Microsoft

ETH zürich

Quantum Computing and Materials Challenges

Matthias Troyer

Beyond exascale computing

Argonne NATIONAL LABORATORY

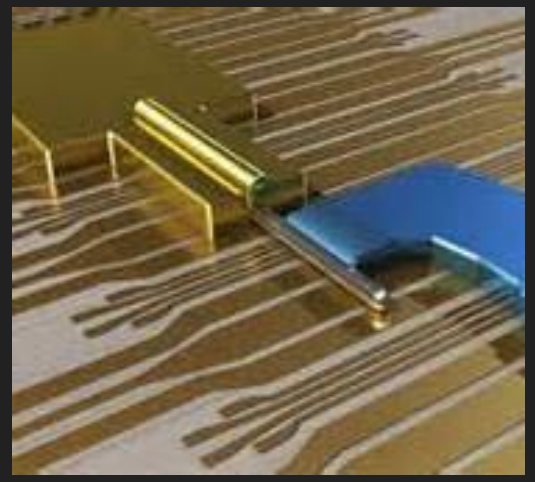
Enabling technologies for beyond exascale computing

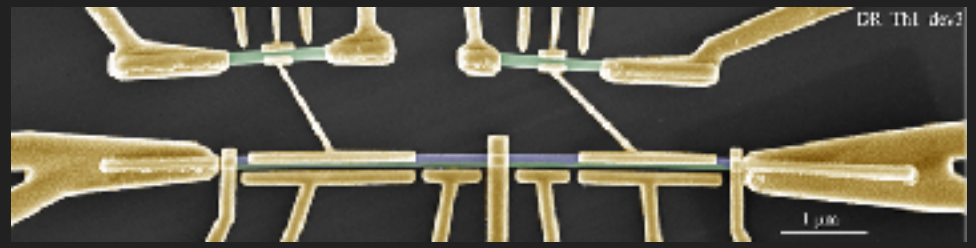
- We are not referring to 10**21 flops
- "Beyond exascale" systems as we are defining them will be based on new technologies that will finally result in the much anticipated (but unknown) phase change to truly new paradigms/methodologies.

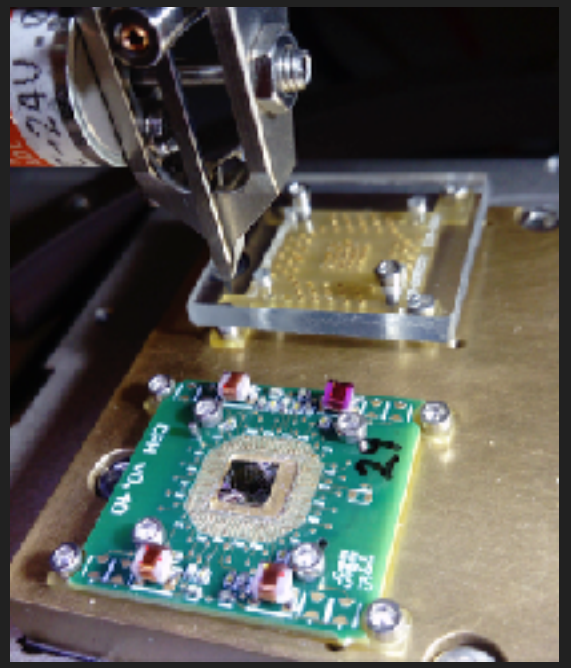
Paul Messina
Director of Science
Argonne Leadership Computing Facility
Argonne National Laboratory

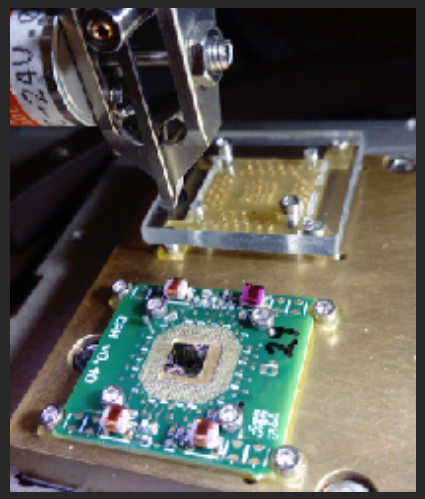
July 9, 2014
Cetraro

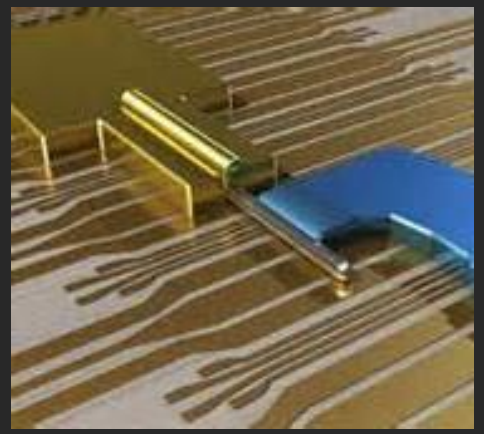
Develop and deploy a scalable, commercial quantum system to solve today's unsolvable problems

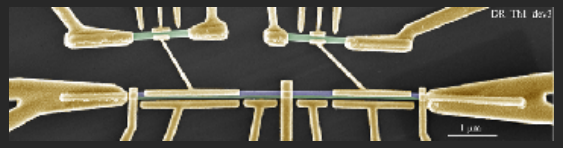












300K ← Room temp

100

Nitrogen →

30

10

Helium →

← Cryogenic Computer

3

Deep Space →

1

0.3

0.1

0.03

Quantum Computer →

← Quantum World

0.01K

APPLICATIONS + SW

CRYOGENIC COMPUTER CONTROL SW

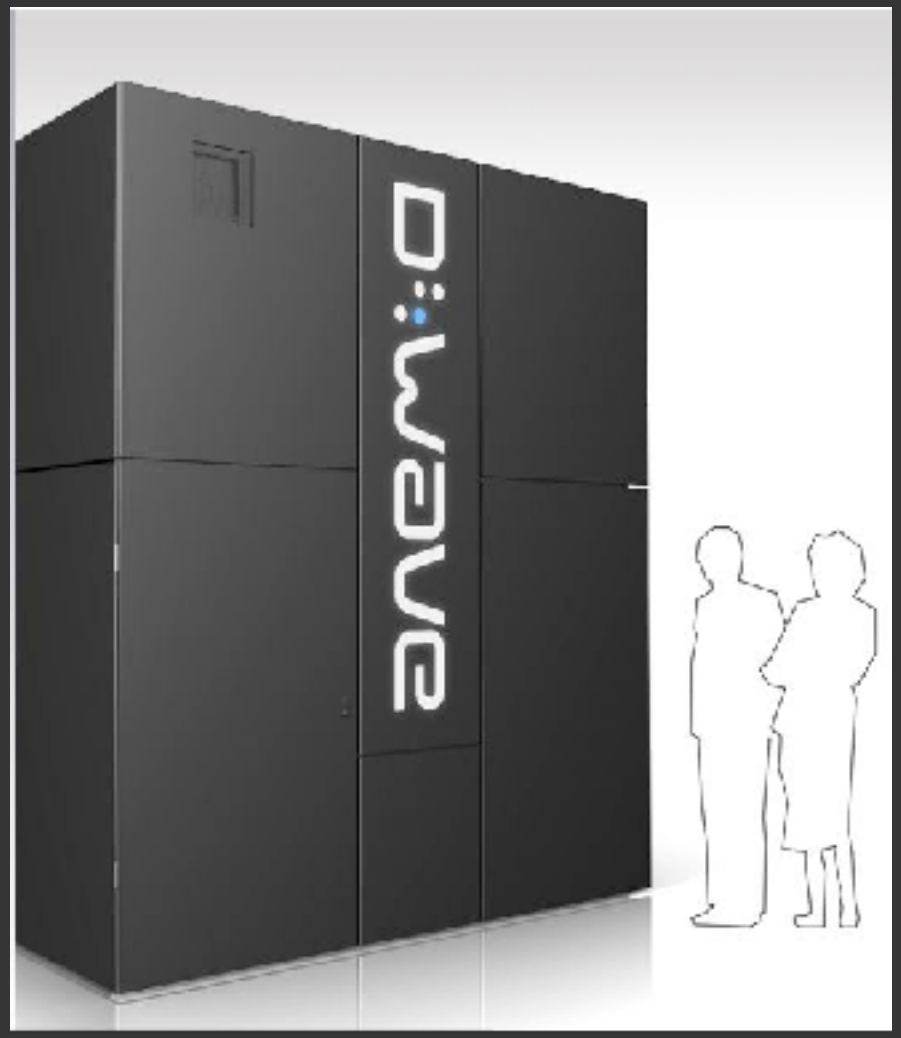
QUANTUM COMPUTER

Developing quantum applications

quantum software engineers

1. Find quantum algorithm with quantum speedup
2. Confirm quantum speedup after implementing all oracles
3. Optimize code until runtime is short enough
4. Embed into specific hardware estimate runtime

