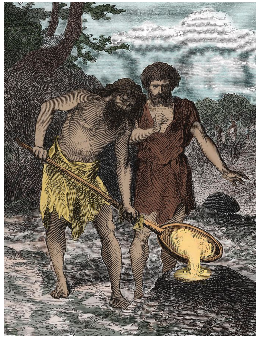
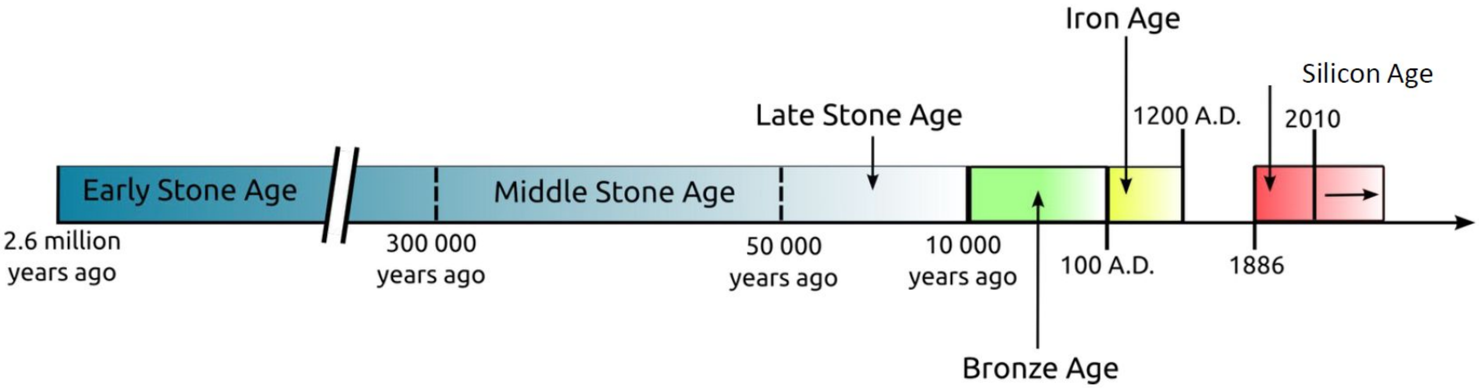
Condensed Matter Experiment & Computation

@ Yale AP&P

Stones, metals, and beyond





The physics of "many"

4 August 1972, Volume 177, Number 4047 **SCIENCE**

More Is Different

Broken symmetry and the nature of the hierarchical structure of science.

P. W. Anderson

The elementary entities of science X obey the laws of science Y.

X	Y
solid state or many-body physics	elementary particle physics
chemistry	many-body physics
molecular biology	chemistry
cell biology	molecular biology
•	•
•	•
•	•
psychology	physiology
social sciences	psychology

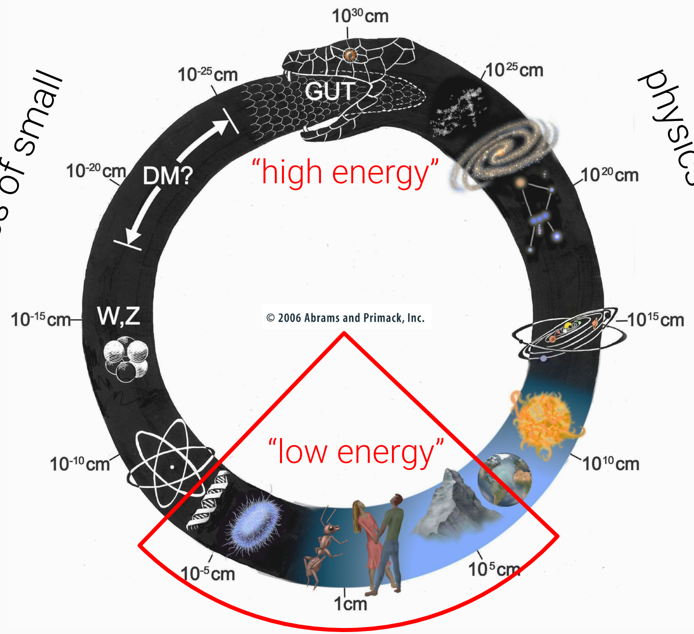
But this hierarchy does not imply that science X is "just applied Y." At each stage entirely new laws, concepts, and generalizations are necessary, requiring inspiration and creativity to just as great a degree as in the previous one.

