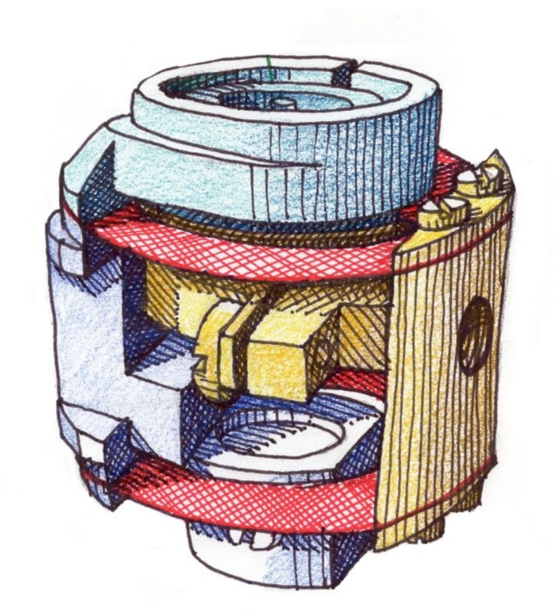
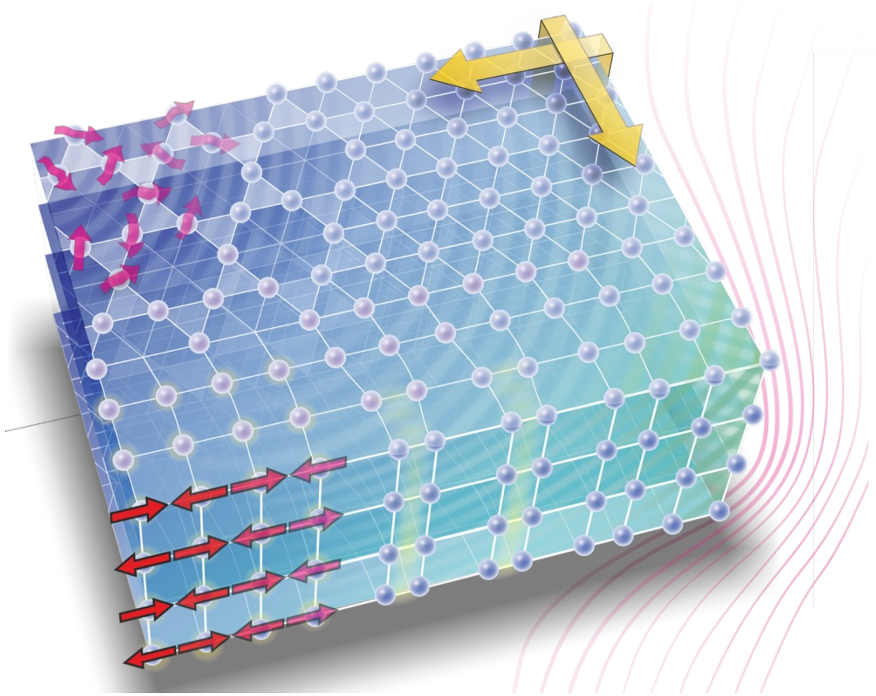
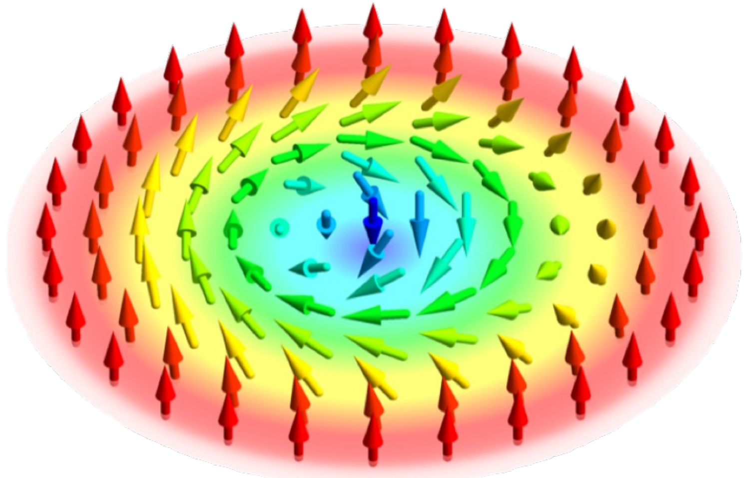
Karlsruhe Institute of Technology

Electronic Properties of Solids - I
Elektronische Eigenschaften von Festkörpern I

Lecturers

Lectures
Tuesday 9.45 - 11.15
Friday 9.45 - 11.15

M. Le Tacon

matthieu.letacon@kit.edu

P. Willke

philip.willke@kit.edu

Exercises
Tuesday 17.30 – 19.00

Paolo Battistoni

paolo.battistoni@kit.edu

Máté Stark

mate.stark@kit.edu

Electronic properties of solids I - ILIAS

Karlsruhe Institute of Technology

4021011 – Electronic Properties of Solids I WS22/23

Actions

Lecture on the electronic properties of solids - part I. The lectures will be given in English and will take place on Tuesdays (09:45 - 11:15) and Fridays (09:45 - 11:15). The lecture hall is the 30.22 Physik-Hörsaal Nr. 4 (Kl. HS B) EXERCISES: The exercise classes are on Tuesdays 17.30 – 19.00 in Seminar room 3.01. Please send the solutions to the exercise sheets by Monday midnight to your tutor via email. You should solve 60% of the exercise sheet at least. Your tutor will choose presenters for the different parts of the exercise sheet and she/he will inform you on the day of the exercise class in advance, so that you can prepare the presentation of the solutions.

Content | Info | Settings | Members | Learning Progress | Metadata | Export | Permissions | Show Member View

General Information

Important Information

Lecture on the electronic properties of solids - part I. The lectures will be given in English and will take place on Tuesdays (09:45 - 11:15) and Fridays (09:45 - 11:15).

The lecture hall is the 30.22 Physik-Hörsaal Nr. 4 (Kl. HS B)

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Password for the lecture: EEFK1
Password to register the in tutorials: EevFk1

- Registration for tutorial groups – max. 20 participants per group
- Exercises are online seven days in advance of the tutorial session
- PPT-files, lecture notes and other documents will be put online at the end of each chapter

Electronic properties of solids I tutorials and certificate

Karlsruhe Institute of Technology

Certificate / Schein (necessary for - nötig für Schwerpunkt-,Ergänzungs- und Nebenfach):

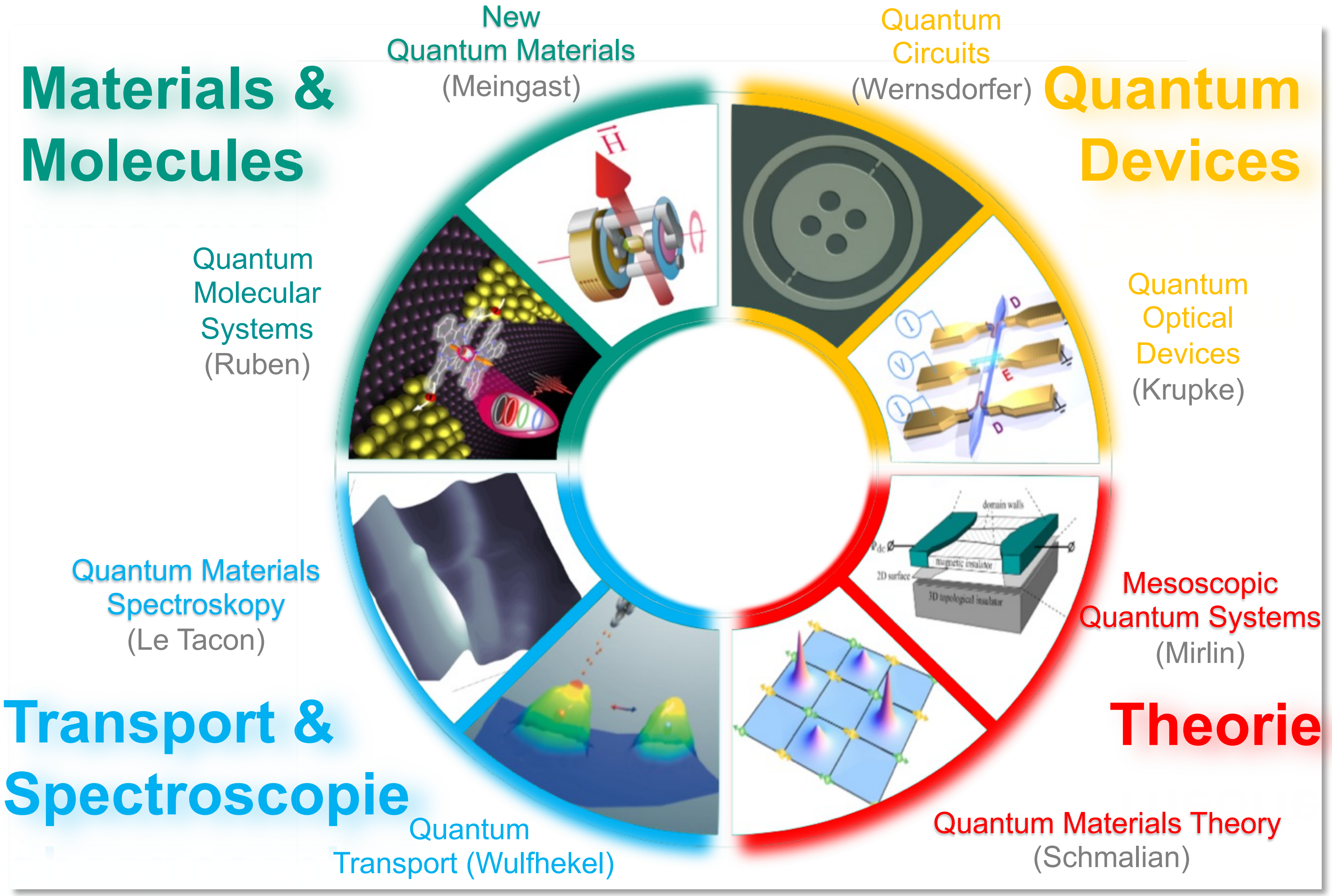
- Compulsory presence
- Submit written solution to 60% of the problems until the day before
  (concretely : 3 out of 4 or 5 problems)
- Tutors will pick up those who will present their solution to the class in the morning on the day of the class (**indicate if you are ready to discuss a problem, and if so which one in you email!**)
- Everyone should be able to discuss a problem at least once in the term

Dates: Nov. 8th/Nov. 22th/Dec. 6th/Dec. 20th/Jan. 17th/ Jan. 31st/ Feb. 14th

Oral Examination

TIME: 17h30-19h00 - Room 3/1 (Physics Hochhaus)

Institute for **Q**uantum **M**aterials & **T**echnologies



- 8 Departments

ca. 115 employees (2022)

- Strong Theory-Exp. collaborations
- Development of novel quantum materials
- Functionalization
- Devices for quantum technologies
- Buiding blocs for quantum computers