A quantum machine to solve hard optimization problems

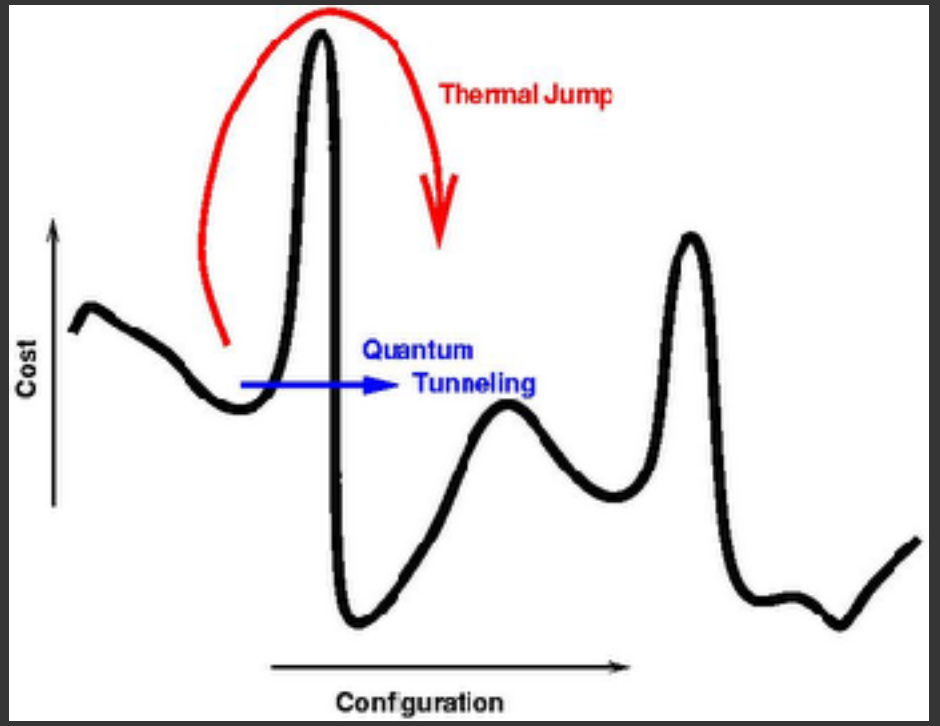


The D-Wave quantum annealer

An analog quantum device to solve quadratic binary optimization problems

$$C(x_1,\ldots,x_N)=\sum_{ij}a_{ij}x_i x_j+\sum_i b_i x_i$$

$$\text{with} \qquad x_i=0,1$$



Can be built with imperfect qubits

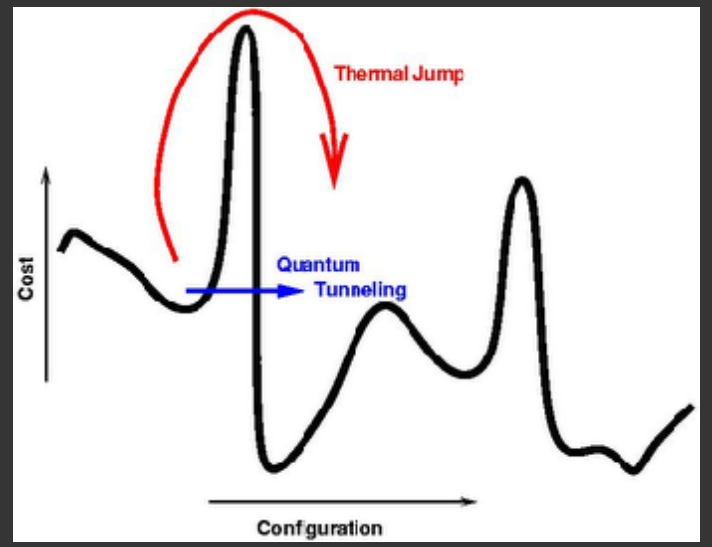
Significant engineering achievement to scale it to two thousand qubits

So far no (scaling) advantage has been observed

Quantum tunneling can be simulated classically!

Early value: quantum inspired optimization

Mimic quantum tunneling
on classical computers today!



Research into quantum algorithms often uncovers new classical algorithms

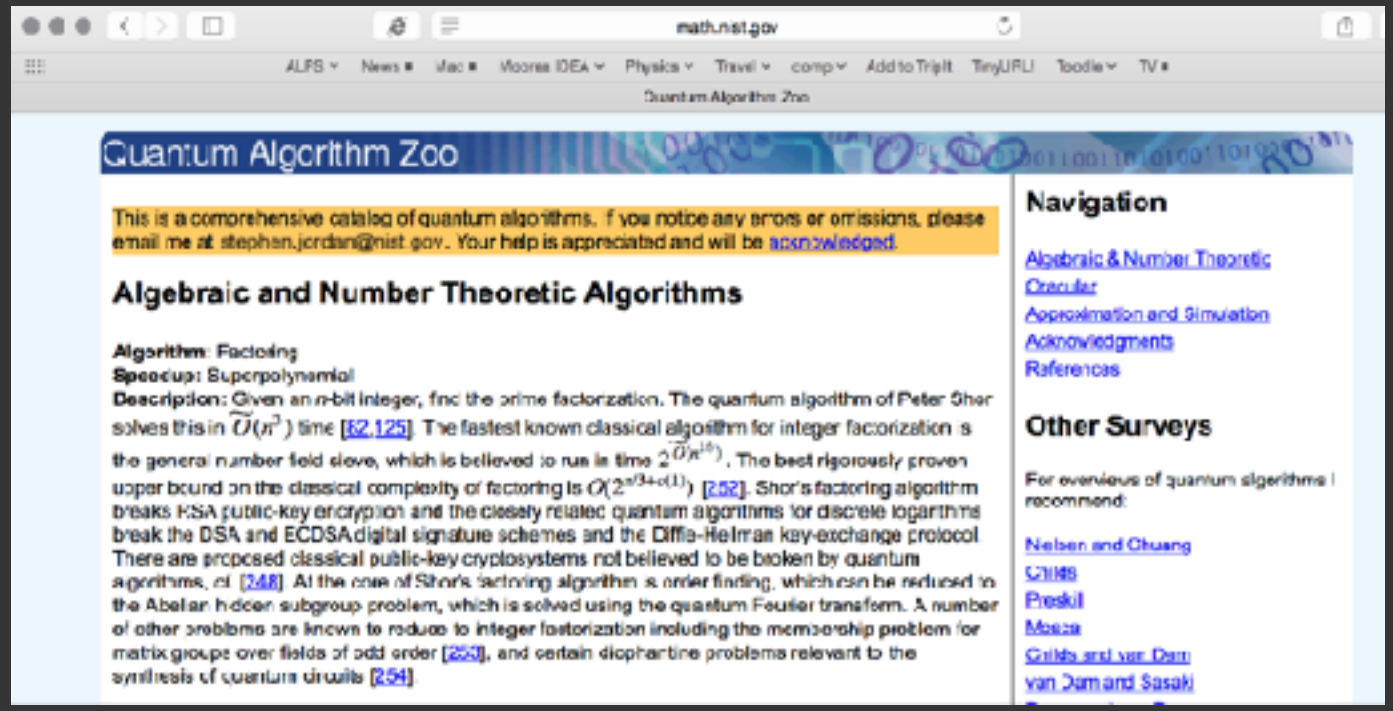
- Better optimization methods
- Better training algorithms
- Better models for machine learning

Yoshihisa Yamamoto, Monday 10:15am

Hidetoshi Nishimori , Tuesday 4:00pm

Developing quantum applications

1. Find quantum algorithm with quantum speedup



Stephen Jordan (Microsoft)

http://math.nist.gov/quantum/zoo/

Impact on Cryptography

Quantum computers break widely used public key encryption

RSA-2048 with 4100 qubits

ECC: Bitcoin with 2330 qubits

New quantum-safe cryptography

Quantum key distribution

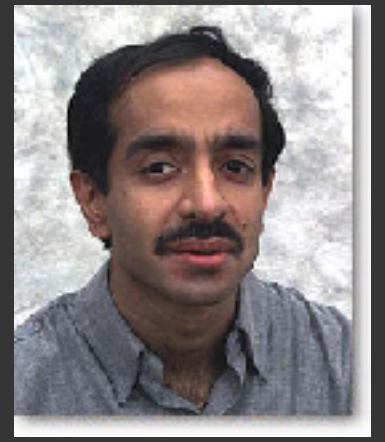
“Post-quantum” classical cryptography

Developing quantum applications

1. Find quantum algorithm with quantum speedup

2. Confirm quantum speedup after implementing all oracles

Grover search



Search an unsorted database of N entries with $\sqrt{N}$ queries

However, the query needs to be implemented!

A single quantum query needs at least $O(N)$ time since all entries must be read! While reading the data *once* we can already find the desired entry!

Only useful if the query result can be efficiently calculated on the fly!

What are the important applications satisfying this criterion?

Developing quantum applications

1. Find quantum algorithm with quantum speedup

2. Confirm quantum speedup after implementing all oracles

3. Optimize code until runtime is short enough

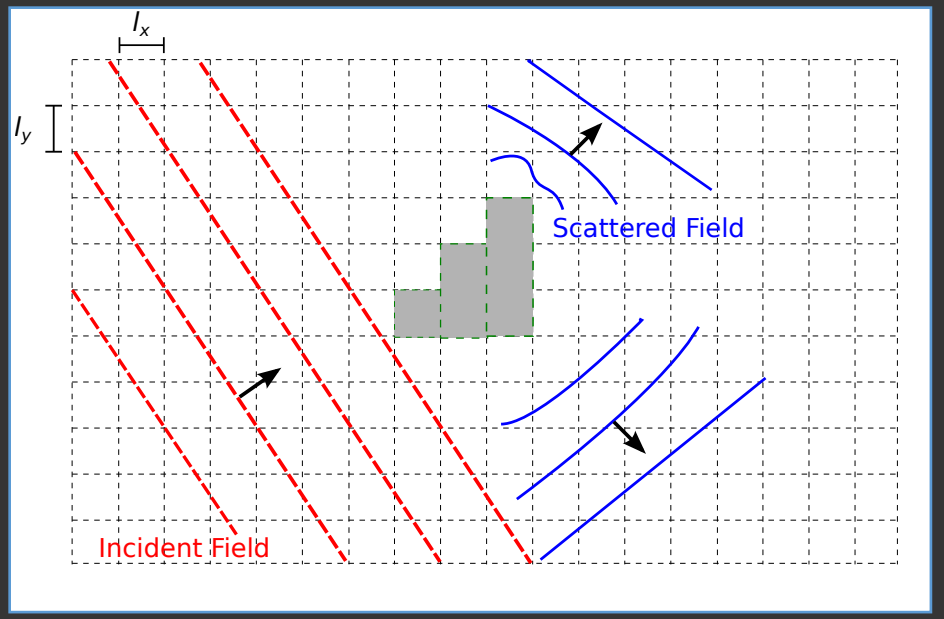
Solving linear systems of equations

Harrow, Hassidim, Lloyd, PRL (2009)

Solve linear system $Ax=b$ in log(N) time

Time evolution using the matrix A needs to be implemented efficiently

$$e^{-iAt}\left|b\right\rangle$$



Exponential speedup for wave scattering problem (Clader et al, PRL, 2013)!

Estimated to use 10^{29} gate operations for a problem that is still tractable on a classical supercomputer (arXiv:1505.06552).