Many-body Physics

aka Approximate-Wisely Physics

Standard Model

physics of small



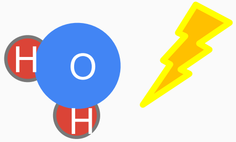
physics of "many"

General Relativity

physics of big

No central command,
simple interactions

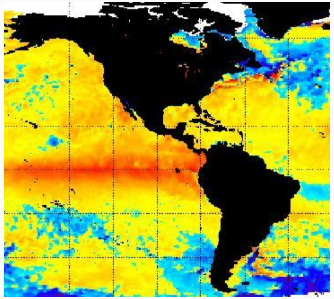
Property "emerges"
beyond brute sum of parts



Water molecule

x 10^{46}

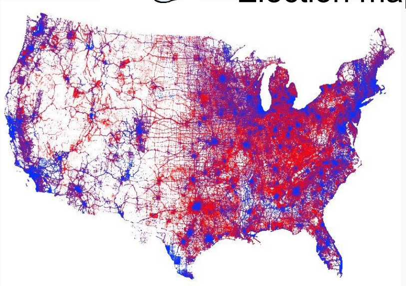
El Niño

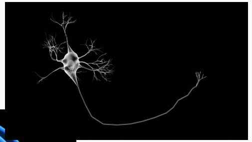


Voter

x 10^{8}

Election map





Neuron

x 10^{11}

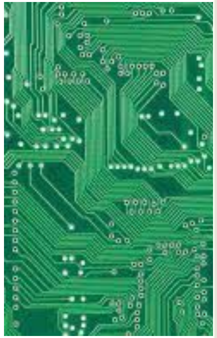
Brain activity

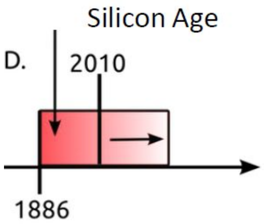
Ant

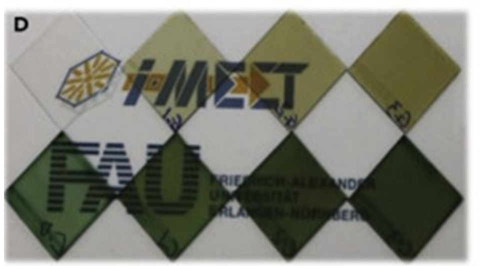
x 10^{8}

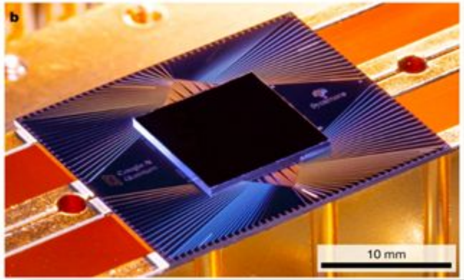
Colony

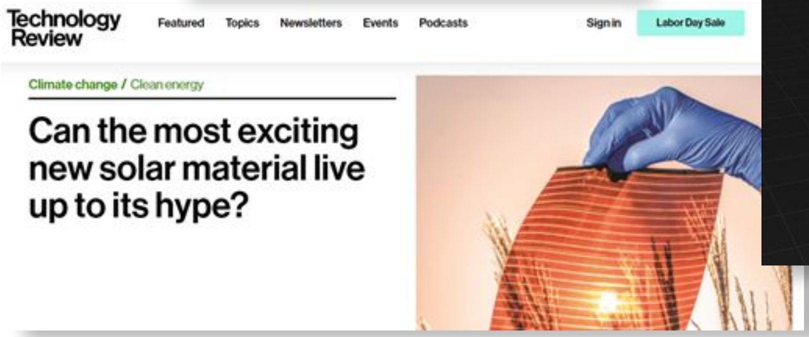
"Quantum" materials engineering





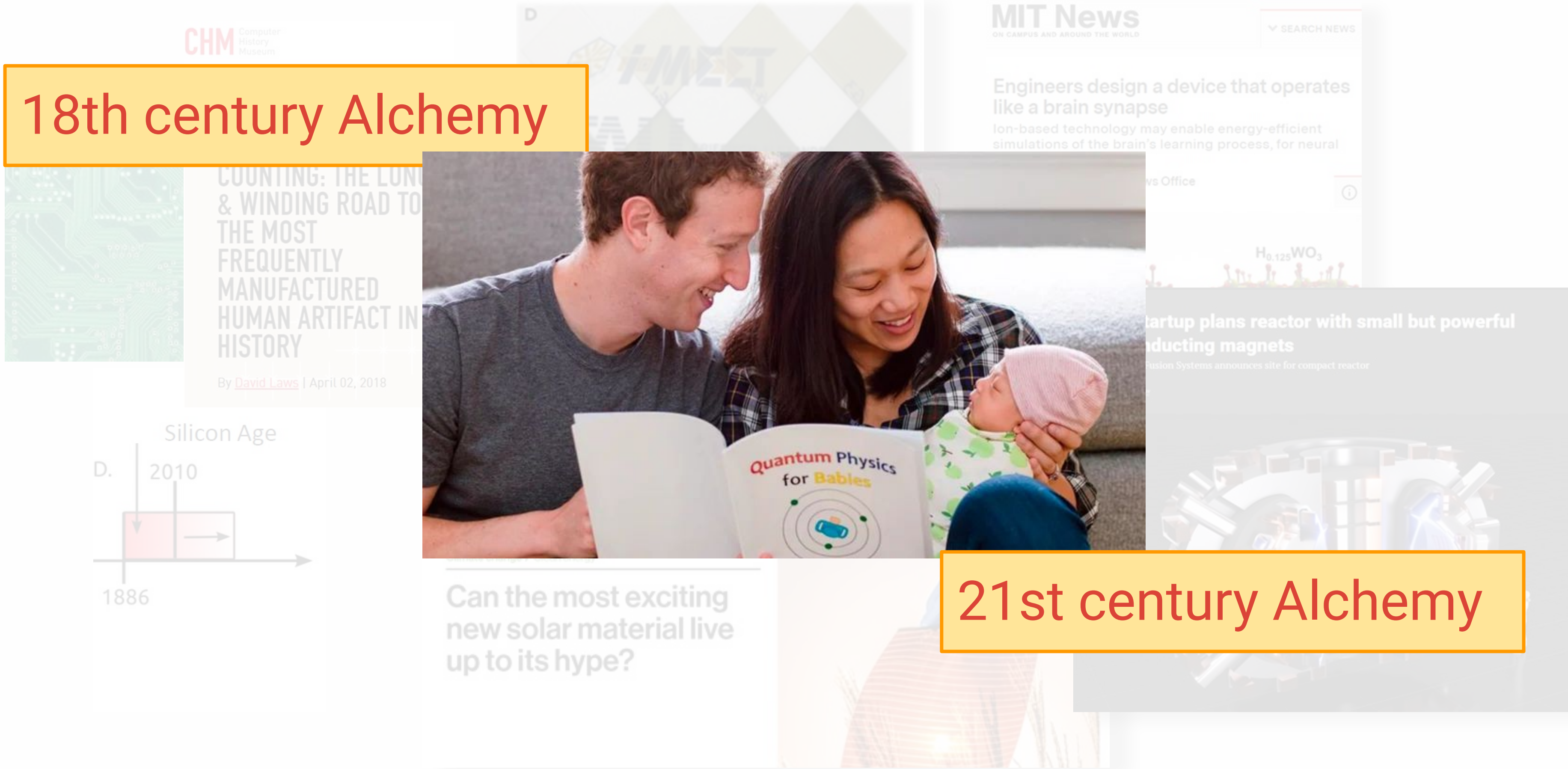






“Quantum” materials engineering

18th century Alchemy