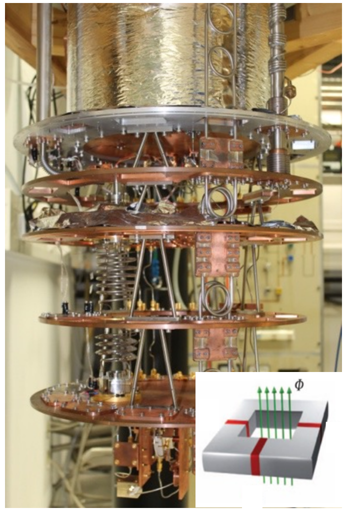
Physikalisches Institut

Karlsruhe Institute of Technology

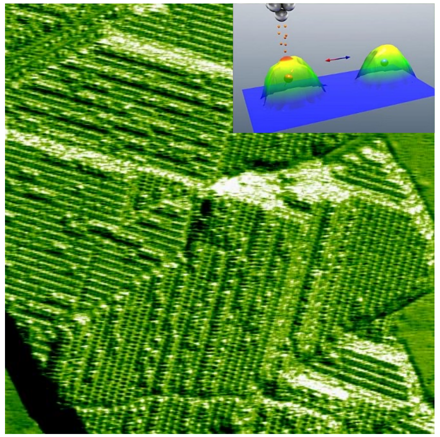
Focus

- Recent Topics in Solid State Physics
- Microscopic Quantum Systems
- Low Temperatures
- Quantum computing and quantum sensors

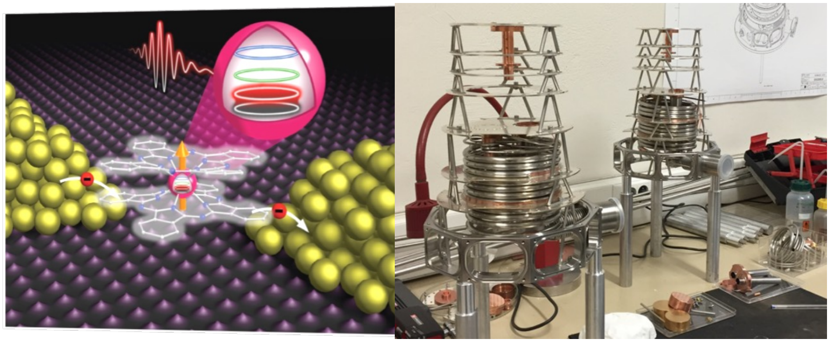
AG Ustinov: Superconducting quantum circuits



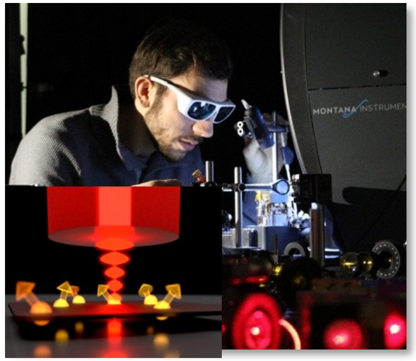
AG Wulfhekel: Scanning Tunneling Microscopy



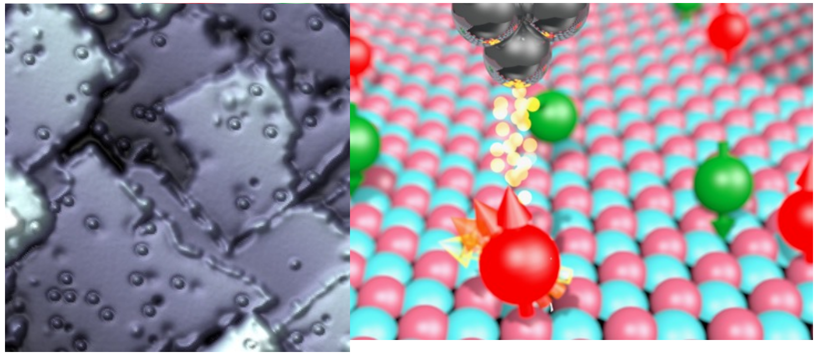
AG Wernsdorfer: Molecular Quantum Spintronics



AG Hunger: Quantum Optics



AG Willke: Control of Atomic Quantum Systems



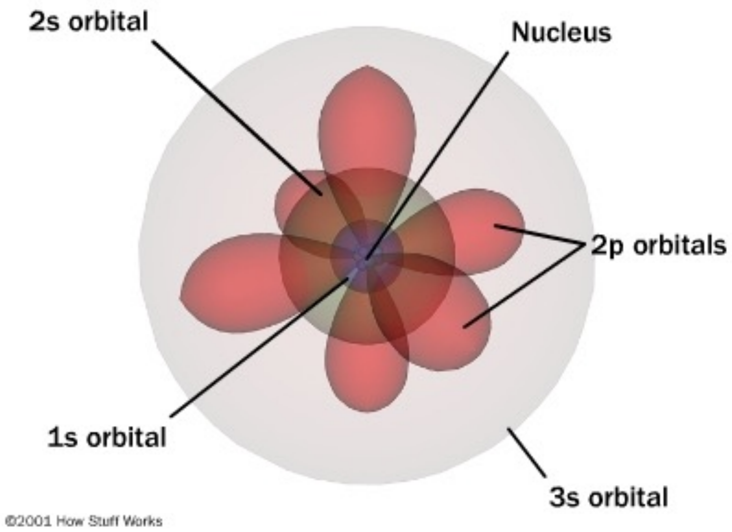
An inspiring quote to start with…

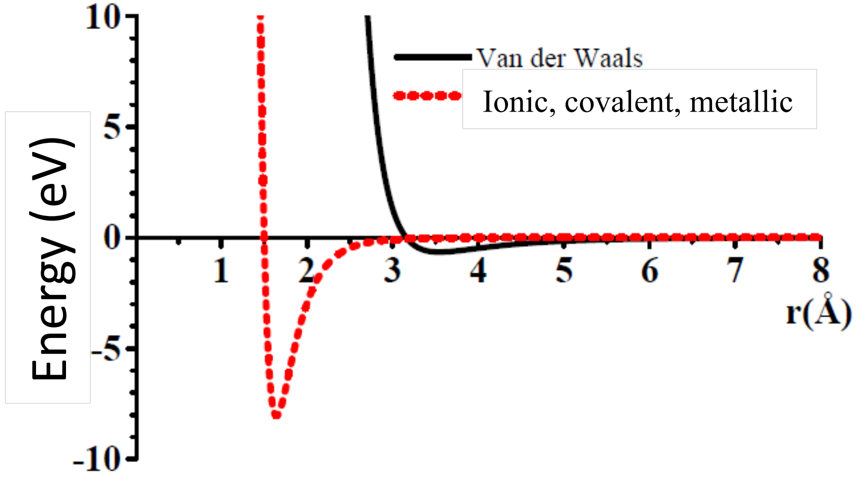
´The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved.´

— Paul A. M. Dirac

'Quantum Mechanics of Many-Electron Systems', *Proceedings of the Royal Society* (1929), A, **123**, 714-733.

From the atomic building block…





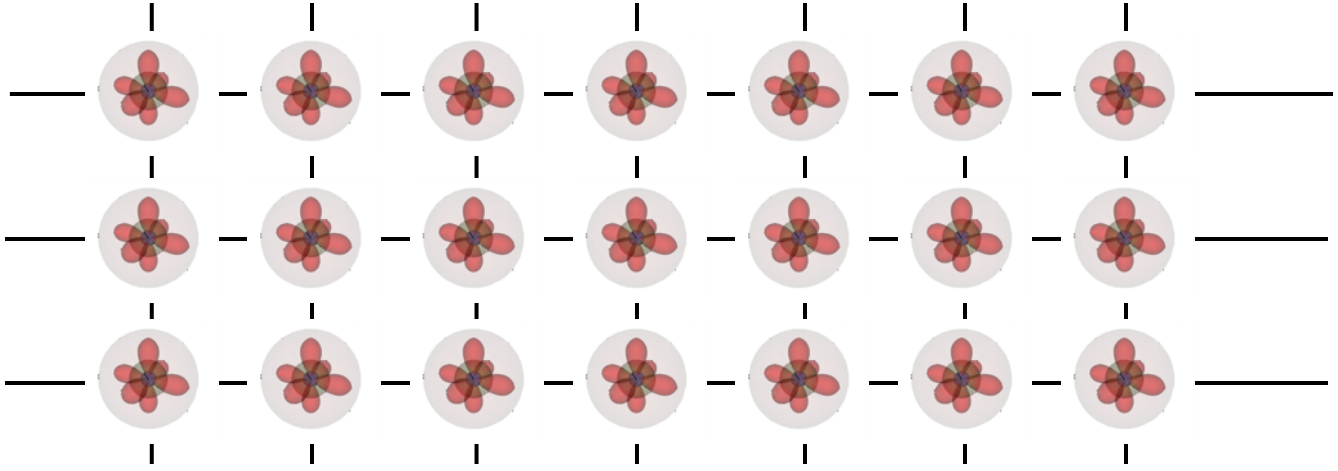
- Nucleus : charge *Ze* + mass
  spin ***I*** (*magnetic moment* $\boldsymbol{M_I} = -g\mu_N \boldsymbol{I}$)

- Electrons : charge *e*
  spin ***S*** (*magnetic moment* $\boldsymbol{M_S} = -g\mu_B \boldsymbol{S}$)

$$\mu_B = \frac{e\hbar}{2m_e}$$

$$\mu_N = \frac{e\hbar}{2M} \ll \mu_B$$

… to the solid



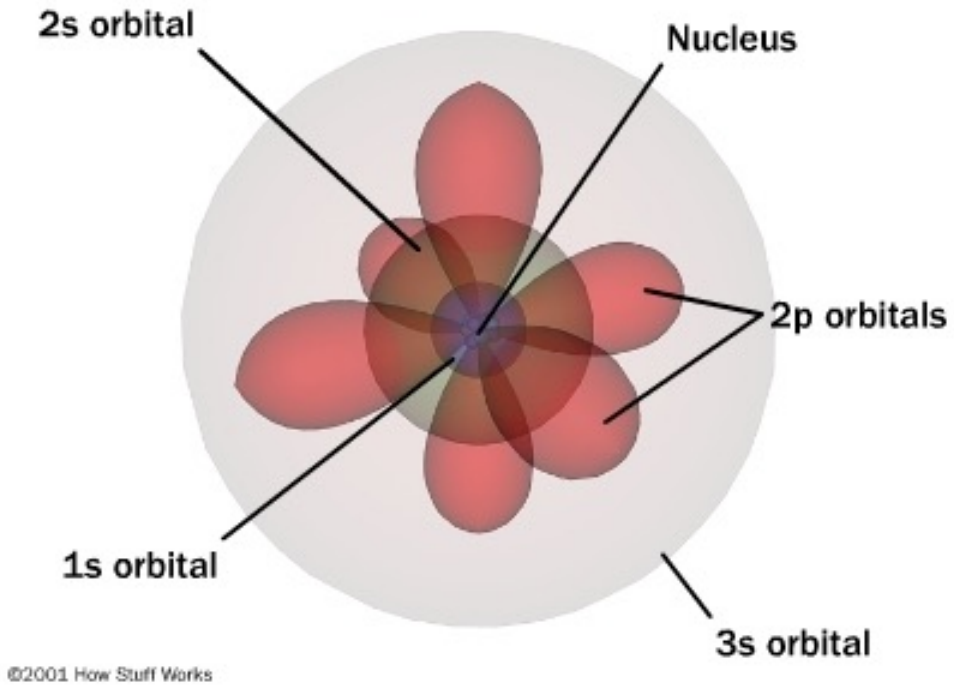
PHYSICAL REVIEW D VOLUME 28, NUMBER 12 15 DECEMBER 1983

