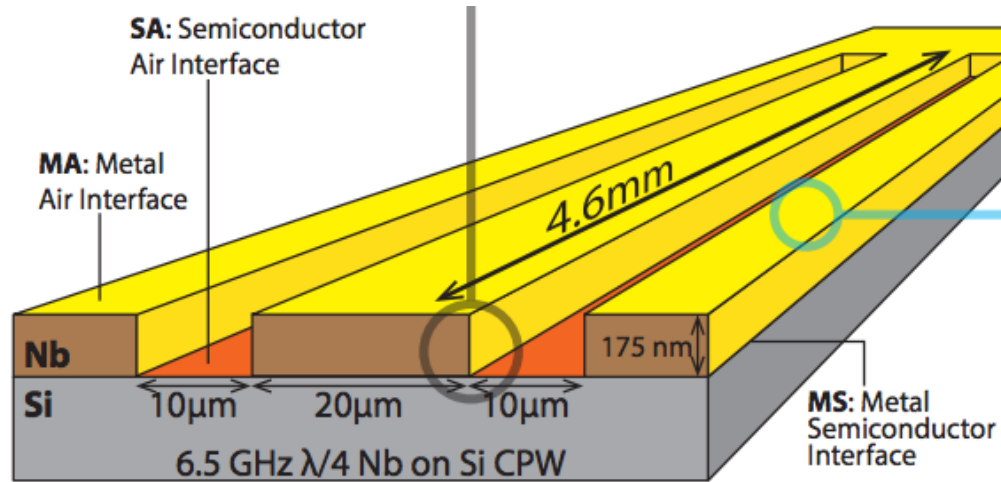


# Computing Needs for Quantum Materials: Science Cases in HEP and QC

Sinéad M. Griffin  
LBNL

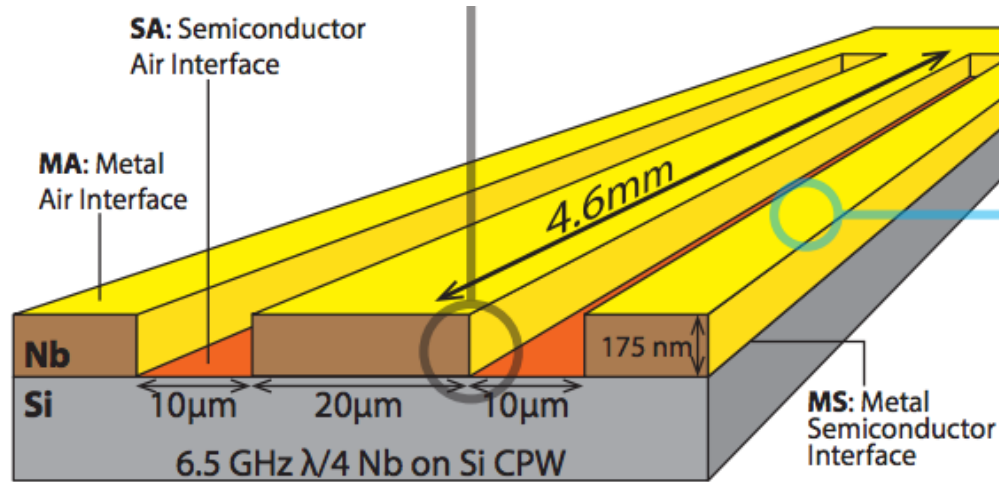
# Why we need high-accuracy quantum materials calculations for Quantum Computing