21st century Alchemy

Predictive power? Only one problem

PNAS Proceedings of the National Academy of Sciences of the United States of America

Home | Articles | Front Matter | News

RESEARCH ARTICLE

The Theory of Everything

R. B. Laughlin and David Pines
+ See all authors and affiliations

PNAS January 4, 2000 97 (1) 28-31; https://doi.org/10.1073/pnas.97.1.28

Contributed by David Pines

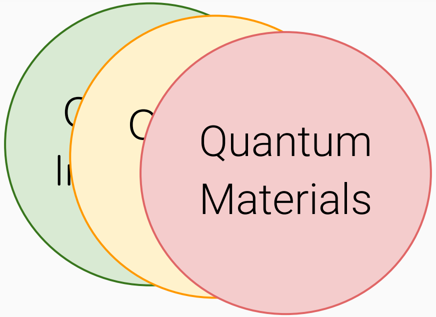
$$i\hbar \frac{\partial}{\partial t} |\Psi > \; = \mathcal{H} |\Psi >$$

where

$$\mathcal{H} = -\sum_{j}^{N_e} \frac{\hbar^2}{2m} \nabla_j^2 - \sum_{\alpha}^{N_i} \frac{\hbar^2}{2M_\alpha} \nabla_\alpha^2 - \sum_{j}^{N_e} \sum_{\alpha}^{N_i} \frac{Z_\alpha e^2}{|\vec{r}_j - \vec{R}_\alpha|} + \sum_{j \ll k}^{N_e} \frac{e^2}{|\vec{r}_j - \vec{r}_k|} + \sum_{\alpha \ll \beta}^{N_j} \frac{Z_\alpha Z_\beta e^2}{|\vec{R}_\alpha - \vec{r}_\beta|}.$$