Wave function of the Universe

J. B. Hartle
Enrico Fermi Institute, University of Chicago, Chicago, Illinois 60637
and Institute for Theoretical Physics, University of California, Santa Barbara, California 93106

S. W. Hawking
Department of Applied Mathematics and Theoretical Physics, Silver Street, Cambridge, England
and Institute for Theoretical Physics, University of California, Santa Barbara, California 93106
(Received 29 July 1983)

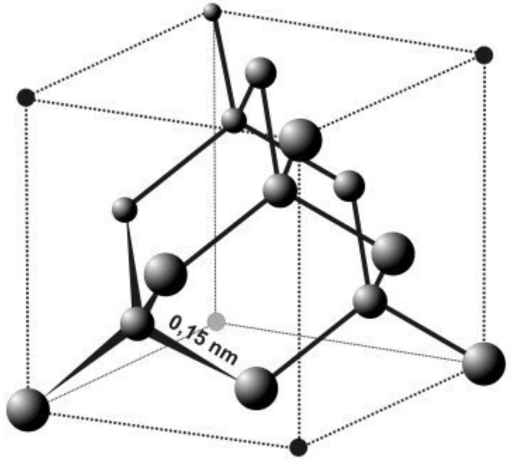
Solve Schrödinger equation: $\mathcal{H}|\psi\rangle = E|\psi\rangle$ $\psi(\boldsymbol{r}_1 \dots \boldsymbol{r}_N, \boldsymbol{R}_1 \dots \boldsymbol{R}_{N'})$ with $N, N' \sim 10^{23}$

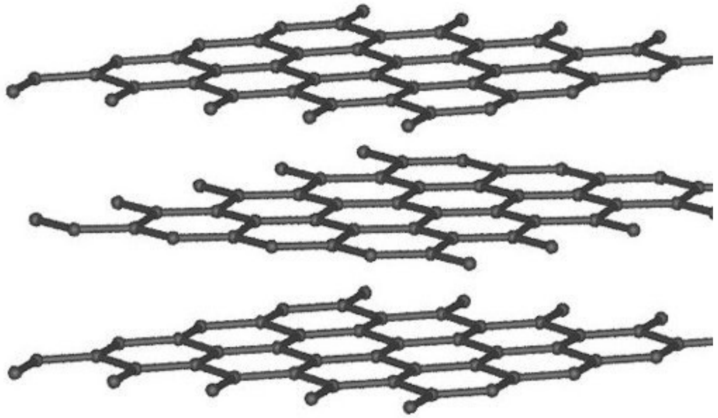


e.g. Carbon (Z=6)

$1s^2 2s^2 2p^2$

Two very different objects made out of C only!





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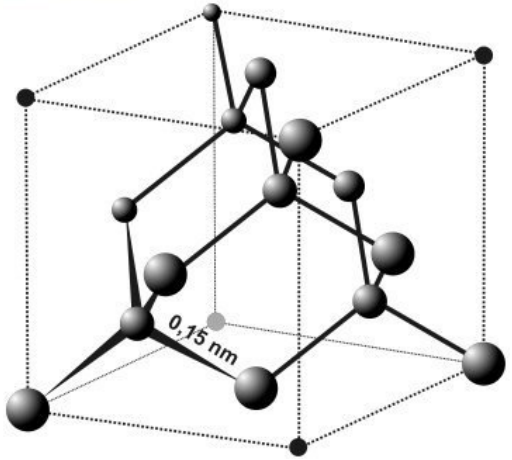
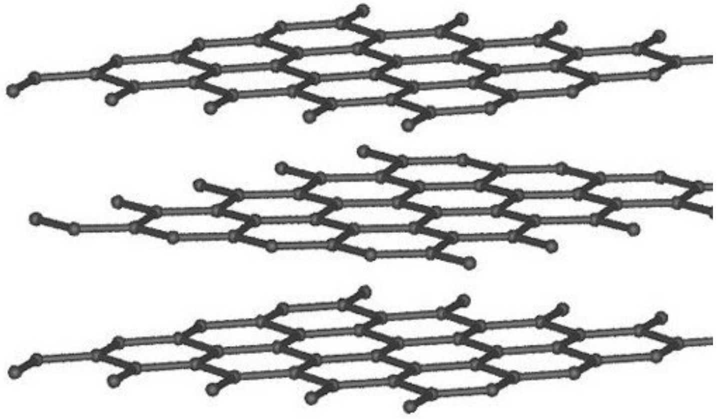
Very different:
- Mechanical properties
  (very hard against friable)
- Electronic properties
  (insulating vs metallish)
- Optical properties
  (Transparent vs opaque)

etc…

Nothing in the electronic structure of isolated Carbon atoms to account for these differences

Two very different objects made out of C only!





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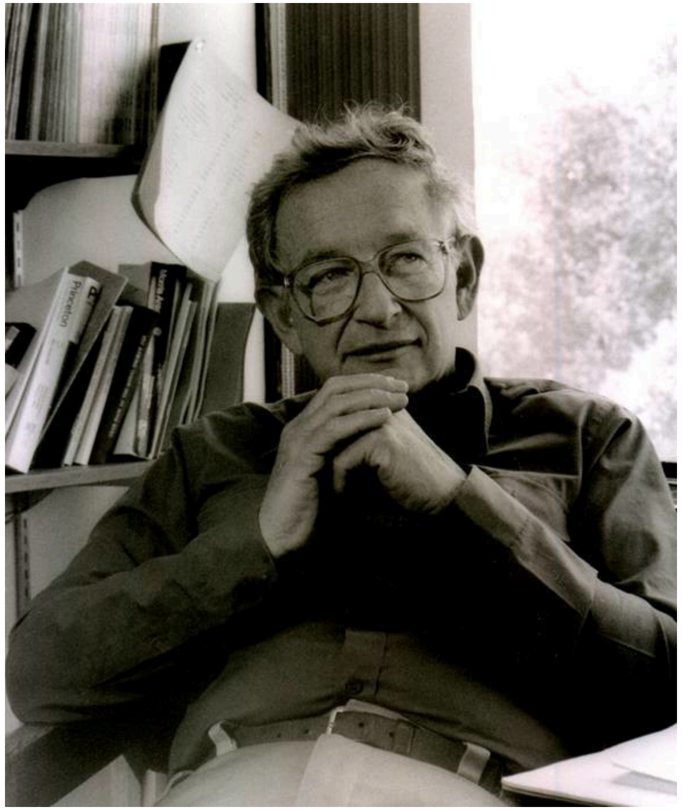

PW Anderson (1923 – 2020)
Nobel 1972

Back to Carbon compounds: Which is which?

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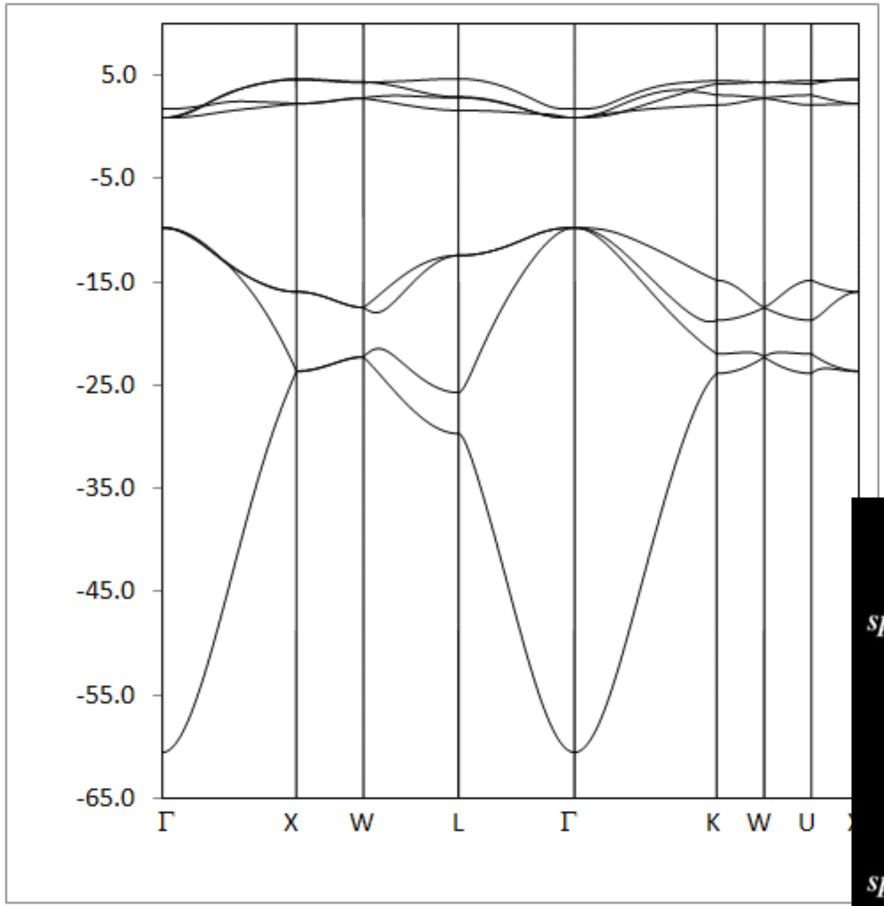
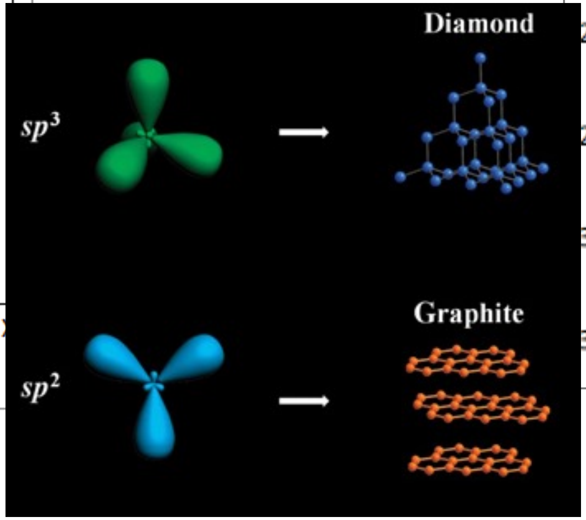
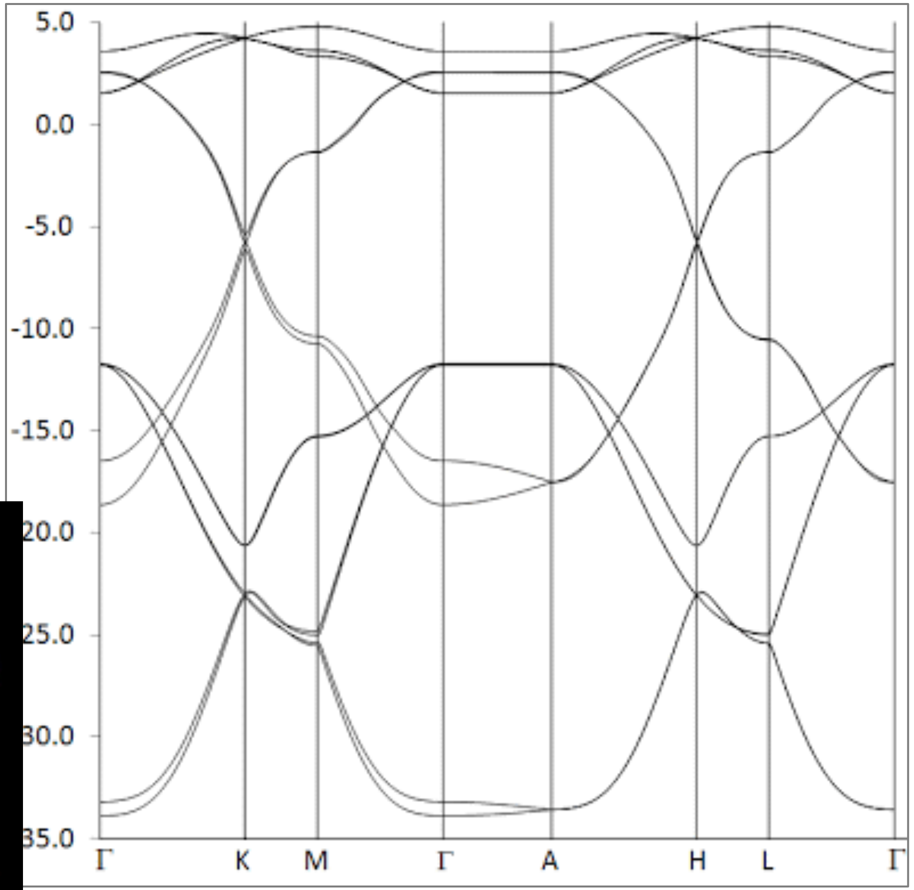