## What Theorists Want

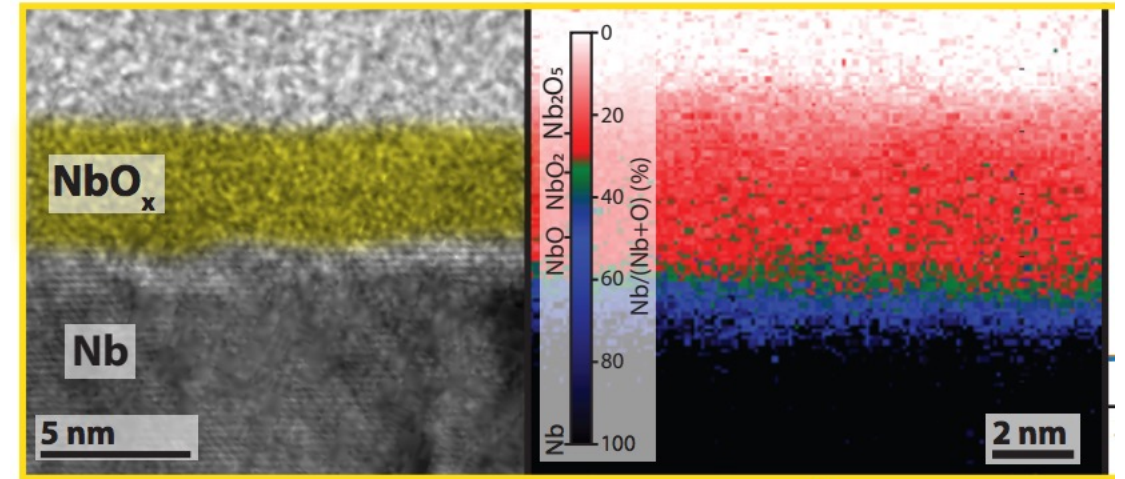


# Why we need high-accuracy quantum materials calculations for Quantum Computing

## What Theorists Want



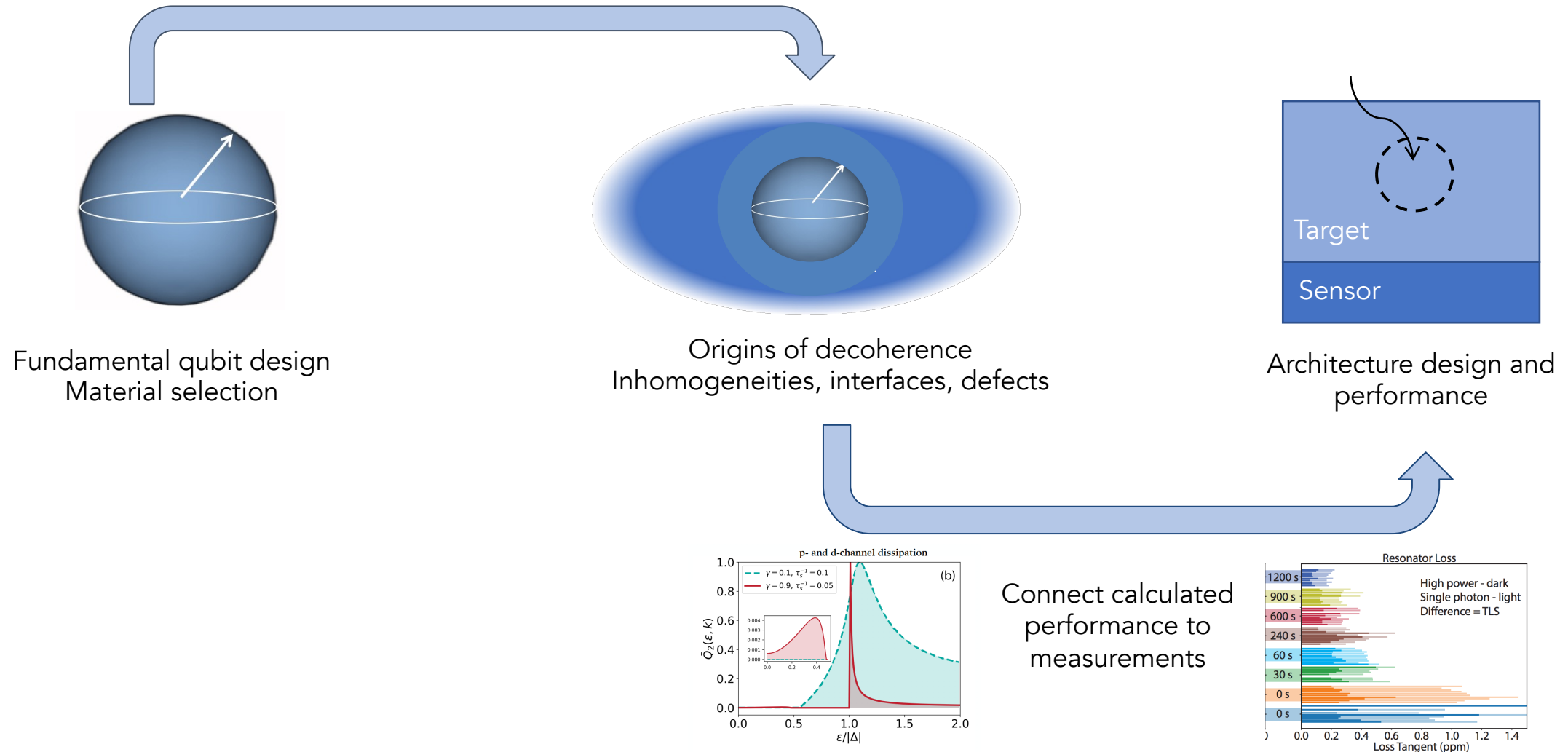
## What We Get



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

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

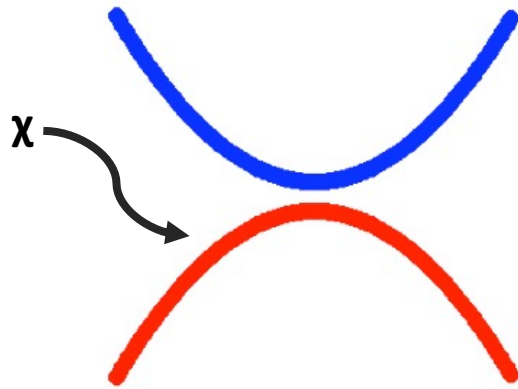
A brief success story: improving superconducting resonator quality factor x5



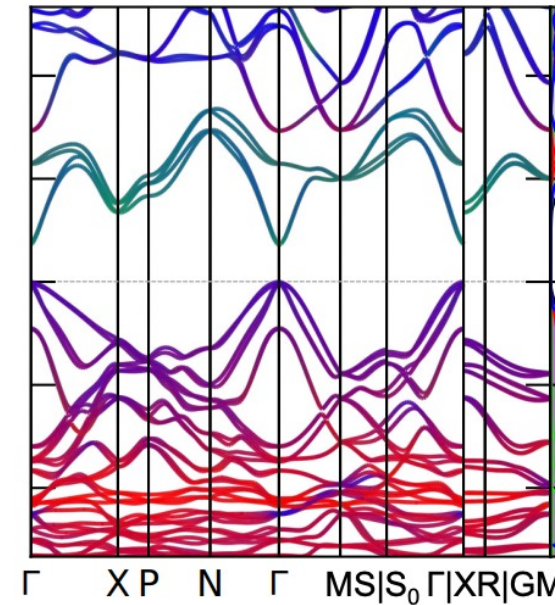
# Why we need high-accuracy quantum materials calculations for High-Energy Physics

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