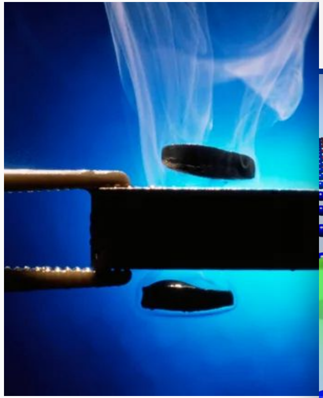
Hydrogen atom □ Hydrogen molecule □ 3-body problem □ **GG**

Condensed Matter Experiment & Computation at Yale AP&P

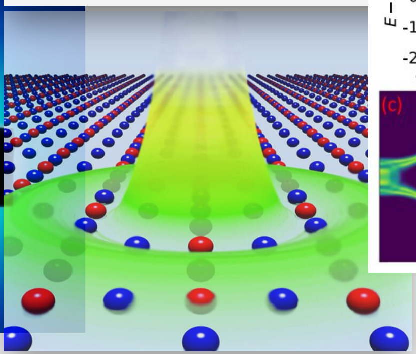


- Understand the microscopic mechanisms behind material properties
- Predict material properties with advanced theory tools
- Control and create material properties with experimental methods

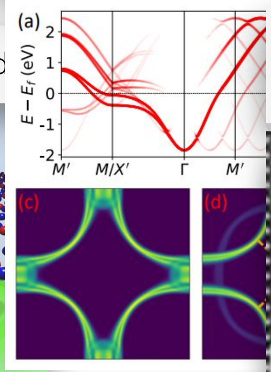
Why is Tc so high?



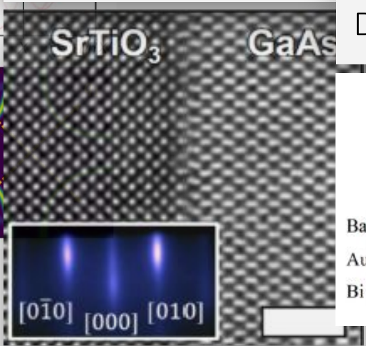
Can F = e^2/ r^2 be twisted



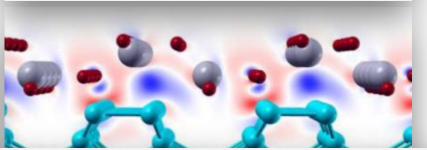
Magnetic order in correlated systems



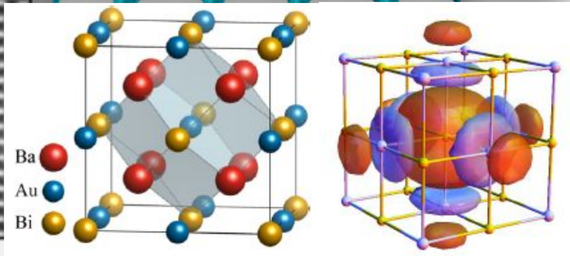
Making wafer-scale 2D quantum materials



How to best functionalize surfaces and interfaces



Designing next gen energy materials



Quantum Materials

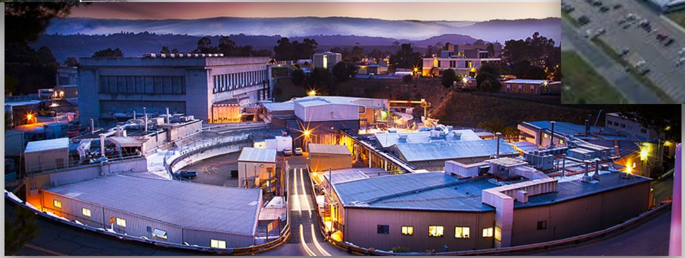
- **EVERY** experimentalist here has a strong tie to the national labs
- Close collaborations with other departments in SEAS and FAS
  - Chemical Engineering, MEMS, Physics, Chemistry, Energy Science Institute...
  - Fengnian Xia, Peijun Guo, Diana Qiu, Mengxia Liu

BROOKHAVEN NATIONAL LABORATORY

SLAC NATIONAL ACCELERATOR LABORATORY

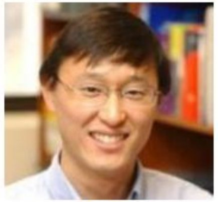
BERKELEY LAB

Argonne NATIONAL LABORATORY



RF Synchrotron

Condensed Matter Experiment & Computation at Yale AP&P



Ahn

Novel complex oxide interfaces:
- water splitting
- artificial neurons
- spintronics & ferroelectrics