First applications that reached a petaflop on Jaguar @ ORNL

Domain area	Code name	Institution	# of cores	Performance	Notes
Materials	DCA++	ORNL	213,120	**1.9 PF**	2008 Gordon Bell Prize Winner
Materials	WL-LSMS	ORNL/ETH	223,232	**1.8 PF**	2009 Gordon Bell Prize Winner
Chemistry	NWChem	PNNL/ORNL	224,196	1.4 PF	2008 Gordon Bell Prize Finalist
Materials	DRC	ETH/UTK	186,624	1.3 PF	2010 Gordon Bell Prize Hon. Mention
Nanoscience	OMEN	Duke	222,720	> 1 PF	2010 Gordon Bell Prize Finalist
Biomedical	MoBo	GaTech	196,608	780 TF	2010 Gordon Bell Prize Winner
Chemistry	MADNESS	UT/ORNL	140,000	550 TF	
Materials	LS3DF	LBL	147,456	442 TF	2008 Gordon Bell Prize Winner
Seismology	SPECFEM3D	USA (multiple)	149,784	165 TF	2008 Gordon Bell Prize Finalist

Source: T. Schulthess

The Theory of Everything

Laughlin & Pines
PNAS 2000

The N-body Schrödinger equation

$$i\hbar\frac{\partial\Psi(\vec{r}_1,....,\vec{r}_N,t)}{\partial t}=H\Psi(\vec{r}_1,....,\vec{r}_N,t)$$

Describes (almost) everything we encounter in daily life with a very simple Hamilton

$$H=\sum_i\left(-\frac{1}{2m_i}\Delta_i+V^{ext}(\vec{r}_i)\right)+\sum_{i,j}\frac{q_iq_j}{\left|\vec{r}_i-\vec{r}_j\right|}$$

It is a simple linear partial differential equation (PDE)

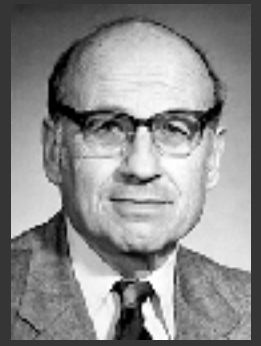
But is exponentially complex since it lives in 3N dimensions

Density functional theory and quantum chemistry

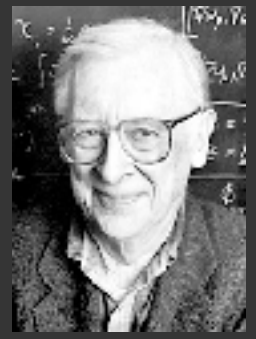
Approximates the *N*-body Schrödinger by a tractable 1-body problem

$$E_0 = \min_{\rho(\vec{r})} \left(F[\rho] + \int d^3\vec{r} V(\vec{r}) \rho(\vec{r}) \right)$$

Successful in calculating properties
many metals, insulators, semiconductors



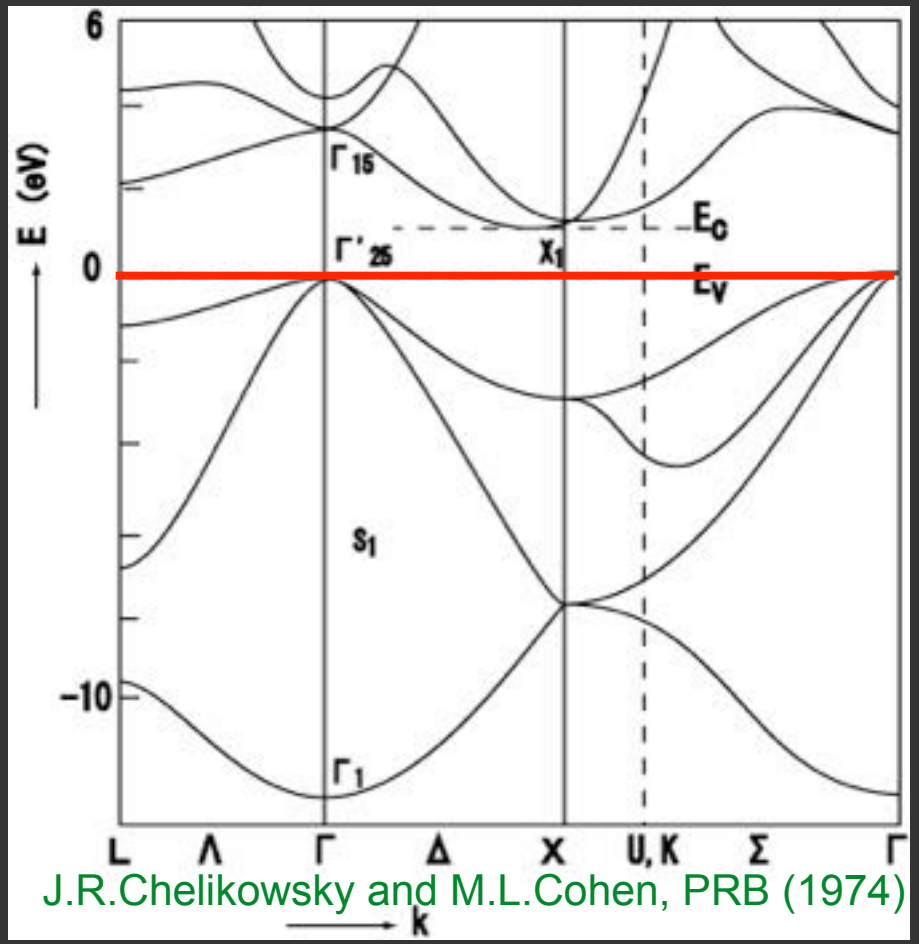
Walter Kohn



John A. Pople

1998 Nobel prize in chemistry

Band structure of silicon



J.R.Chelikowsky and M.L.Cohen, PRB (1974)

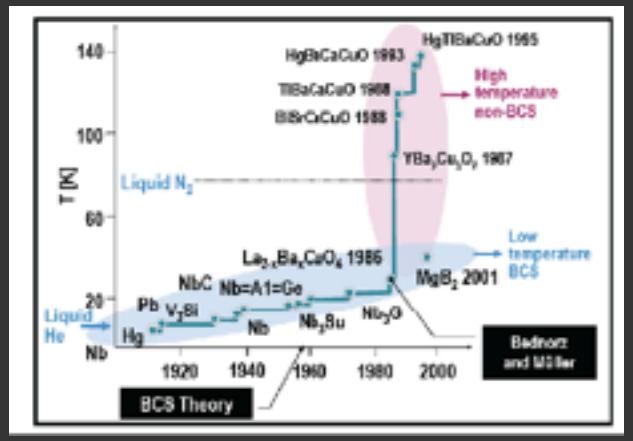
Cuprate high temperature superconductors

Undoped materials:

half-filled band and metal according to DFT

but antiferromagnetic insulator in experiment!

Band structure calculation breaks down!

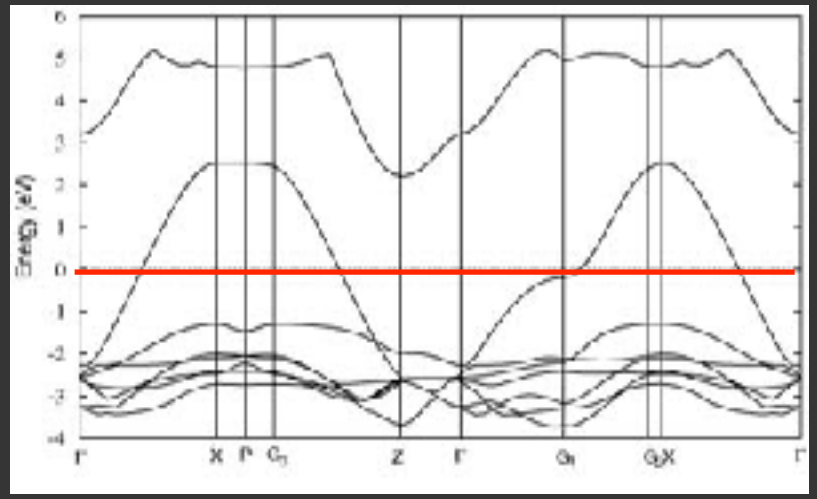


Doped materials:
high-temperature superconductors

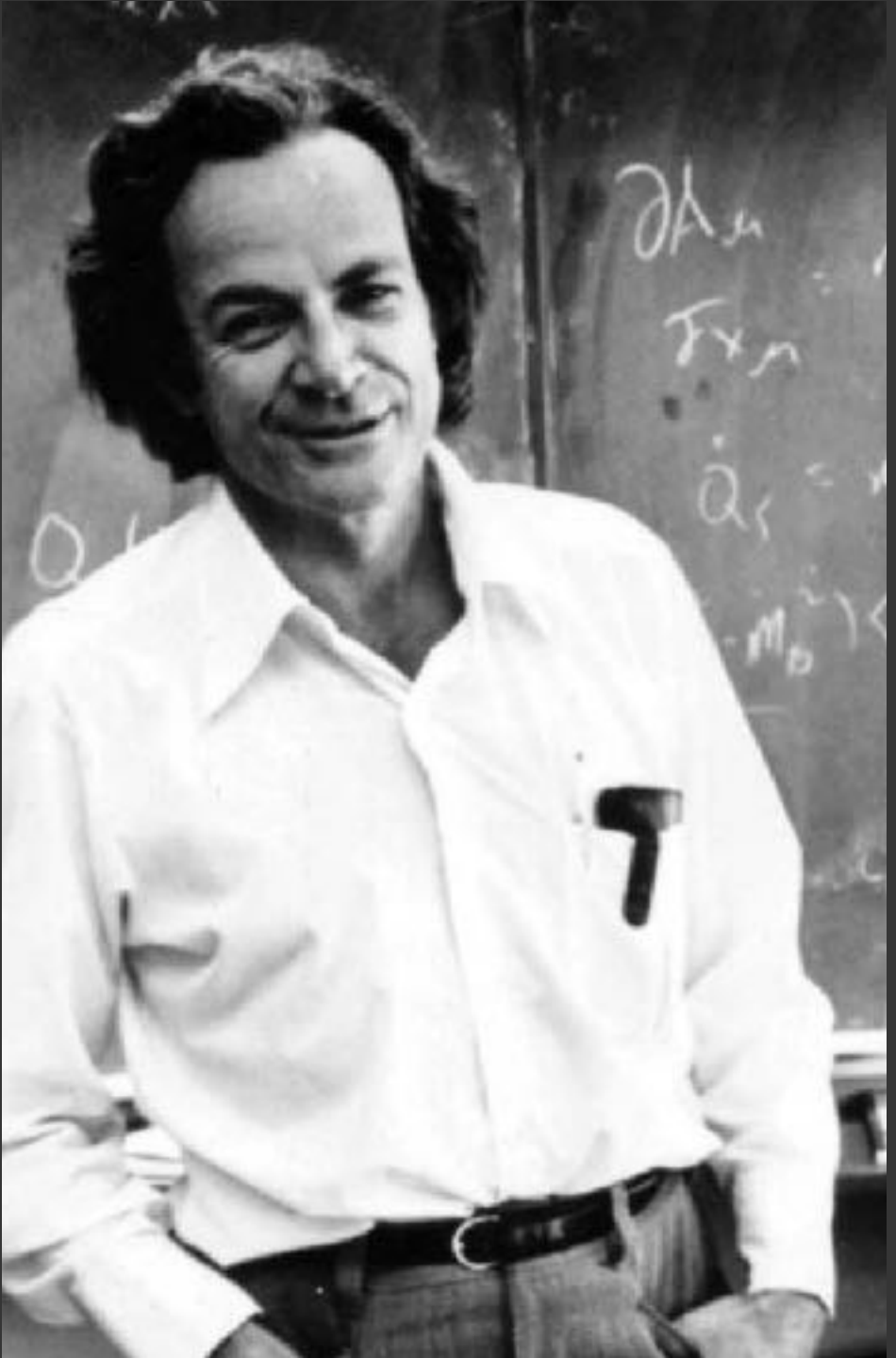
What causes superconductivity?