Model electronic structure

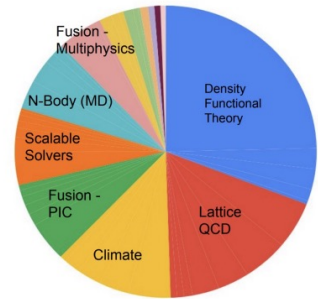


Real electronic structure

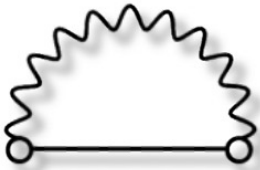


1. Real Hamiltonians are complex – can result in processes/signals not considered
2. Materials design can now optimize materials selection to maximize cross section

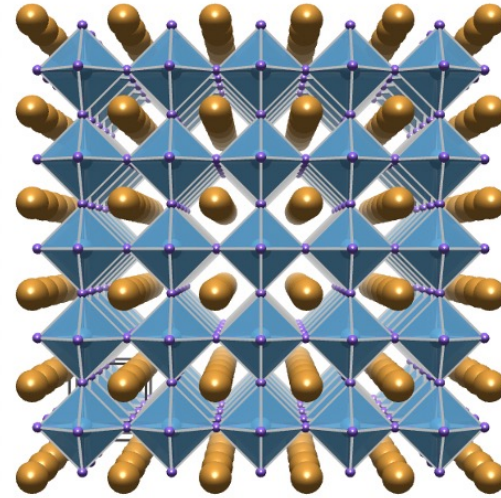
# The Landscape of Quantum Materials Theory & Calculations



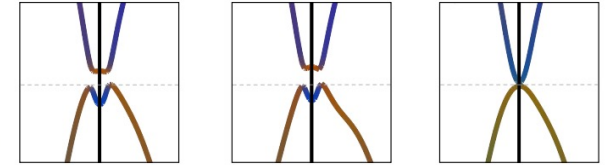
simulations  
theoretical models



DESCRIPTION



DESIGN  
mechanisms  
optimizing functionality  
physical/chemistry  
engineering