MBE, RIXS, XRD, transport…

He

Momentum resolved electronic states:
- high-Tc superconductivity
- magnetic metals and vdW materials
- correlated electronic systems

ARPES, IXS, INS, growth…

da Silva Neto

Atomically resolved electronic states:
- topological state of matter
- nematicity and superconductivity
- vortex and density waves

STS, SNOM, RIXS, ARPES…

Ismail-Beigi

Electronic structure w/ first principles:
- solid-gas/solid-solid interfaces
- electron correlation in oxides
- 2D material and nanostructure

DFT, Green's function, slave boson…

Ozolins

Electronic property w/ numerical methods:
- materials for energy applications
- machine learning in materials physics
- exotic magnetism

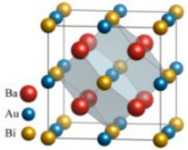
DFT, MD, Monte Carlo, Machine learning…

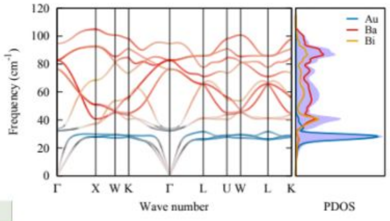
Vidvuds Ozolins

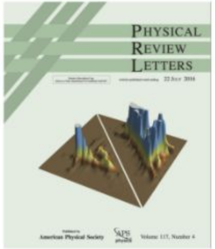
Theory of electronic structure & energy materials

Theory of real electronic materials

Applications in energy storage, generation and conversion



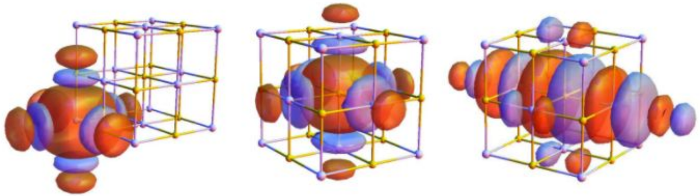


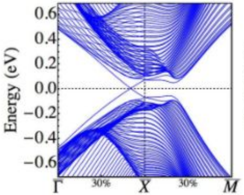


- Electron-phonon interactions in solids
- Transport of heat and electrical current
- Thermoelectric effect
- Exotic magnetism – spin liquids

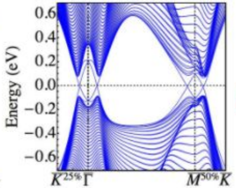
Machine learning for quantum mechanics:

- Solving the Schrödinger equation
- Localized basis for electron correlation
  - Wannier functions
- Deep Boltzmann machines and Convolutional Neural Nets for Quantum Monte Carlo

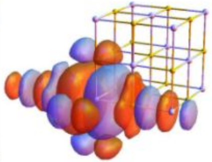




(a)(001) surface with SOC



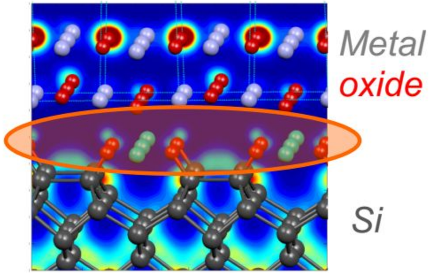
(c)(111) surface with SOC

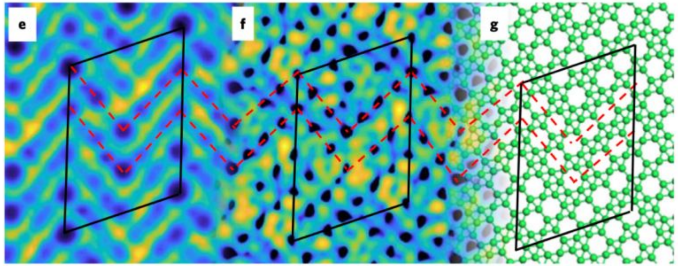


Sohrab Ismail-Beigi

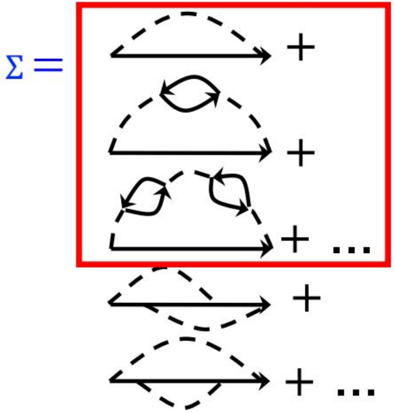
Electronic structure & materials theory from first principles

Interfaces between two materials: How is the interfacial region different from either side? What do electrons do in such an asymmetric environment?