Are there room temperature superconductors?

Fermi level



Band structure of La_2CuO_4



International Journal of Theoretical Physics, Vol. 21, Nos. 6/7, 1982

Simulating Physics with Computers

Richard P. Feynman

Department of Physics, California Institute of Technology, Pasadena, California 91107

Received May 7, 1981

Feynman proposed to use quantum computers to simulate quantum physics

Simulating quantum materials on a quantum computer

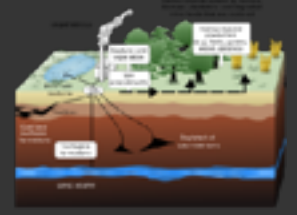
Can we use quantum computers to design new quantum materials?

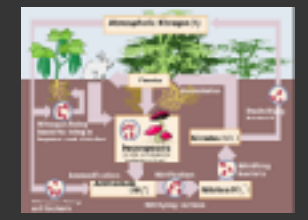
A room-temperature superconductor?

Non-toxic designer pigments?

A catalyst for carbon fixation?

Better catalysts for nitrogen fixation (fertilizer)?





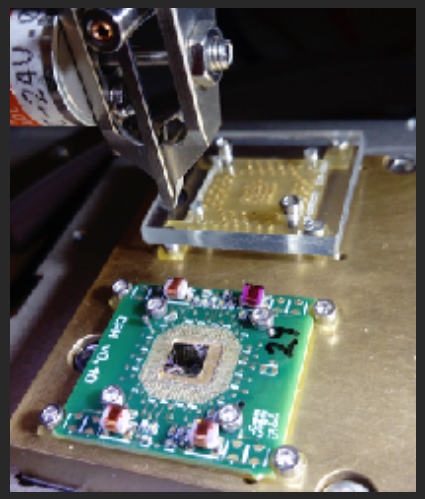
Solving materials challenges with strong correlations has

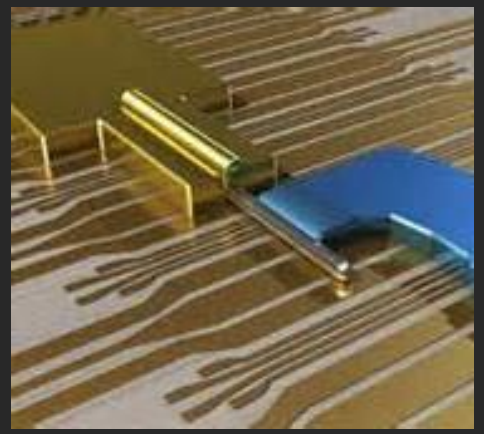
exponentially complexity on classical hardware

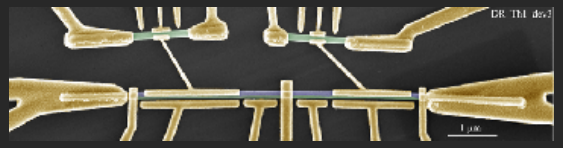
polynomial complexity on quantum hardware!

Garnet Chan, Monday 11:30am

Markus Reiher , Tuesday 9:00am







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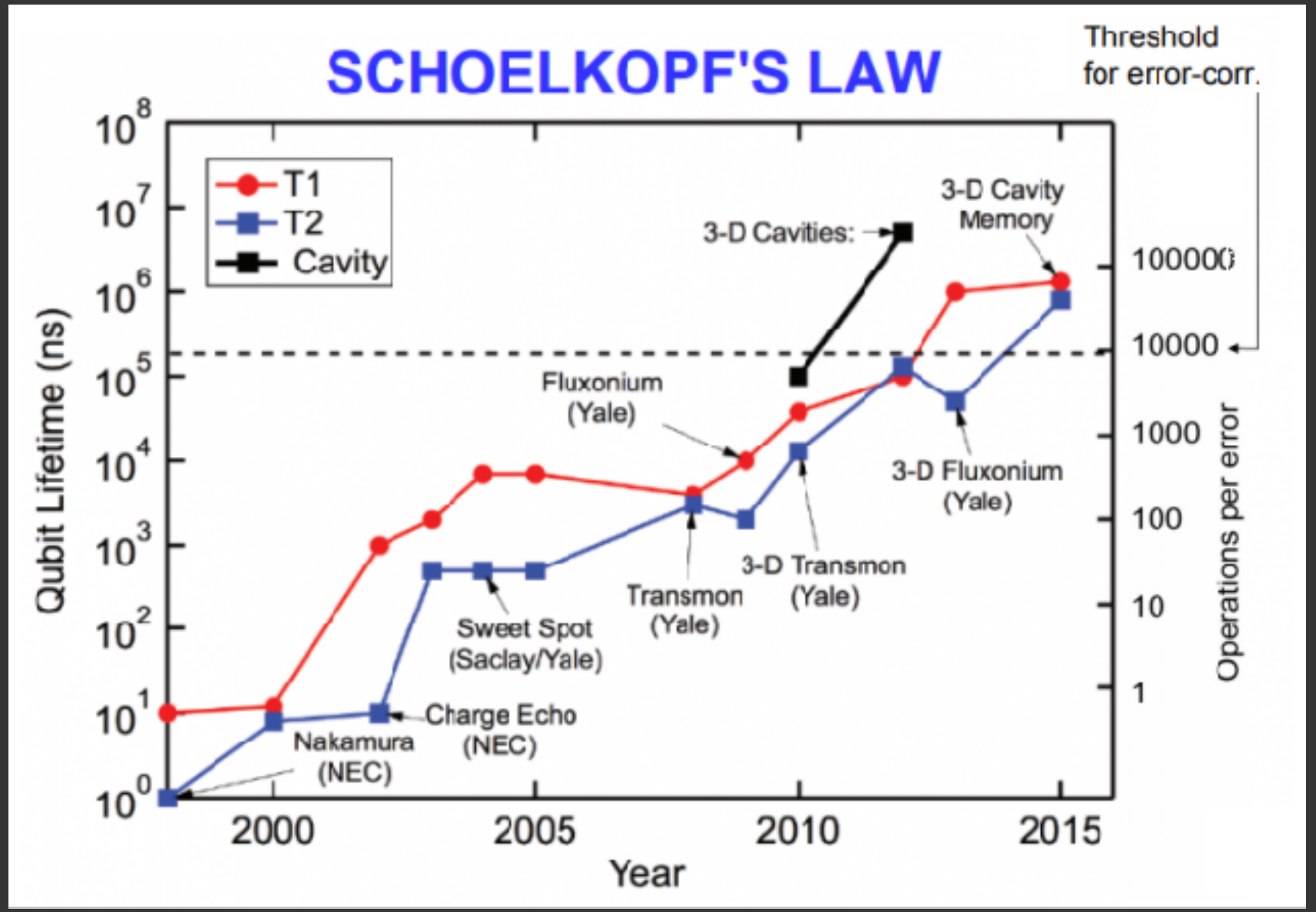
0.01K

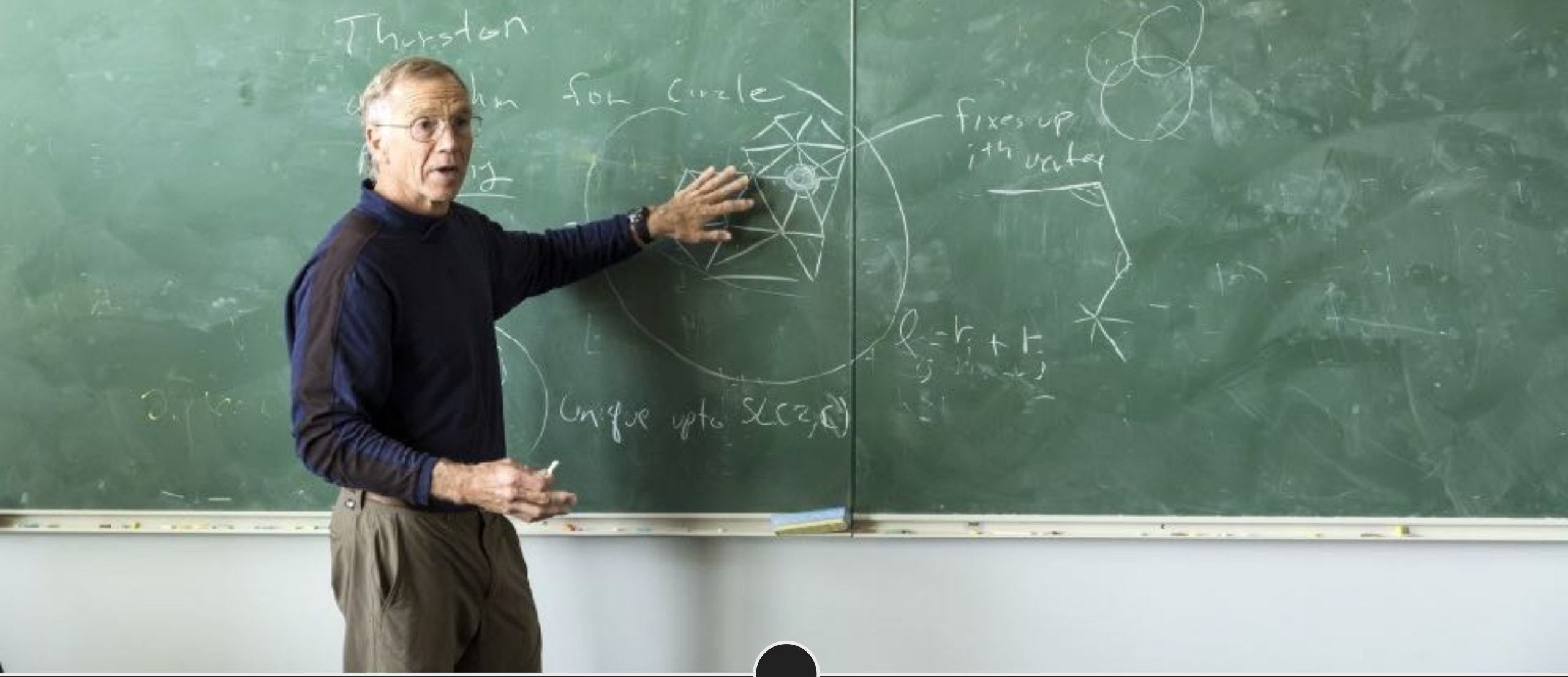
APPLICATIONS + SW

CRYOGENIC COMPUTER CONTROL SW

QUANTUM COMPUTER



Significant progress in qubit quality is to a large extent due to progress in materials quality