DISCOVERY

experimental guides  
high-throughput

PERIODIC TABLE																	
1 IA H Hydrogen 1.0079	2 IIA Li Lithium 6.941	3 IIIB Na Sodium 22.990	4 IVB K Potassium 39.098	5 VB Ca Calcium 40.078	6 VIB Sc Scandium 44.956	7 VIIB Ti Titanium 47.88	8 VIIIB V Vanadium 50.942	9 VIIIB Cr Chromium 51.996	10 VIIIB Mn Manganese 54.938	11 VIIIB Fe Iron 55.845	12 VIIIB Co Cobalt 58.933	13 IIIB Ni Nickel 58.69	14 IIIB Cu Copper 63.546	15 IIIB Zn Zinc 65.38	16 IIIB Ga Gallium 69.723	17 IIIB Ge Germanium 72.63	18 IIIB As Arsenic 74.922



**MATERIALS  
PROJECT**



# The Landscape of Quantum Materials Theory & Calculations

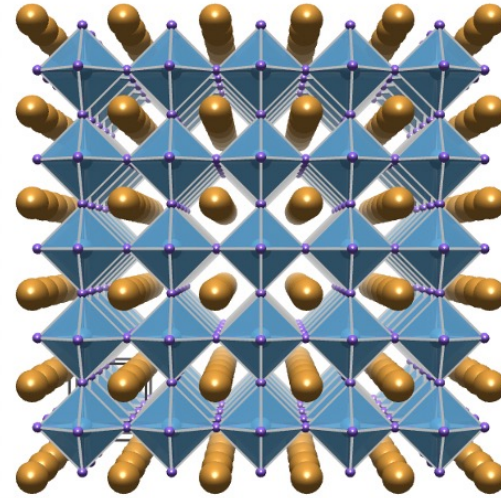
Expansion of classical calculations to larger and more complex systems

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

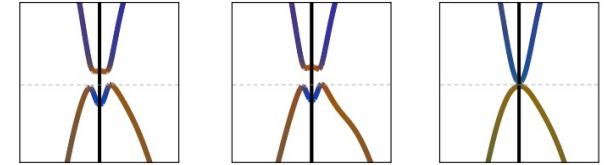
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1 IA												14 IVA									
H Hydrogen 1.0079		2 IIA												Group IUPAC Group CAS							
Li Lithium 6.941		Be Beryllium 9.012												Atomic Number Symbol Name Element Configuration		6 C Carbon 6.001		Selected Oxidation States			
Na Sodium 22.990		Mg Magnesium 24.305		3 IIIB		4 IVB		5 VB		6 VIB		7 VIIB		8 VIII							
K Potassium 39.098		Ca Calcium 40.078		Sc Scandium 44.956		Ti Titanium 47.867		V Vanadium 50.942		Cr Chromium 51.996		Mn Manganese 54.938		Fe Iron 55.845		Co Cobalt 58.933					
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**MATERIALS  
PROJECT**

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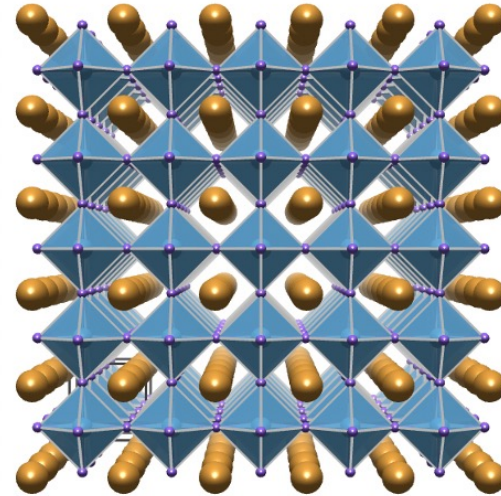
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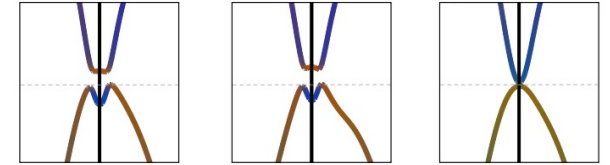
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engineering