Nanoscale/low-dimensional materials
- 2D materials: synthesis, bonding, electronic & optical response, topology
- Ferroelctric surface chemistry

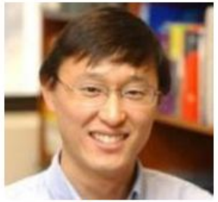


Electron correlation especially in transition metal oxides
(many-body Green functions; slave bosons)

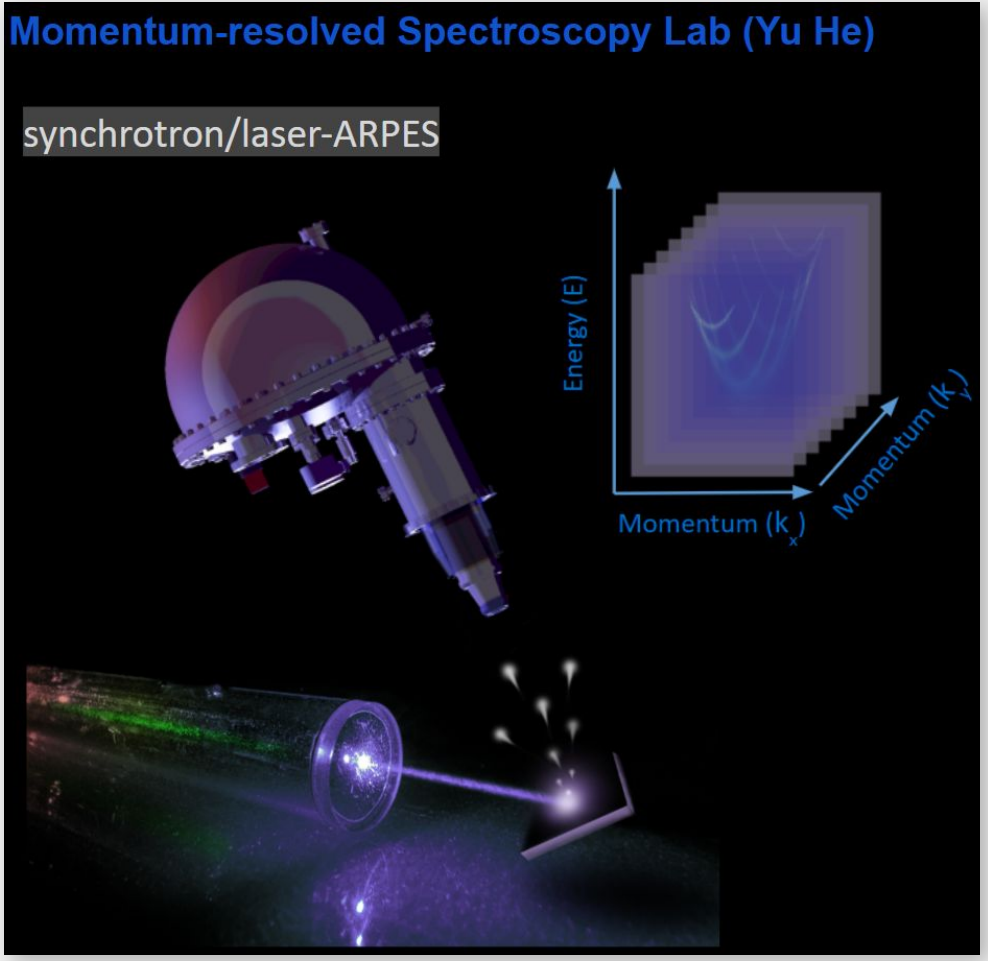
Ahn Research Group

- Synthesis using molecular beam epitaxy.
- Characterization using synchrotron x-rays.