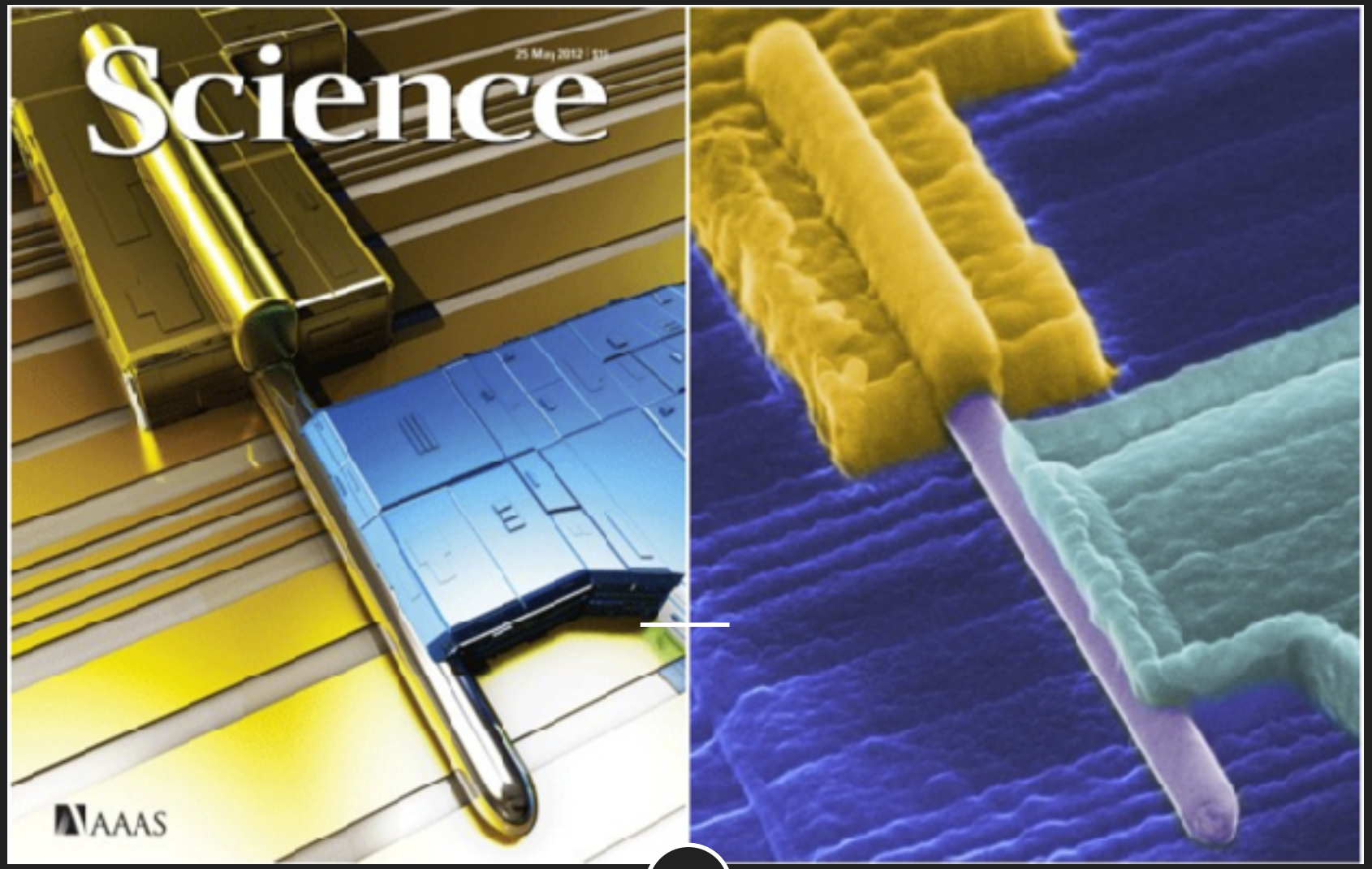
Topological qubits will be another step forward

Yasuyuki Kawahigashi, Wednesday 10:15am

Zhenghan Wang, Wednesday 2:00pm

Majorana Fermions

Predicted by Ettore Majorana in 1937

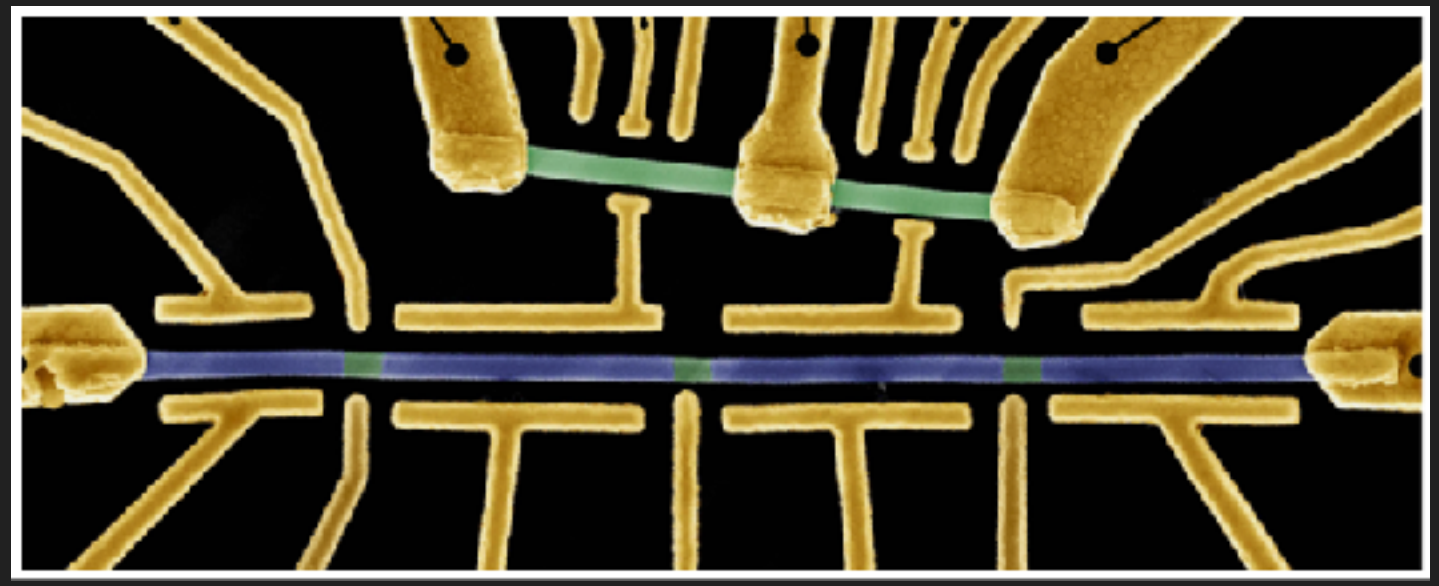


2012

Majorana qubits: split the information

Store a qubit in a superposition of 0 or 1 electrons

Split 0 or 1 electrons into two “Majorana” particles

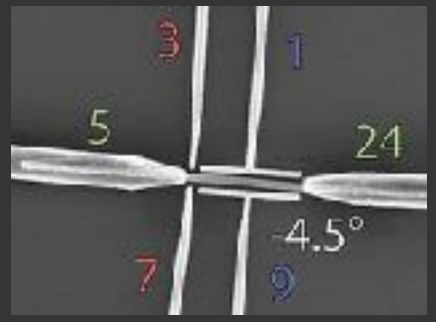


Bela Bauer, Tuesday 10:15am

Roman Lutchyn, Tuesday 11:30am

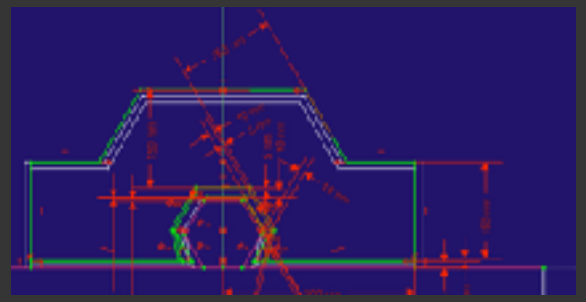
Qubit modeling and design optimization

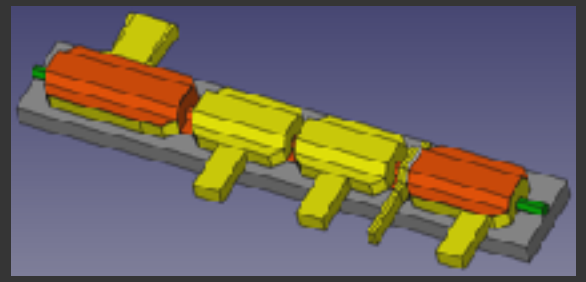
2D Design



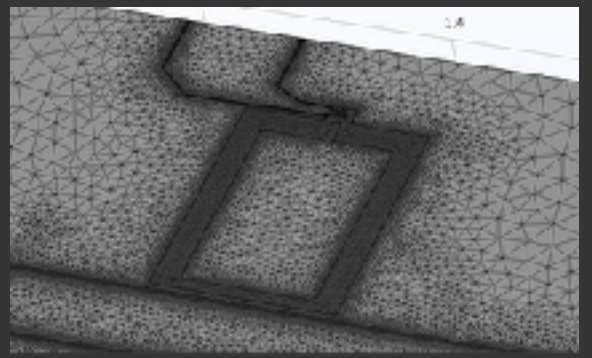
Automatic rendering of 3D CAD from 2D designs and images.