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

DISCOVERY

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high-throughput

PERIODIC TABLE																	
1																	
1A	2															14	15
H	He															IVA	VA
Hydrogen	Helium															Carbon	Nitrogen
1.0079	4.0026															6.0024	14.0064
1	2															6	7
Li	Be															C	N
Lithium	Beryllium															Carbon	Nitrogen
6.941	9.0122															12.011	14.0064
11	12															11	12
Na	Mg															Na	Mg
Sodium	Magnesium															22.990	24.305
19	20															19	20
K	Ca															K	Ca
Potassium	Calcium															39.098	40.078
37	38															37	38
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**MATERIALS  
PROJECT**



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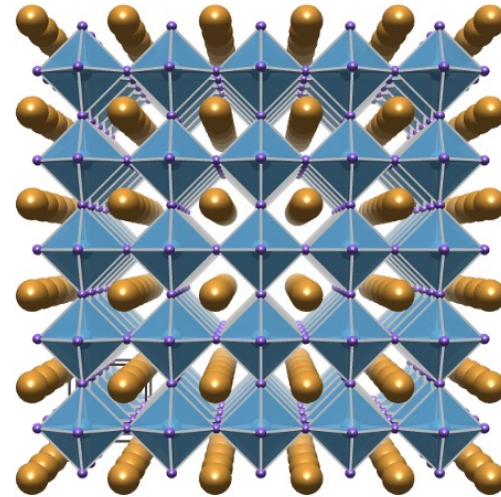
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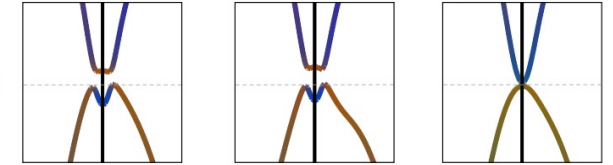
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**MATERIALS  
PROJECT**

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

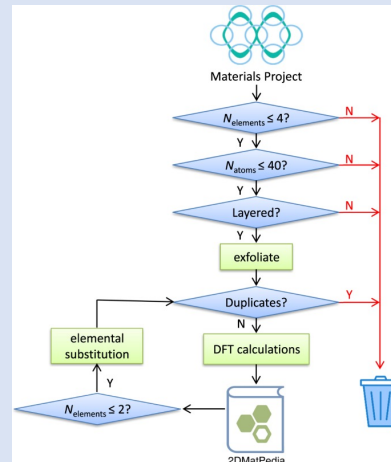
### Quantum calculations:

- 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

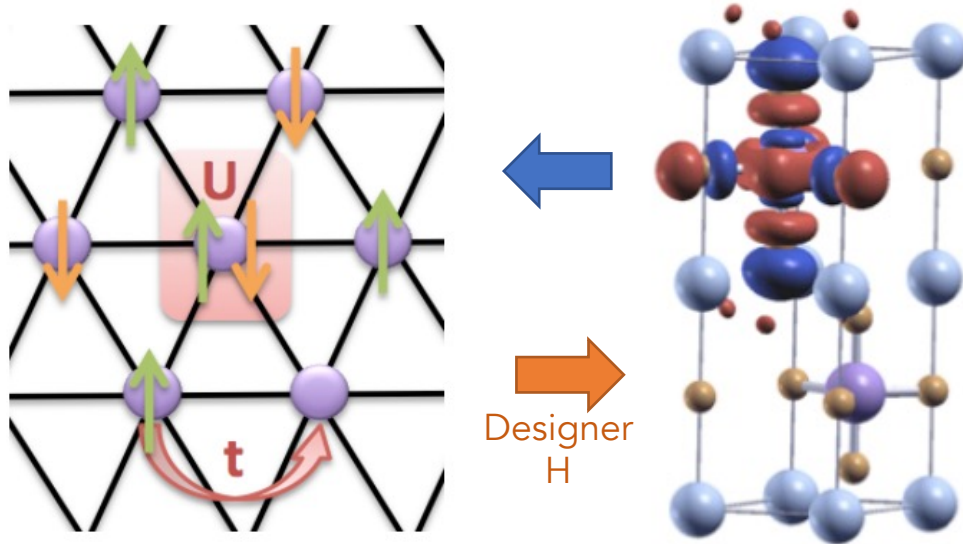


## Targeted programs focused on quantum materials for HEP and QC

### 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