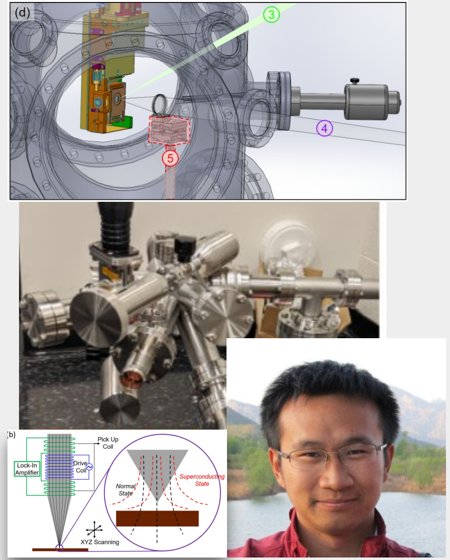
- Picoscale Engineering
- To invent new materials
- Apply to:
- Photo electro chemical water splitting
- Neuromorphic computing



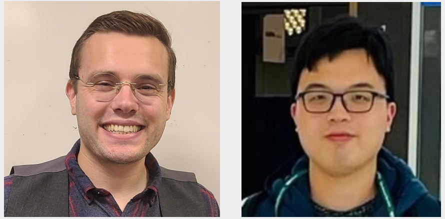
Ahn



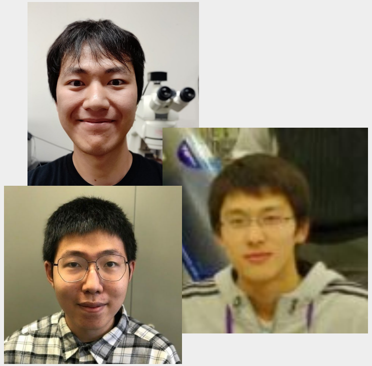
Tool development for Solid State Quantum Simulation



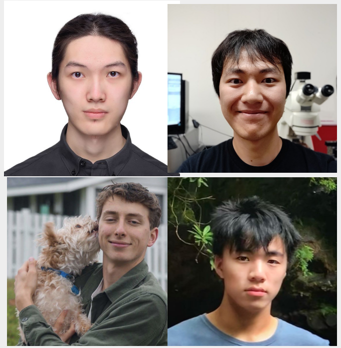
2D Magnetism



Metal to insulator transitions



Superconductivity



da Silva Neto Lab

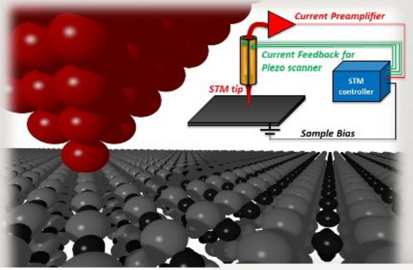
Investigating Novel Quantum States of Matter