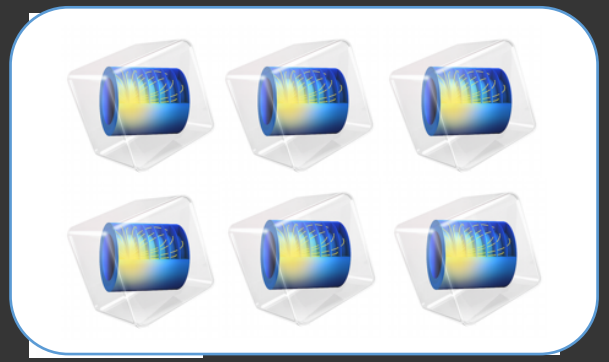
Parametric 3D CAD





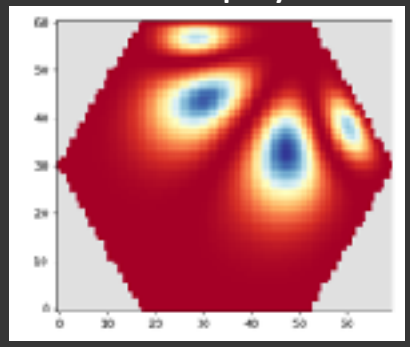
Batch Simulations





Automatic cross-sectional slices

Advanced physics

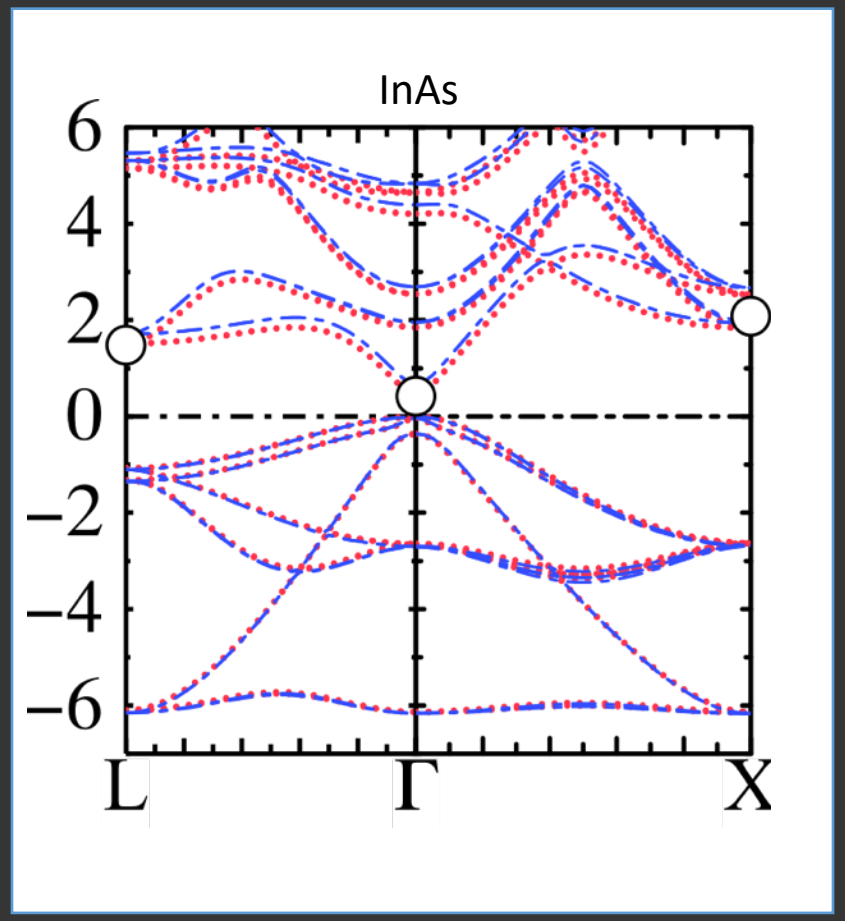


Edwin Barnes, Monday 4:00pm

Susan Coppersmith, Tuesday 2:30pm

Rick Muller, Wednesday 9:00am

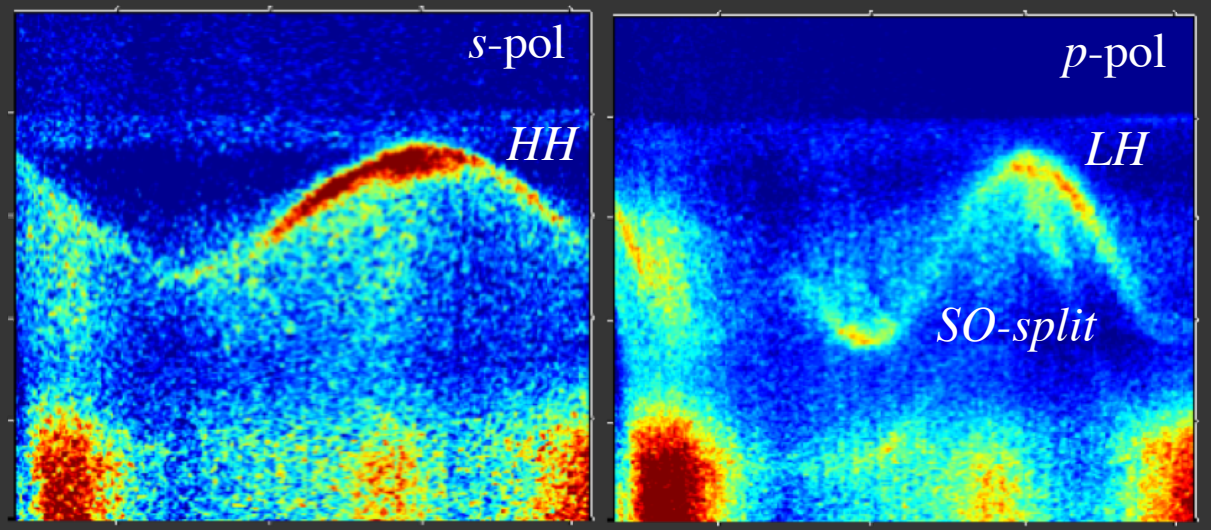
Materials Simulations and Characterization



Band structure calculations

ARPES experiments

InAs/Al interfaces

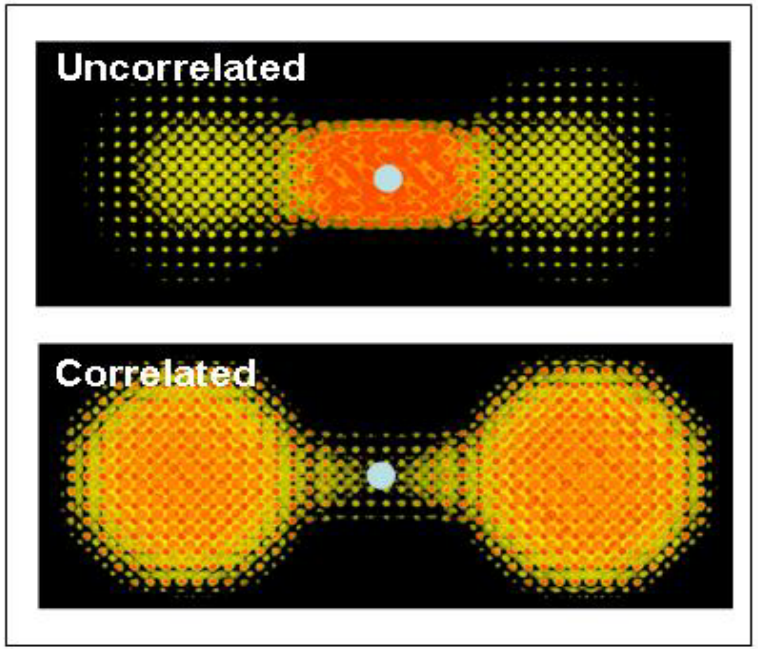


First principles simulations of nano devices?

Journal of Physics: Conference Series **46** (2006) 292–298
SciDAC 2006

Predicting the electronic properties of 3D, million-atom semiconductor nanostructure architectures

A. Zunger, A. Franceschetti, G. Bester,
Materials Science Center, NREL.
W.B. Jones, Kwiseon Kim and P. A. Graf,
Scientific Computing Center, NREL.
L-W. Wang, A. Canning, O. Marques, C. Voemel
Computational Research Division, LBNL.
J. Dongarra, J. Langou and S. Tomov
Dept. of Computer Science, University of Tennessee.