$1s^2 2s^2 2p^2$

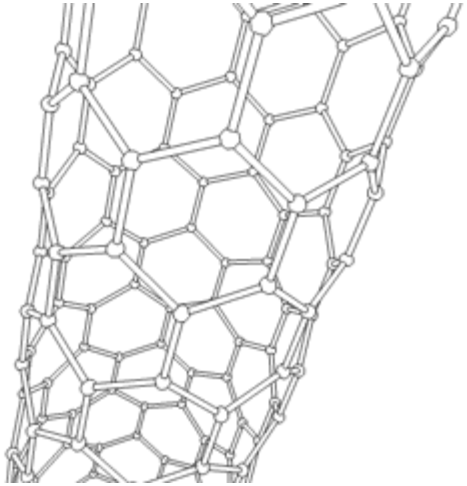




http://openmopac.net/

Other ‘C-only’ materials…

Nanotubes



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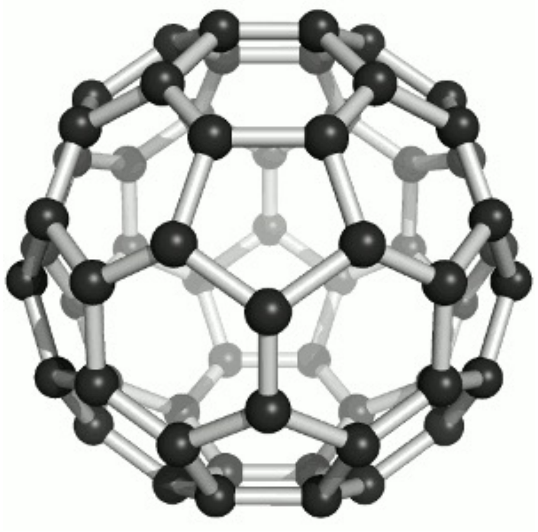
Fullerenes



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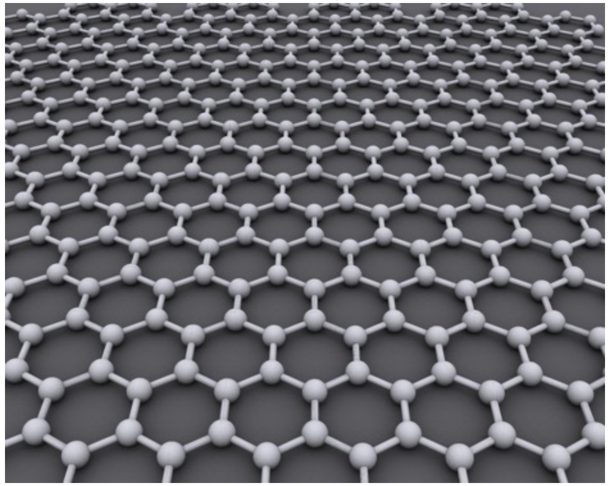
Graphene



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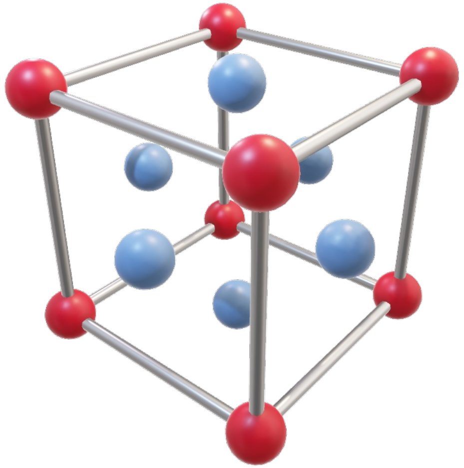
… that all have properties very different from that of diamond or graphite

Physics of electrons in Condensed Matter

Karlsruhe Institute of Technology



Vacuum	Gas	Liquid	Solids

Density of particles →

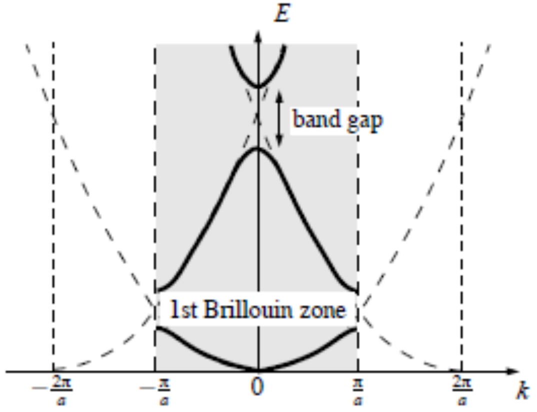
Band Insulator	Semiconductor	Metals	
	No/little interactions between particles	interactions between particles	Instabilities and new electronic phases

Condensed Matter Hamiltonian

Objective:
Understand and predict the physical properties of materials

Approach #1: Effective 'low-energy' Model

What are the relevant physical ingredients required to capture the important physics of the system?

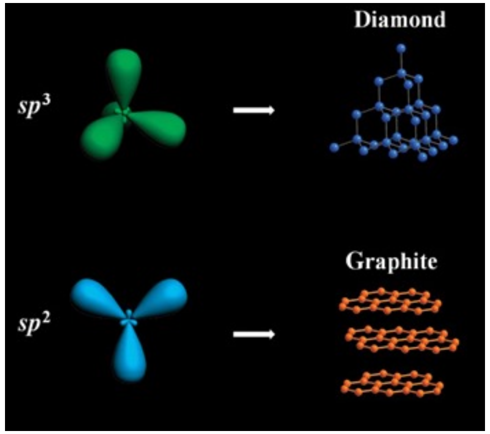


- Free electrons $\mathcal{H} = \sum_i \frac{\boldsymbol{p}_i{}^2}{2m_i}$ + scattering (Drude) + Fermi-Dirac statistic (Sommerfeld)

- Electrons in a weak periodic potential

$$\mathcal{H} = \sum_i \frac{\boldsymbol{p}_i{}^2}{2m_i} + V(\boldsymbol{r}_i)$$

- Tight binding models (LCAO), variational approaches etc…



Condensed Matter Hamiltonian

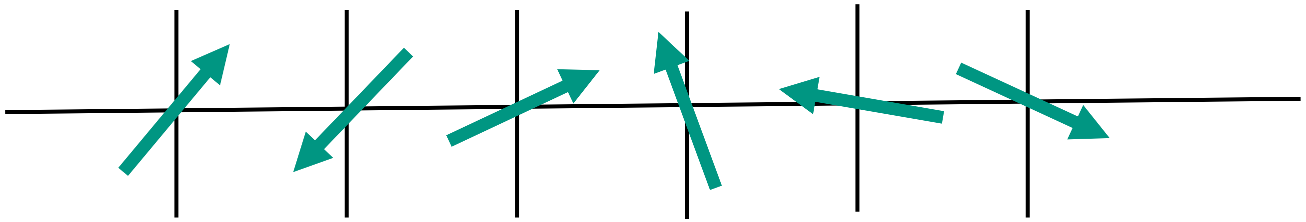
Objective:
Understand and predict the physical properties of materials

Approach #1: Effective 'low-energy' Model

What are the relevant physical ingredients required to capture the important physics of the system?

Other example to deal with magnetic degrees of freedom only

- Magnetism (e.g. Heisenberg Model) $\mathcal{H} = \sum_{i,j} J_{i,j}\, \boldsymbol{S}_i . \boldsymbol{S}_j$



Condensed Matter Hamiltonian

Objective:
Understand and Predict the physical properties of Materials

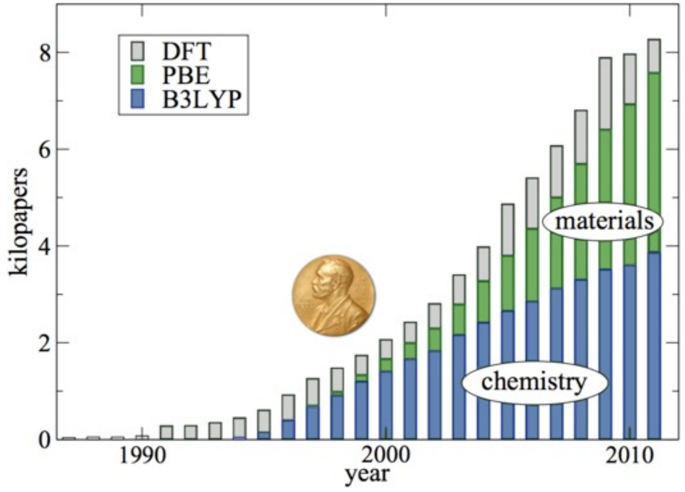
Approach #2: ab-initio [Density Functional Theory + approx.]
Calculates the ground-state from first principles

$$\psi(\boldsymbol{r}_1 \dots \boldsymbol{r}_N, \boldsymbol{R}_1 \dots \boldsymbol{R}_{N'}) \rightarrow \psi[n(\boldsymbol{r})] \qquad E = |\langle\psi|\mathcal{H}|\psi\rangle|$$

'Trick': find a good approximation to estimate $n(\boldsymbol{r})$

Advice to the interested:
https://www.nobelprize.org/nobel_prizes/chemistry/laureates/1998/kohn-lecture.pdf

https://arxiv.org/pdf/1201.3679.pdf



Condensed Matter Hamiltonian

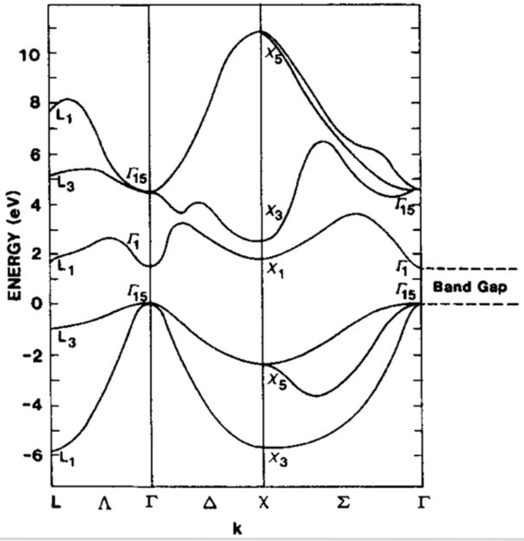
Objective:
Understand and Predict the physical properties of Materials

Approach #2: ab-initio [Density Functional Theory + approx.]