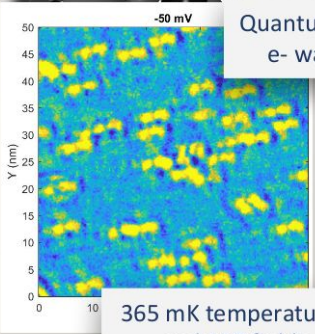
Department of Physics

Energy Sciences Institute

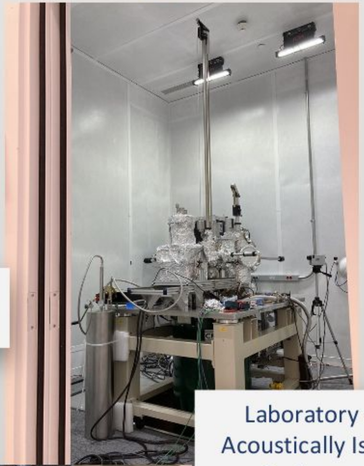
Yale

STM/S Laboratory @ the Energy Sciences Institute

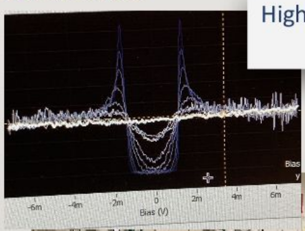




Quantum interference e- wavefunctions

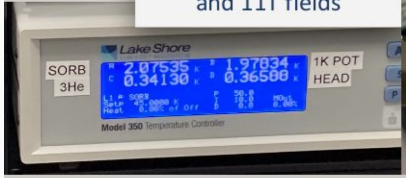


Laboratory with Acoustically Isolated Environment

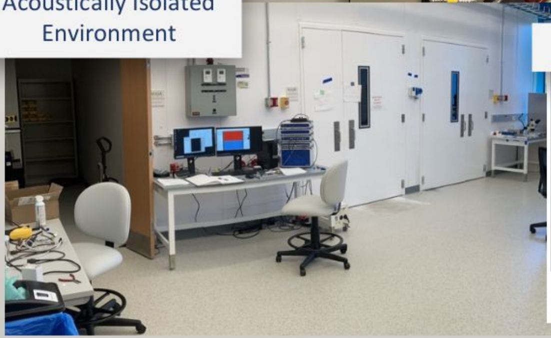


High energy-resolution spectroscopy

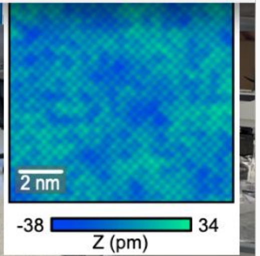
Helium Recycling System



365 mK temperatures and 11T fields



Atomic Resolution



Science

Current Issue First release papers

HOME > SCIENCE > VOL. 365, NO. 6459 > "WEYL"ING AWAY TIME-REVERSAL SYMMETRY

PERSPECTIVE | TOPOLOGICAL MATTER

“Weyl”ing away time-reversal symmetry

EDUARDO H. DA SILVA NETO

SCIENCE • 20 Sep 2019 • Vol 365, Issue 6459 • pp. 1248-1249 • DOI: 10.1126/science.aax6190

REVIEWS OF MODERN PHYSICS

Recent Accepted Authors Referees Search Pres

Angle-resolved photoemission studies of q

Jonathan A. Sobota, Yu He, and Zhi-Xun Shen

Rev. Mod. Phys. **93**, 025006 – Published 26 May 2021

nature materials

Explore content ⌄ About the journal ⌄ Publish with us ⌄

nature > nature materials > news & views > article

News & Views | Published: 03 May 2023

Quantum materials

High-temperature superconductivity survives

Yu He

Nature Materials **22**, 671–672 (2023) | Cite this article

nature materials

Explore content ⌄ About the journal ⌄ Publish with us ⌄

nature > nature materials > articles > article

Article | Published: 18 January 2021

Tuning spin excitations in magnetic films by confinement

Jonathan Pelliciari, Sangjae Lee, K

Charles H. Ahn, Frederick J. Walker &

Nature Materials **20**, 188–193 (2021

4453 Accesses | **3** Citations | **69**

Explore content ⌄ About the journal ⌄ Publish with us ⌄

nature > nature chemistry > articles > article

Article | Published: 31 January 2022

Micrometre-scale single-crystalline borophene on a square-lattice Cu(100) surface

Rongting Wu, Stephen Eltinge, Ilya K. Drozdov, Adrian Gozar, Percy Zahl, Jerzy T. Sadowski, Sohrab Ismail-Beigi & Ivan Božo

Nature Chemistry (2022)

ScienceAdvances

Current Issue First release papers Archive

HOME > SCIENCE ADVANCES > VOL. 9, NO. 27 > SUPERCONDUCTING $ND_{1-x}EU_xNIO_2$ THIN FILMS USING IN SITU SYNTHESIS

RESEARCH ARTICLE | MATERIALS SCIENCE

Superconducting $Nd_{1-x}Eu_xNiO_2$ thin films using in situ synthesis

WENZHENG WEI, DUNG VU, ZHAN ZHANG, FREDERICK J. WALKER, AND CHARLES H. AHN Authors Info & Affiliations

SCIENCE ADVANCES • 5 Jul 2023 • Vol 9, Issue 27 • DOI: 10.1126/sciadv.adh3327

npj | computational materials

Explore content ⌄ About the journal ⌄ Publish with us ⌄

nature > npj computational materials > articles > article

Article | Open Access | Published: 25 March 2021

Optimal band structure for thermoelectrics wit realistic scattering and bands

Junsoo Park, Yi Xia, Vidvuds Ozoliņš & Anubhav Jain

ature materials

ore content ⌄ About the journal ⌄ Pub

re > nature materials > perspectives > article

pective | Published: 03 May 2021

Designing and controlling the properties of transition metal oxide quantum materials

Charles Ahn, Andrea Cavalleri, Antoine Georges, Sohrab Ismail-Beigi, Andrew J. Millis & Jean-Marc Triscone

ELSEVIER

Journa

A variational framework for computing Wannier functions using dictionary learning

Bradley Magnetta [a, b], Vidvuds Ozoliņš [a, b]

Condensed Matter Experiment & Computation at Yale AP&P

Quantum Materials

- Understand the microscopic mechanisms behind material properties
- Predict material properties with advanced theory tools
- Control and create material properties with experimental methods

We do theory with...

- First principles calculation for electronic structure prediction
- Machine learning for quantum mechanics
- Supercomputing facilities for high performance computing

We do experiment with ...

- Molecular beam epitaxy
- Bulk single crystal synthesis
- Nano-fabrication
- Scanning tunneling spectroscopy
- Photoemission spectroscopy
- Synchrotron X-ray scattering
- Magnetic imaging and low-T transport
- Scanning nearfield optical microscopy ...