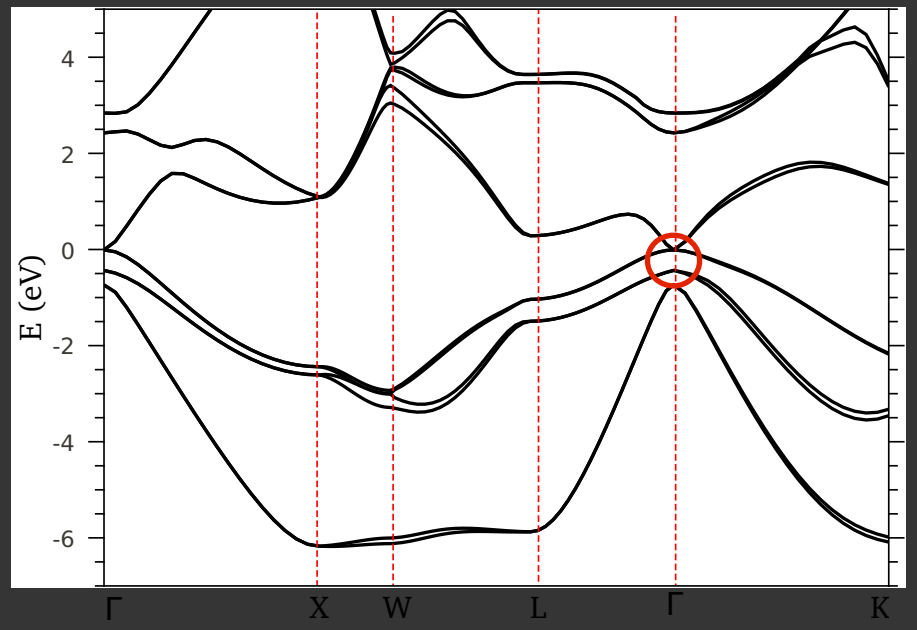
Eric Cances, Monday 2:30pm

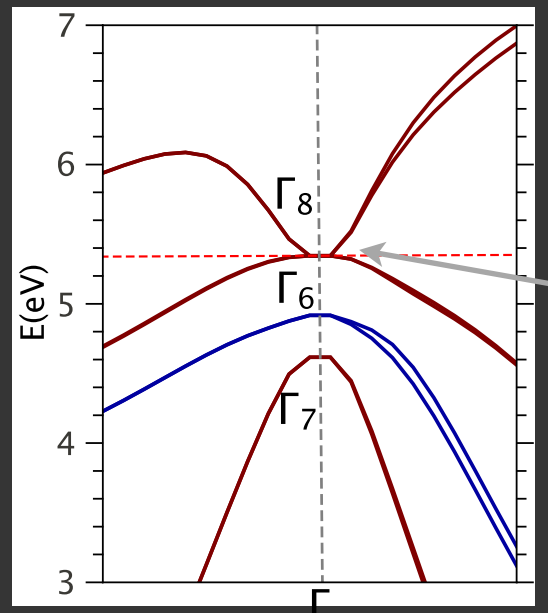
Sophia Economou , Wednesday 11:30

First-principles calculations of InSb band structure

Simple functionals fail in most of the zincblende semiconductors

InSb is gapless using LDA and GGA due to wrong band ordering



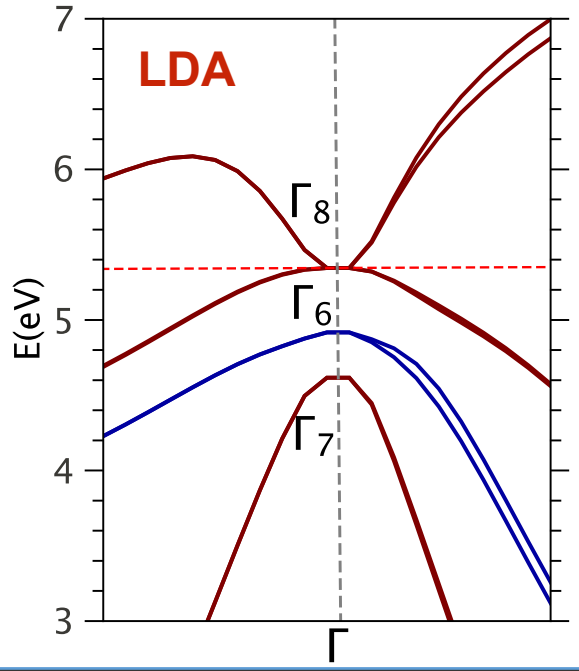


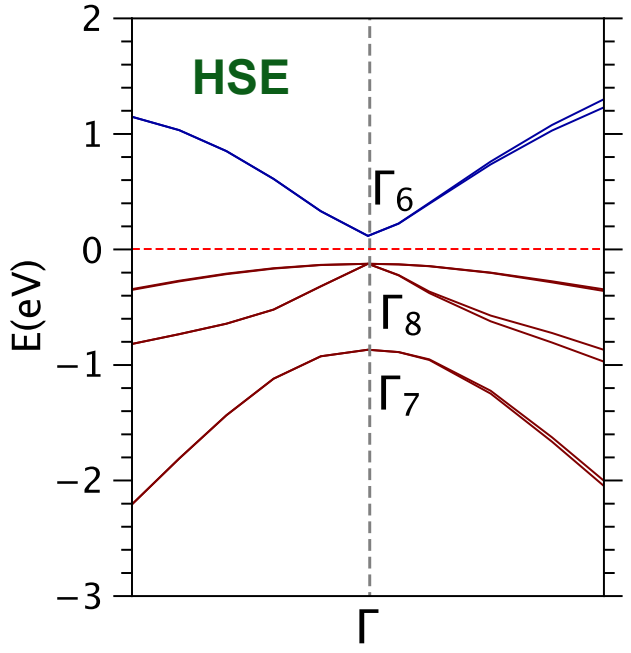
zero
band gap

Using hybrid functionals

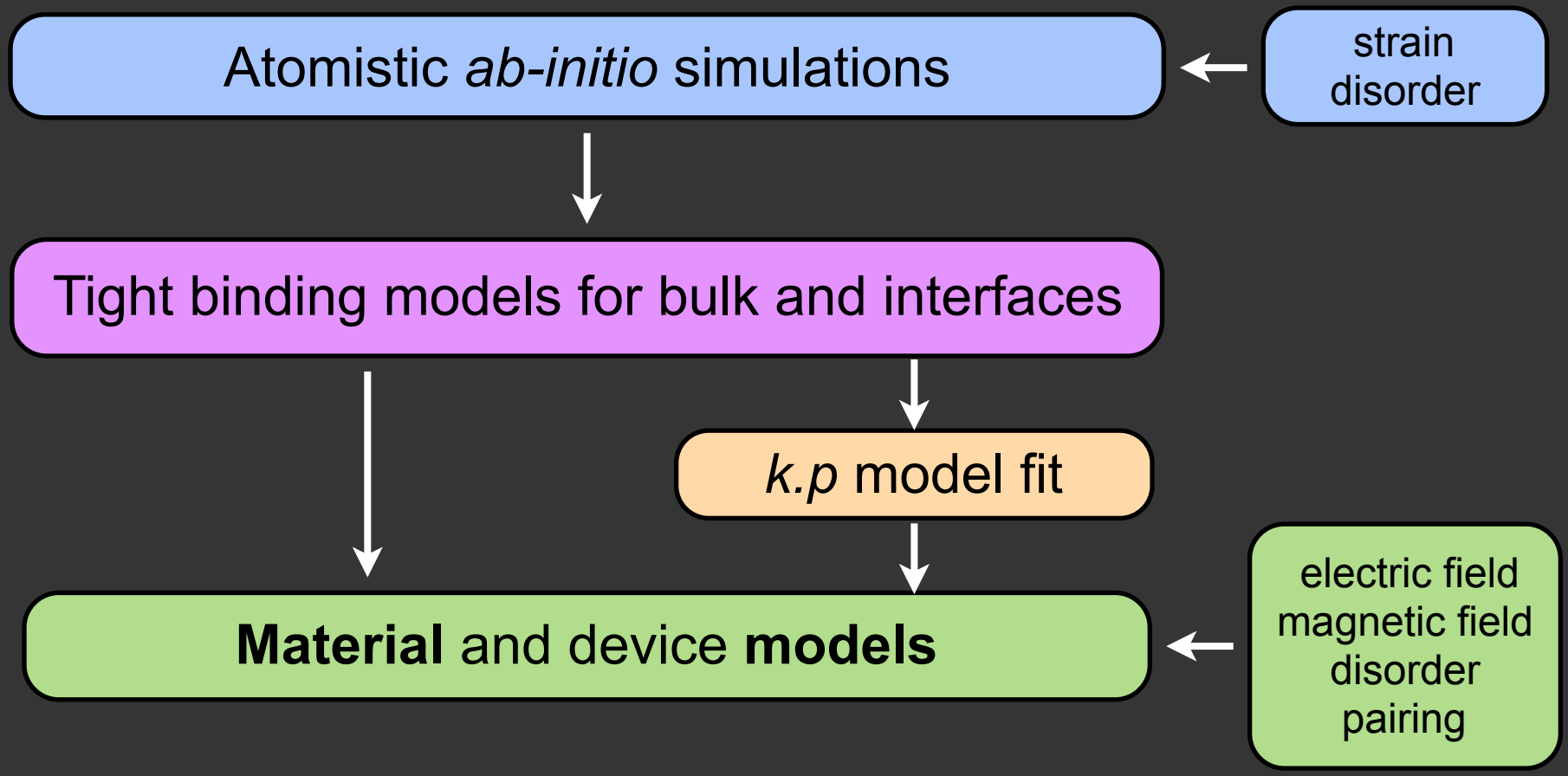
Admix some Hartree-Fock exchange energy for the short range part of the interaction

$$E_{\mathrm{xc}}^{\mathrm{HSE}} = E_{\mathrm{xc}}^{\mathrm{LDA}}(\mu) - \frac{1}{4}(E_{\mathrm{xc}}^{\mathrm{LDA}}(\mu) + E_{\mathrm{x}}^{\mathrm{HF}}(\mu)) \qquad \mu = 0.2\mathring{A}^{-1}$$