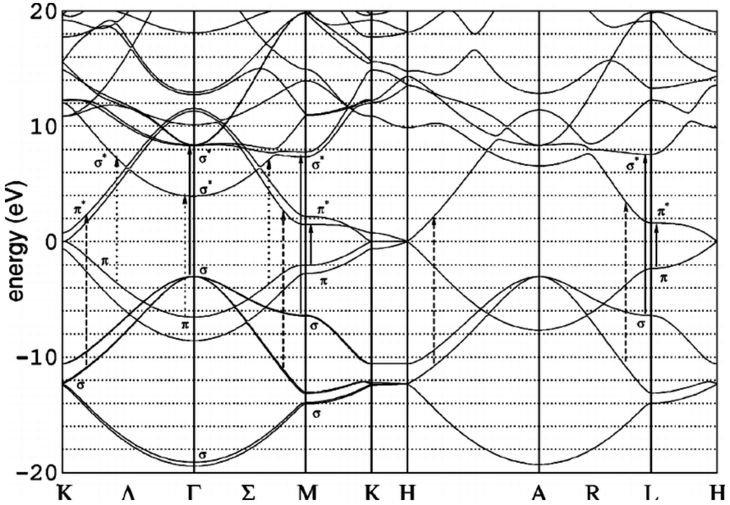
Calculates the ground-state from first principles

very successful (Crystal & Electronic structures, Dynamics) !

Diamond



Graphite



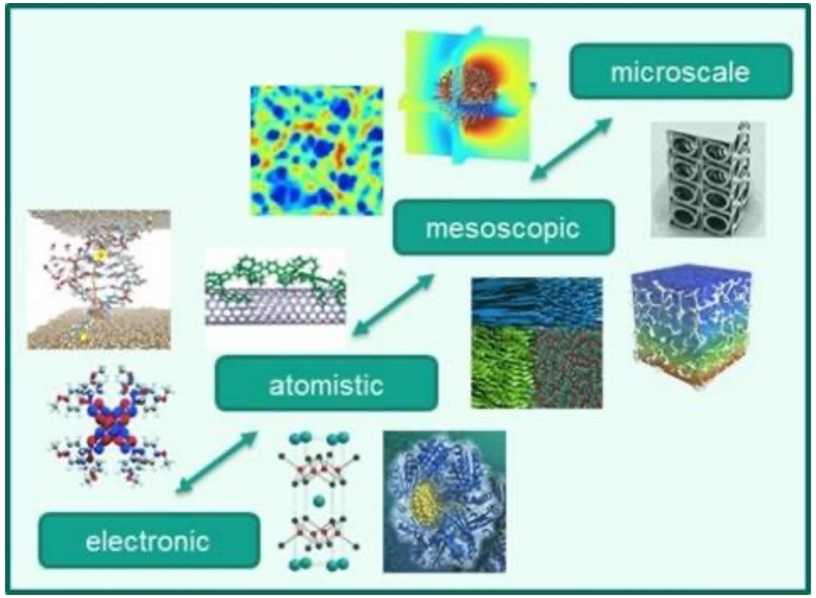
Condensed Matter Hamiltonian

Objective:
Understand and Predict the physical properties of Materials

Approach #2: ab-initio [Density Functional Theory + approx.]

Calculates the ground-state from first principles
very successful (Crystal & Electronic structures, Dynamics)!

Towards the design of novel materials with tailored electronic properties



Joint Laboratory Virtual Materials Design
Coordinator: W. Wenzel

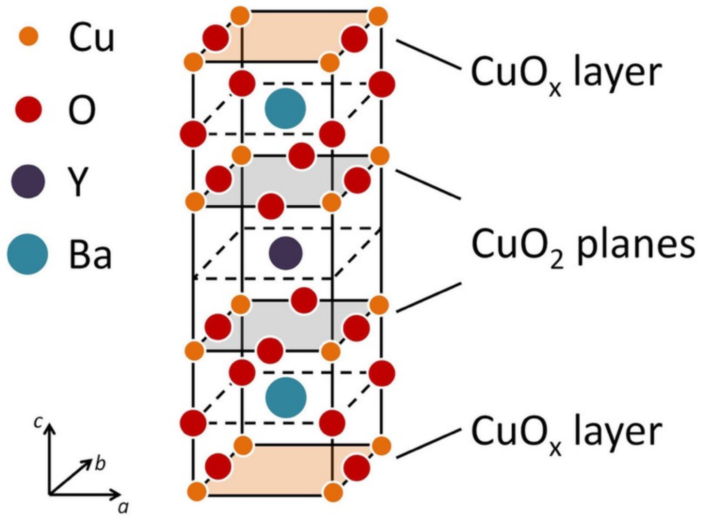
Condensed Matter Hamiltonian

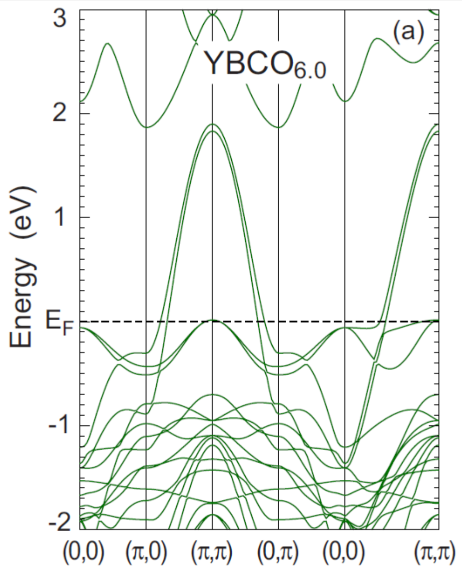
Karlsruhe Institute of Technology

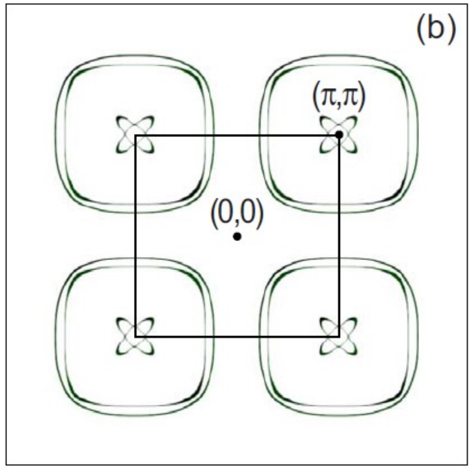
Objective:
Understand and Predict the physical properties of Materials

Approach #2: ab-initio [Density Functional Theory + approx.]
Calculates the ground-state from first principles
very successful **but** hard with some interactions e.g. strong Coulomb repulsion between electrons

A Nobelprize-worth fail:
Electronic Structure of $YBa_2Cu_3O_6$

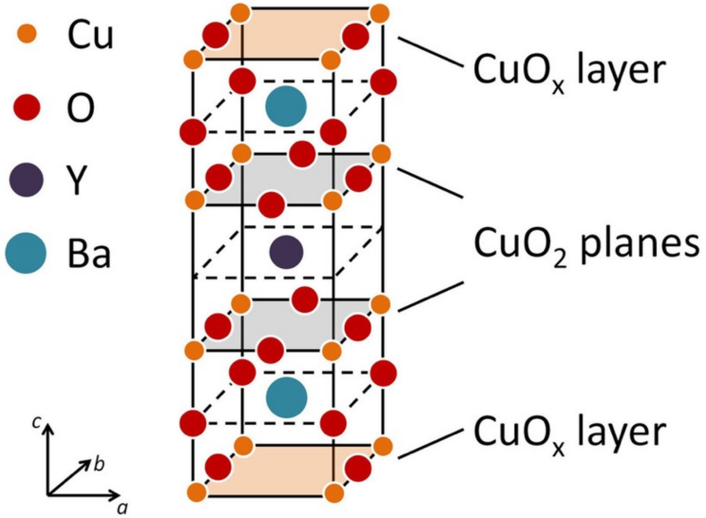


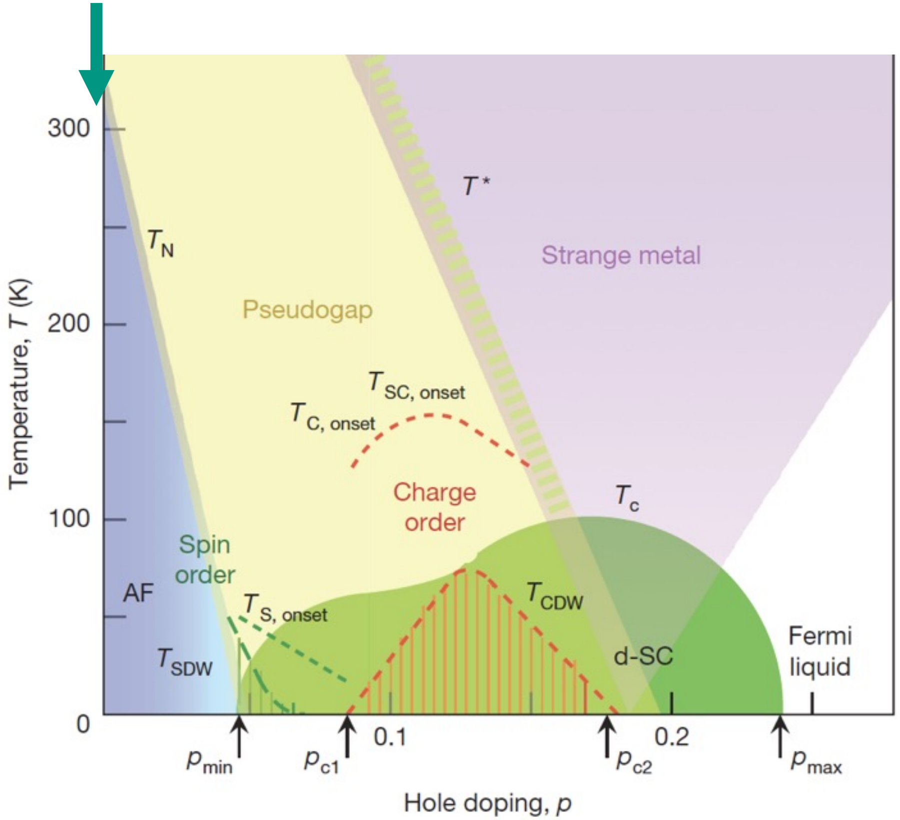




Eflimov et al. PRB **77** R060504 (2008)

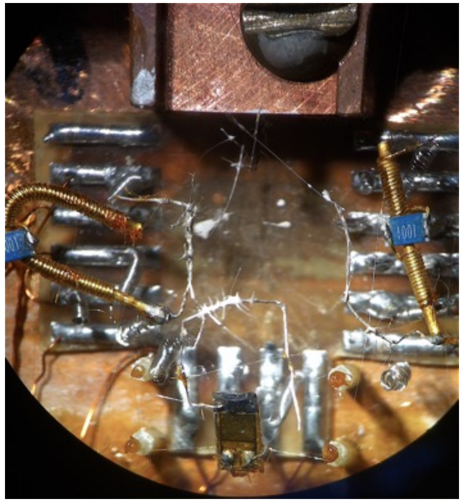
$YBa_2Cu_3O_6$ is in fact a *magnetic Insulator*





Biased Conclusion #1:

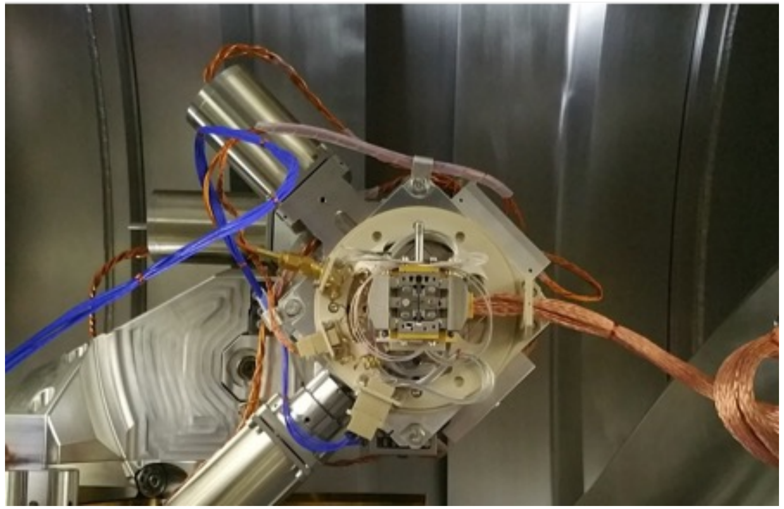
This is physics - Theory is good, but **in the end Experiment wins**

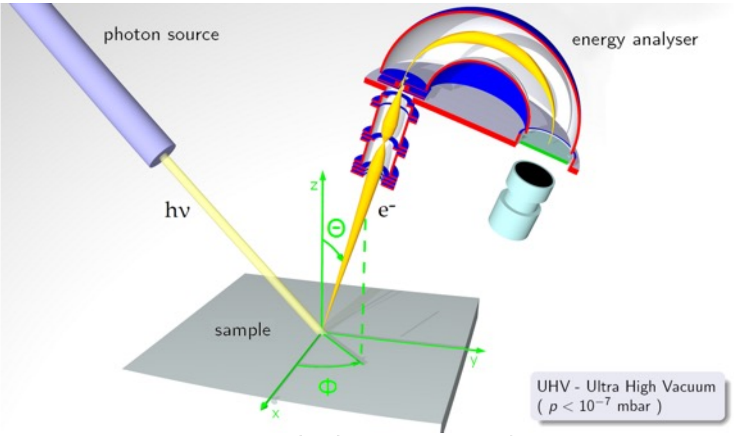


B. Michon, PhD Thesis

www.vulgarisation.fr

https://horizon-magazine.eu/





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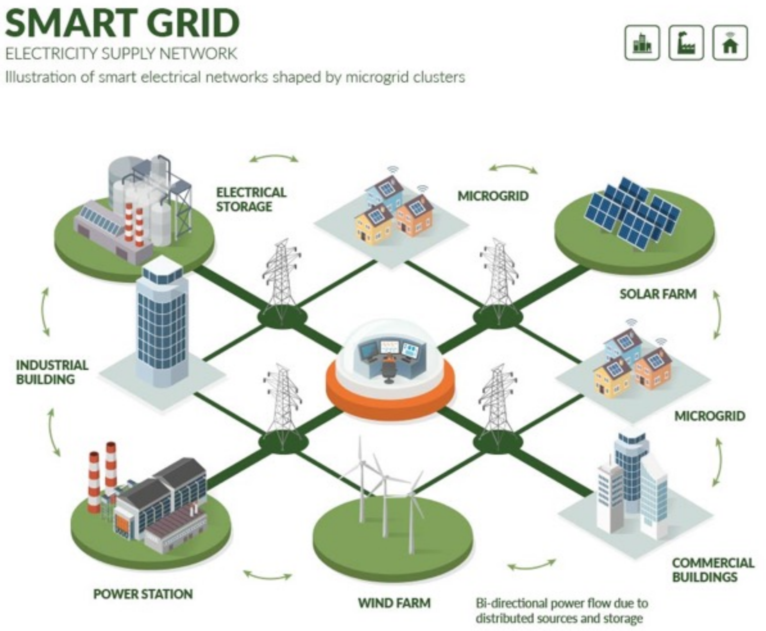
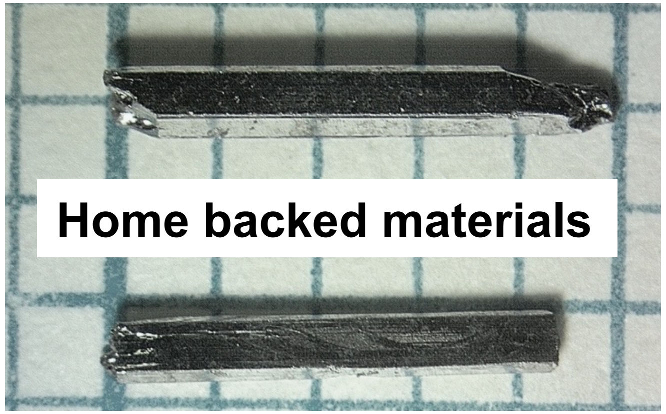
Why do we do all this?



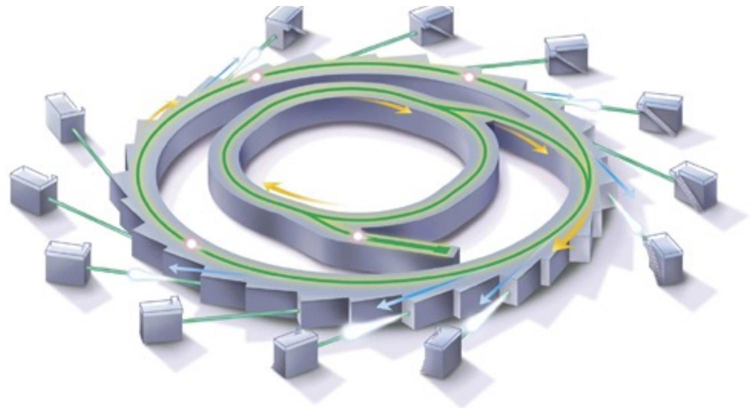
1) Because our technological world relies deeply on electronic properties of solids

2) Because it is **FUN**



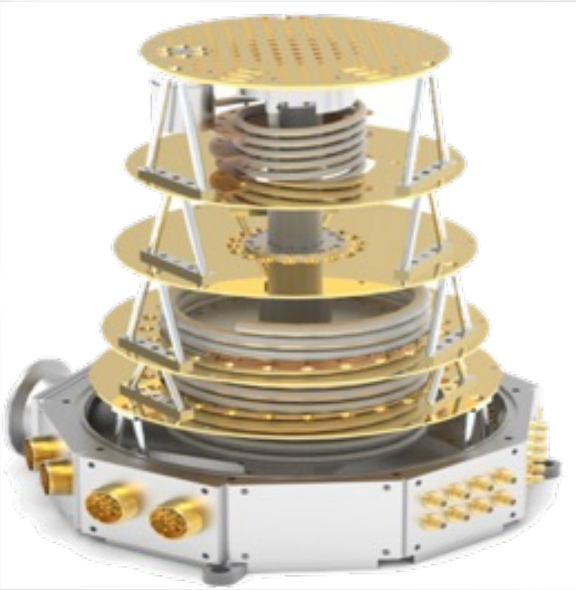
A. Haghighirad

Brightest Light/x-ray Sources



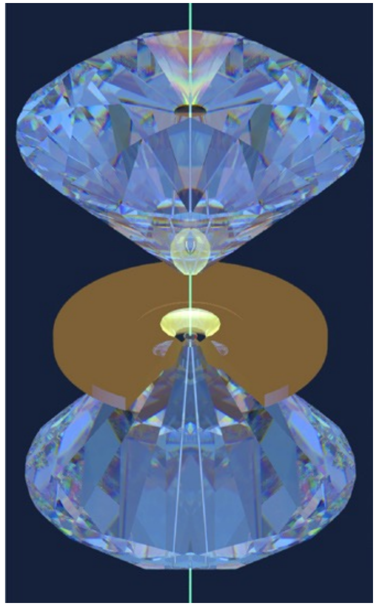
http://www.synchrotron.org.au/images/stories/beamline_illustation.jpg

Temperatures colder than Anything available in the universe



Large Magnetic fields

Extreme Pressures



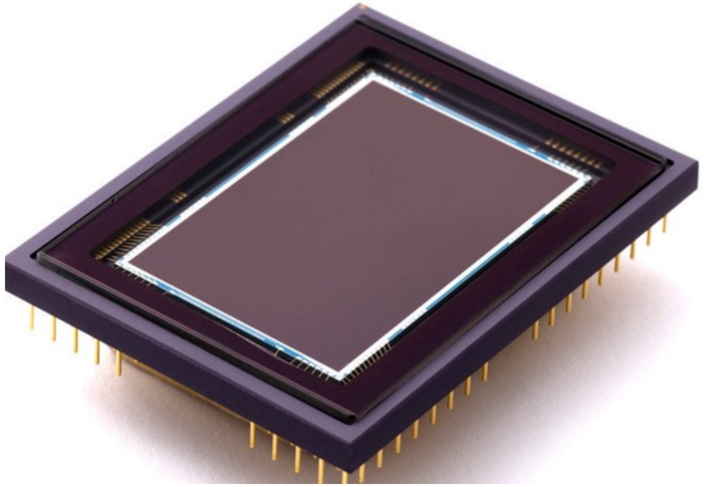
New electronic properties

The Nobel Prize in Physics 2007

Photo: U. Montan
Albert Fert
Prize share: 1/2

Photo: U. Montan
Peter Grünberg
Prize share: 1/2

The Nobel Prize in Physics 2007 was awarded jointly to Albert Fert and Peter Grünberg *"for the discovery of Giant Magnetoresistance"*



The Nobel Prize in Physics 2009

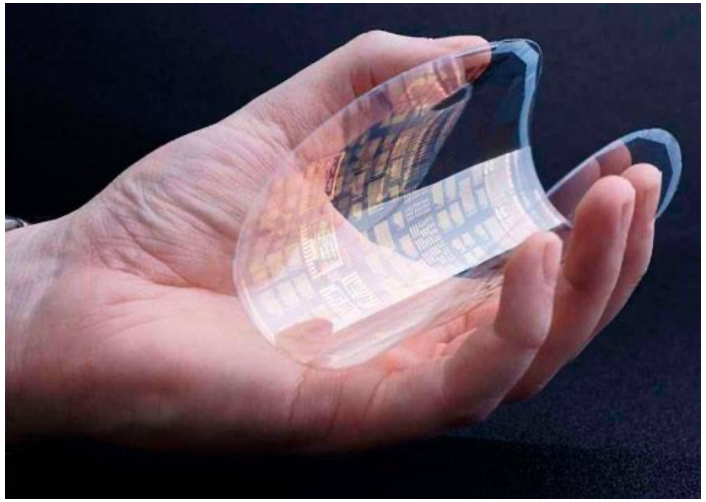
Photo: U. Montan
Charles Kuen Kao
Prize share: 1/2

Photo: U. Montan
Willard S. Boyle
Prize share: 1/4

Photo: U. Montan
George E. Smith
Prize share: 1/4

The Nobel Prize in Physics 2009 was divided, one half awarded to Charles Kuen Kao *"for groundbreaking achievements concerning the transmission of light in fibers for optical communication"*, the other half jointly to Willard S. Boyle and George E. Smith *"for the invention of an imaging semiconductor circuit - the CCD sensor"*.