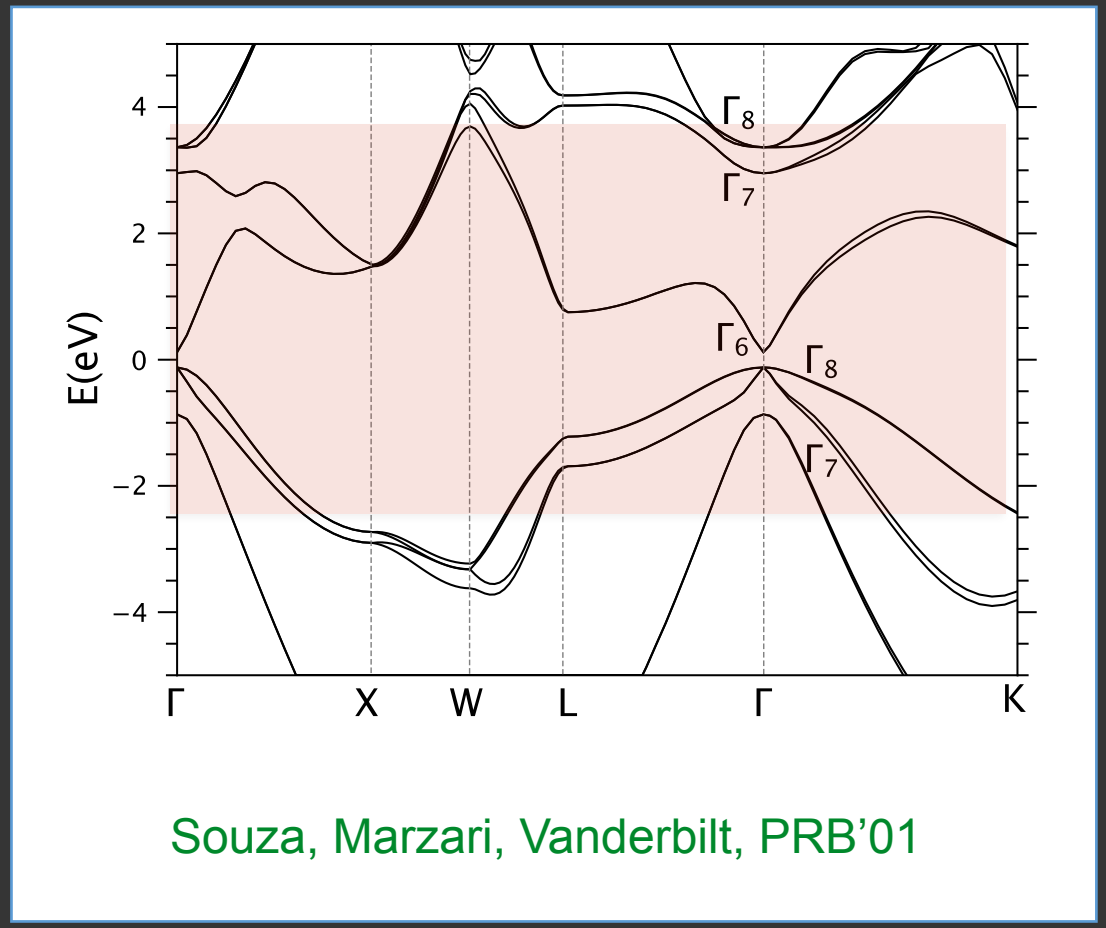


Strategy for numerical simulations



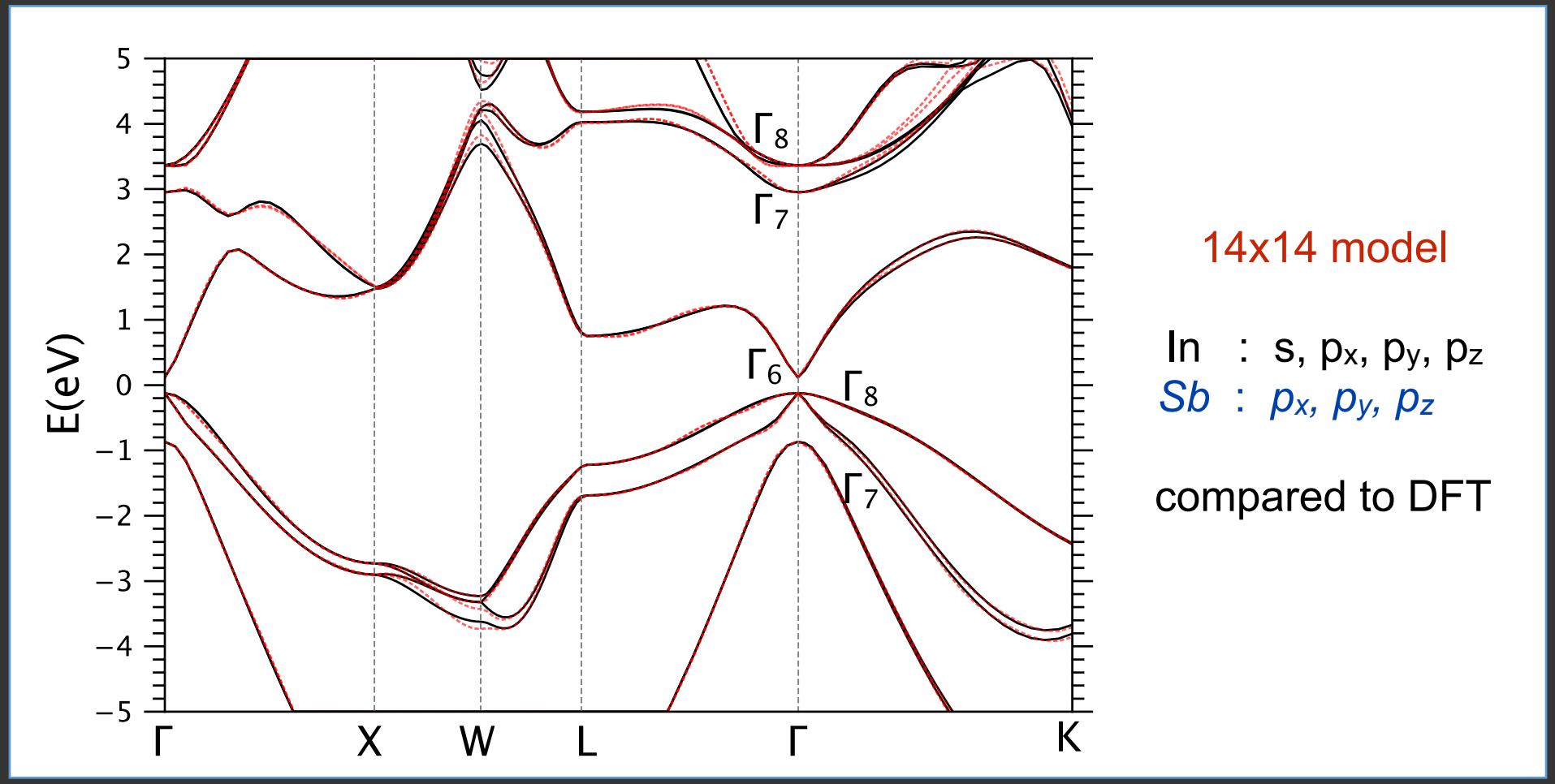
Constructing tight-binding models

Choose an energy window and build a tight binding model



Souza, Marzari, Vanderbilt, PRB'01

Accurate tight-binding models respecting symmetries



14x14 model

In : s, p_x, p_y, p_z

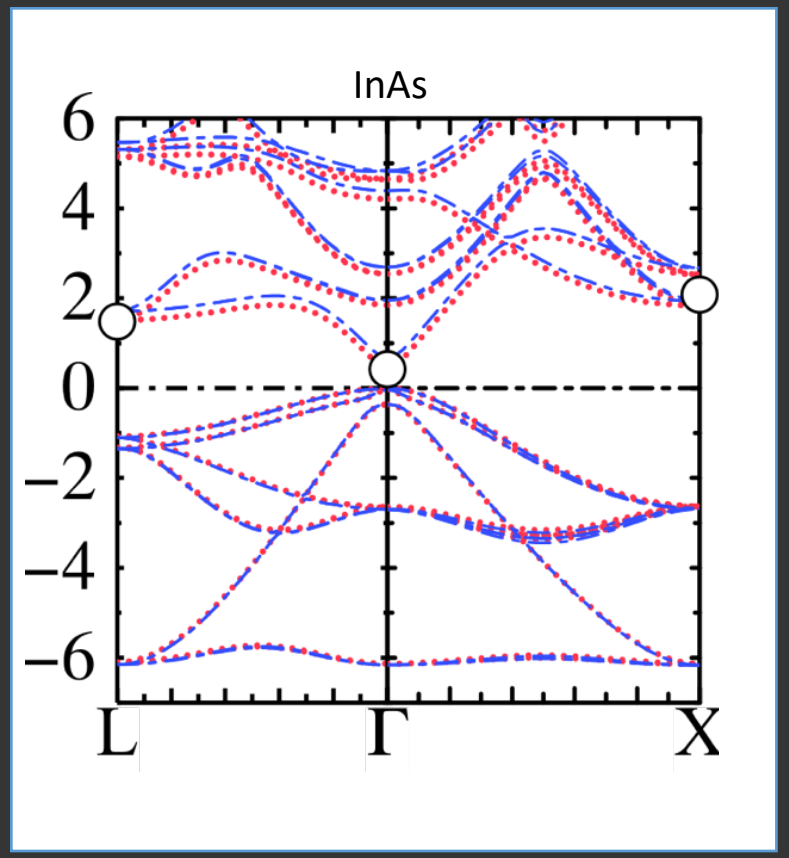
Sb : *p_x, p_y, p_z*

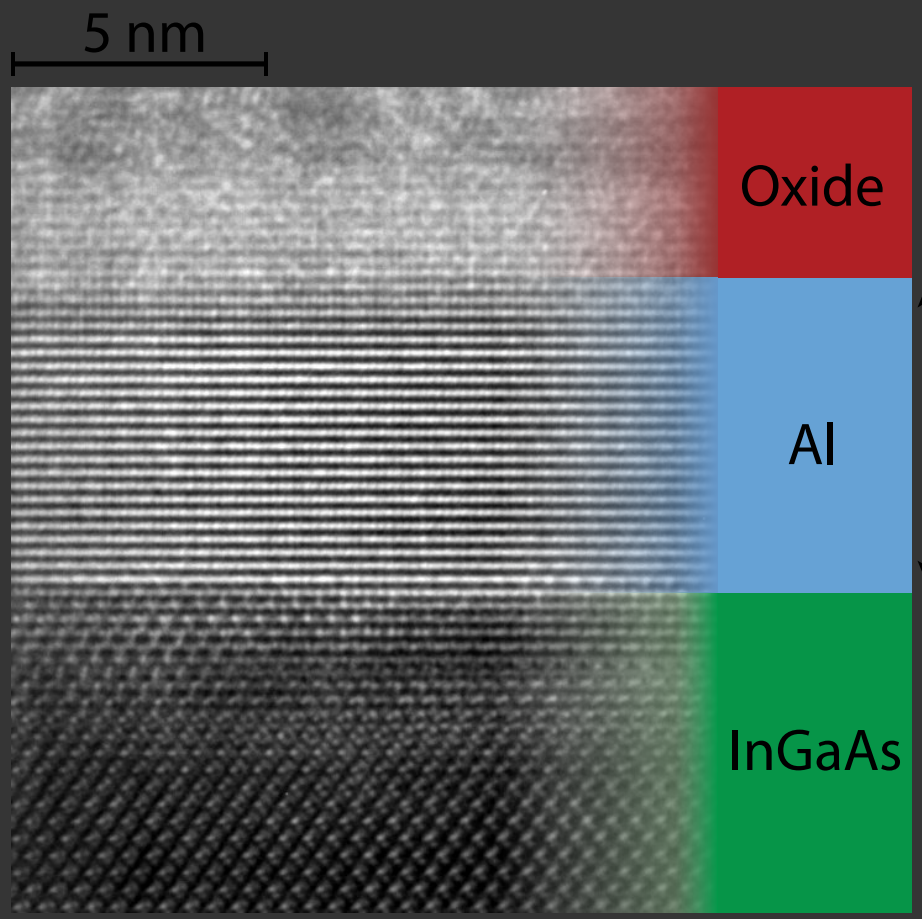
compared to DFT

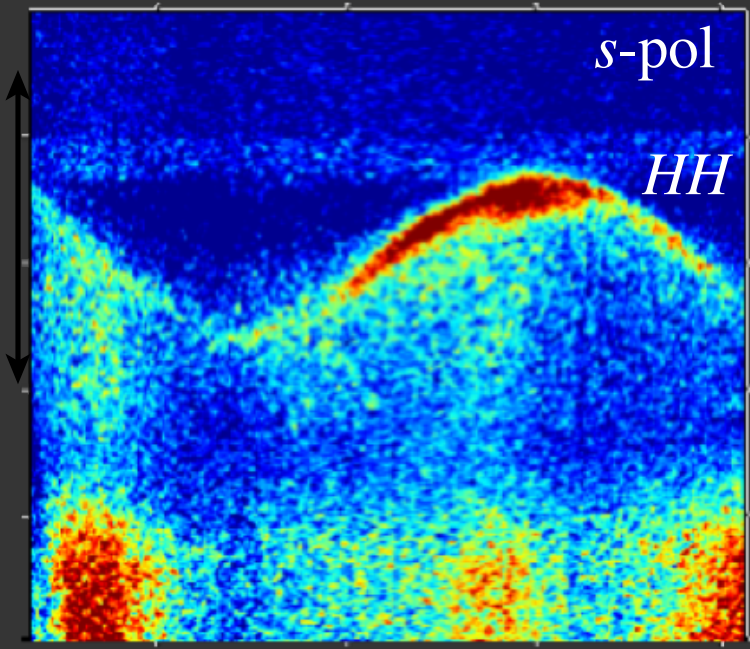
Bela Bauer, Tuesday 10:15am

Roman Lutchyn, Tuesday 11:30am

Better materials will be important for better qubits







Imagine the quantum future of materials …

Nitrogen Fixation

cheap fertilizer everywhere

Carbon Capture

mitigate global warming

Materials Science

lossless power lines

better batteries

smart materials

Machine learning