New electronic properties

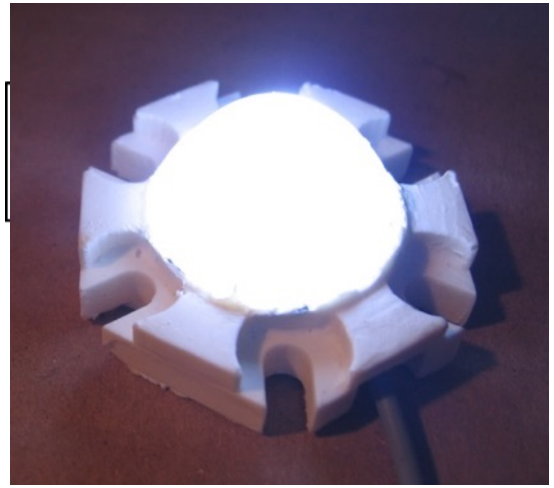


The Nobel Prize in Physics 2010

Photo: U. Montan
Andre Geim
Prize share: 1/2

Photo: U. Montan
Konstantin Novoselov
Prize share: 1/2

The Nobel Prize in Physics 2010 was awarded jointly to Andre Geim and Konstantin Novoselov *"for groundbreaking experiments regarding the two-dimensional material graphene"*



The Nobel Prize in Physics 2014

Isamu Akasaki, Hiroshi Amano and Shuji Nakamura

"for the invention of efficient blue light-emitting diodes which has enabled bright and energy-saving white light sources"

The Nobel Prize in Physics 2016

© Trinity Hall, Cambridge University. Photo: Kiloran Howard

David J. Thouless

Prize share: 1/2

Photo: Princeton University, Comms. Office, D. Applewhite

F. Duncan M. Haldane

Prize share: 1/4

Ill: N. Elmehed. © Nobel Media 2016

J. Michael Kosterlitz

Prize share: 1/4

The Nobel Prize in Physics 2016 was divided, one half awarded to David J. Thouless, the other half jointly to F. Duncan M. Haldane and J. Michael Kosterlitz *"for theoretical discoveries of topological phase transitions and topological phases of matter"*.

… all of this has to do with the way electron behave in materials

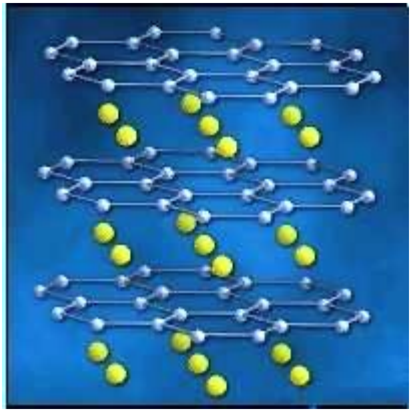
(Biased) Conclusion #2:

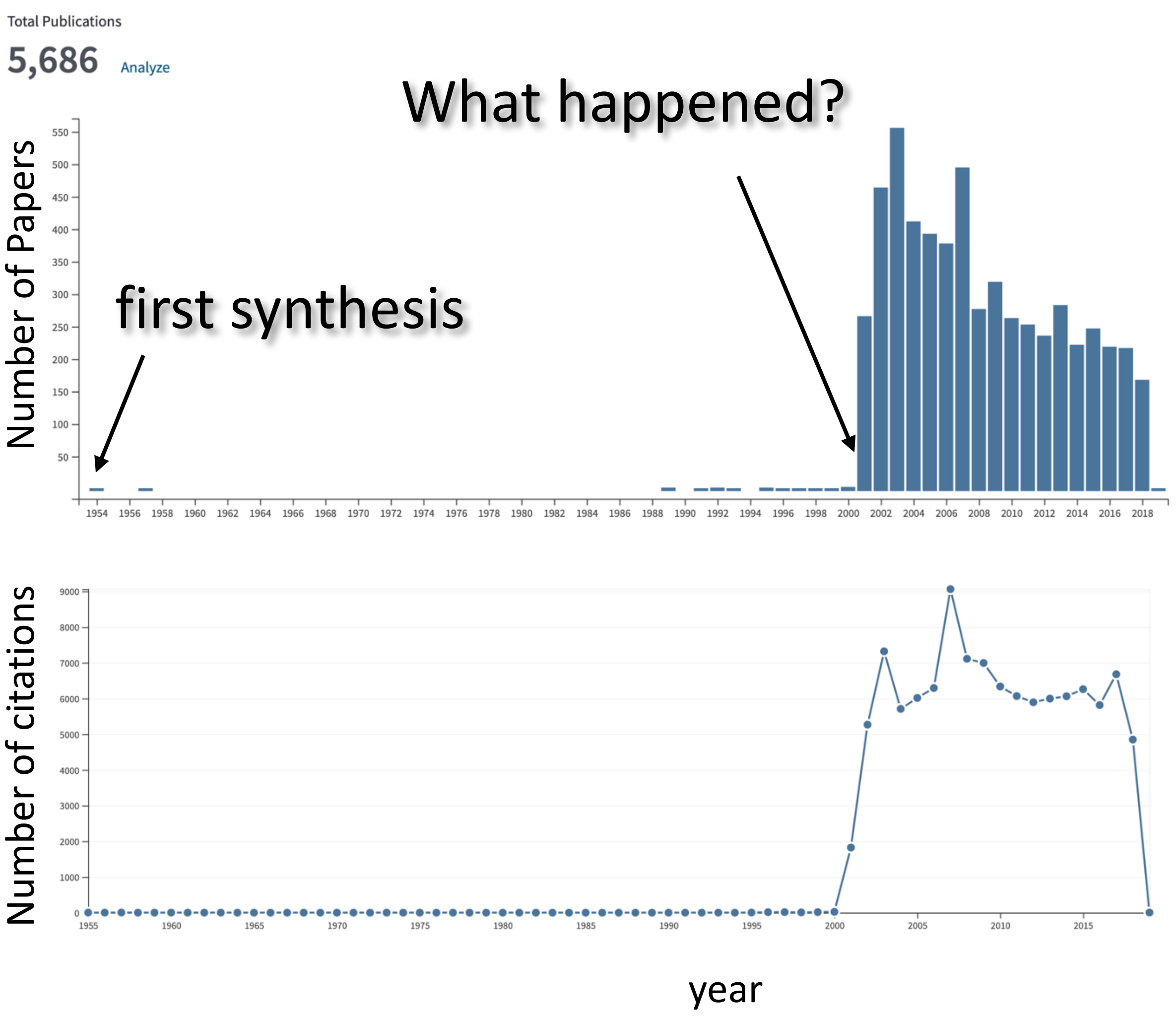
Original physical properties are game changer and **always** yield useful applications

Electronic Properties of Solids

New materials:
synthesis/design

MgB_2

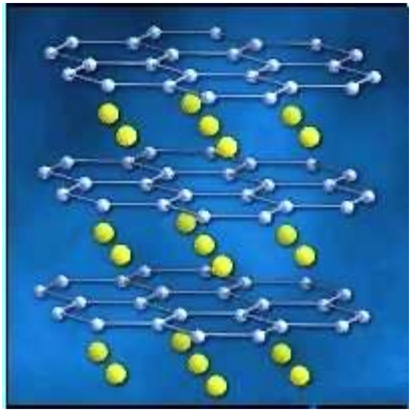




Electronic Properties of Solids

New materials: synthesis/design

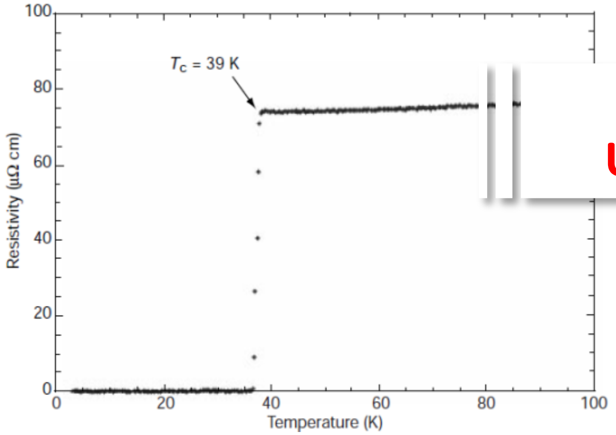
MgB_2



Original Physical Properties

Superconductivity at 39 K in magnesium diboride

Jun Nagamatsu*, Norimasa Nakagawa*, Takahiro Muranaka*, Yuji Zenitani* & Jun Akimitsu*†



Nature **410**, 63 (2001)

Quantitative Understanding

Technological applications

…en The MRI 0.5T cryogenic free magnet

… transport of green power: First successful testing … 20 kA superconducting cable

Electronic Properties of Solids

Karlsruhe Institute of Technology

Crystal/Magnetic Structure
x-ray /Neutrons

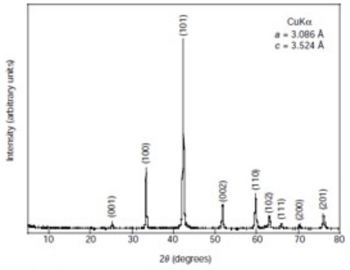
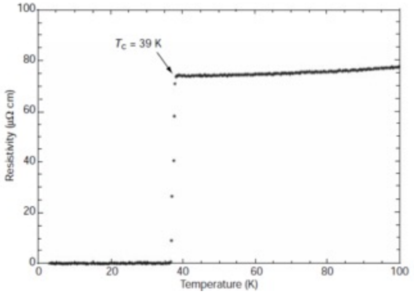


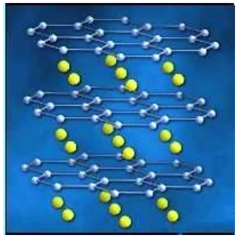
Figure 1 X-ray diffraction pattern of MgB_2 at room temperature.

Nagamatsu et al.
Nature **410**, 63 (2001)

Transport (U = R I)

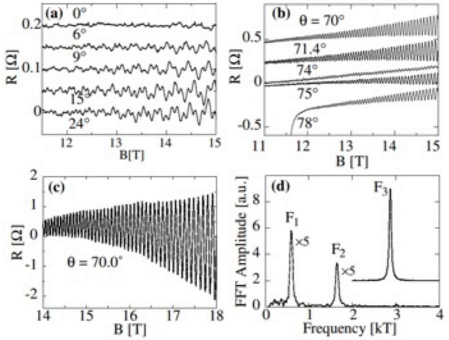


MgB_2

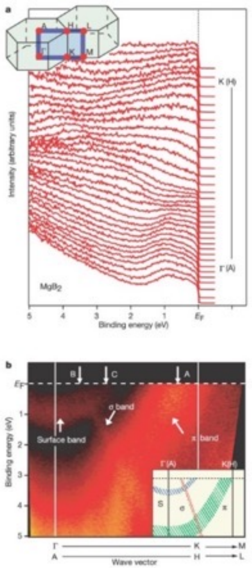


Electronic Structure
Quantum Oscillations

ARPES

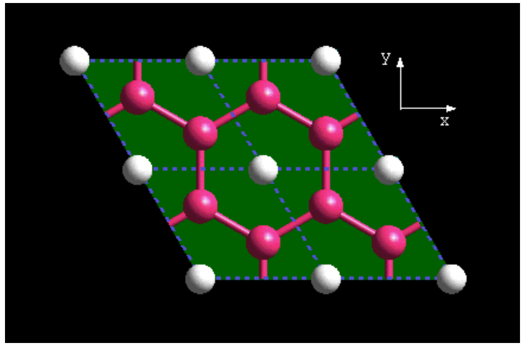


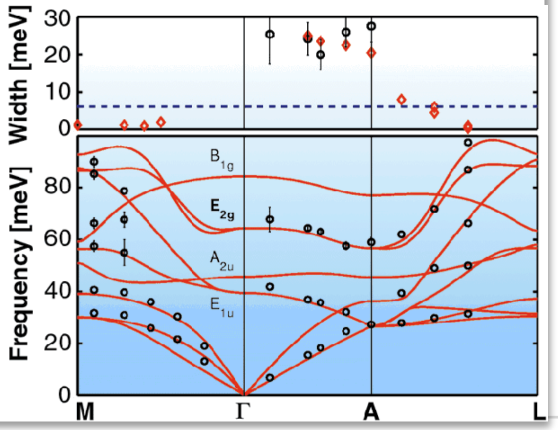
Yelland et al.
PRL **88**, 217002 (2002)



Souma et al.
Nature **423** 65(2003)

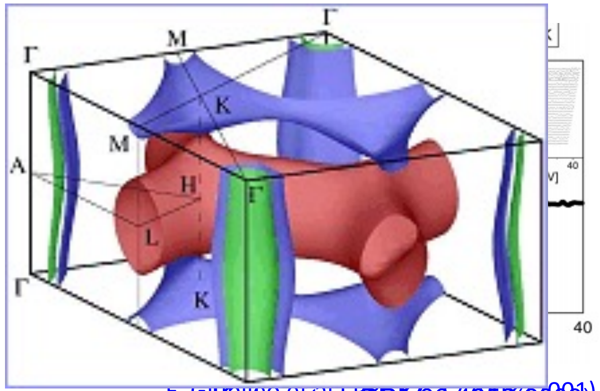
Dynamical properties
Charge electrodynamics: optics
Phonon (lattice vibrations): optics, Raman, INS, IXS.





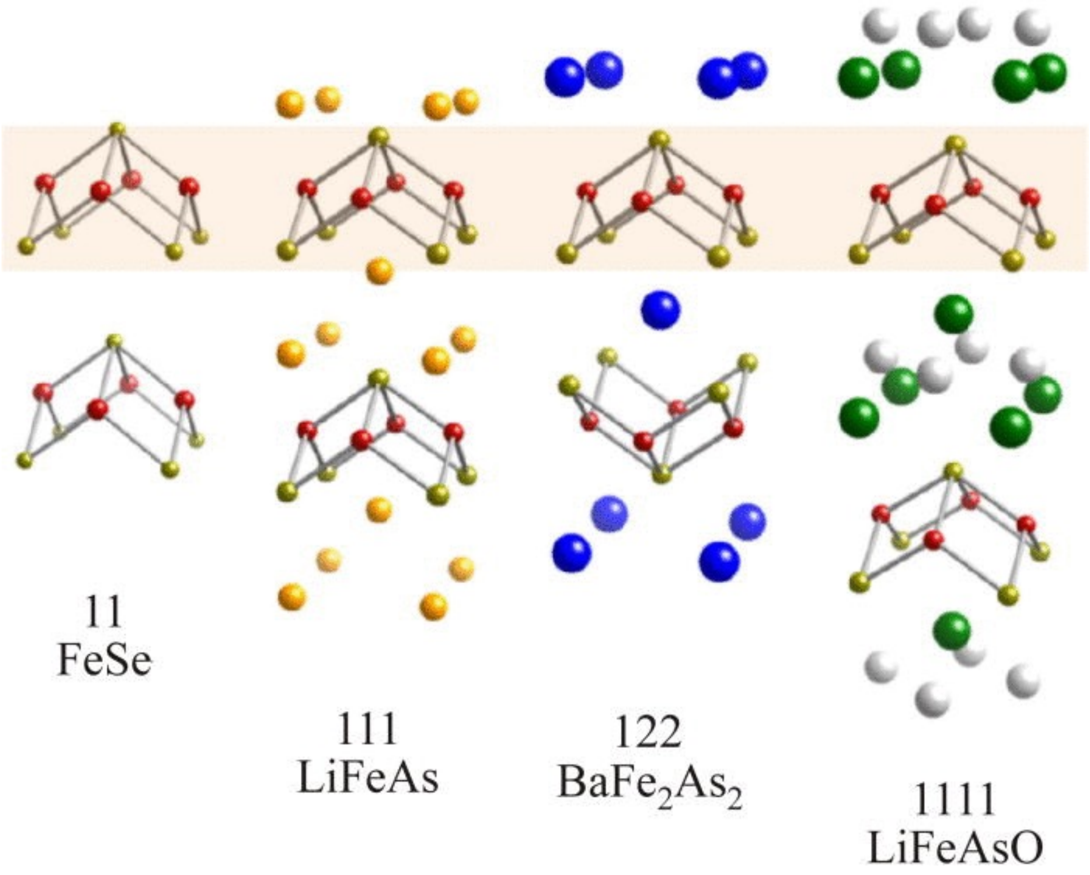
Shukla, et al. PRL 90, 095506 (2003)

Ab-initio Calculations



Kortus et al. PRL 86 4656(2003)

Fe-based superconductors (discovery 2008)



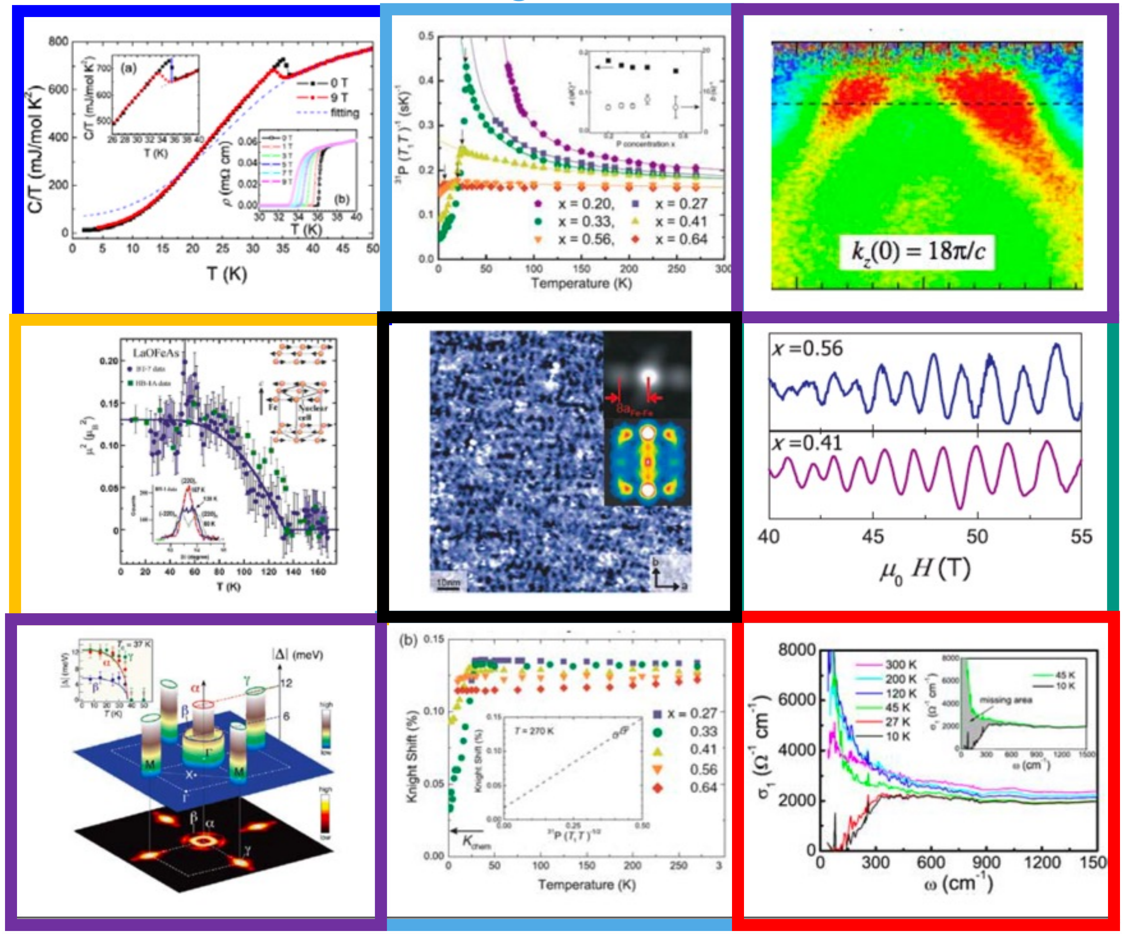
Fe-based superconductors (discovered 2008)

Nuclear Magnetic Resonance

Specific heat

Magnetic Neutron Diffraction

Angle-Resolved Photoemission



Scanning Tunneling Microscope

Quantum Oscillations

Optical Conductivity

From J. Bobroff

Mesurer les proprétés électroniques des solides

Electronic Transport (MLT ~ 10 Lectures)

Electrons in metals

- Revision: Bloch model and band structure
- Boltzman Equation
- Scattering mechanisms
- Magnetotransport
- Experimental determination of the Fermi Surfaces (quantum oscillations, ARPES)

Phase transitions (MLT ~ 4 Lectures)

Generalities and Landau Theory of phase transitions

- Landau Free energy
- Order parameters
- Critical exponents

Application: Charge Density Wave Instabilities in metals

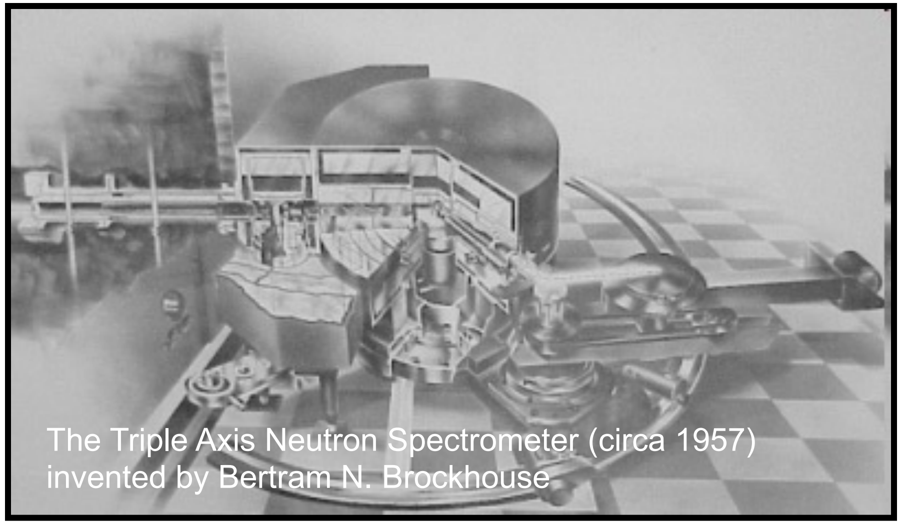
Magnetism (P. Willke – 14 lectures)

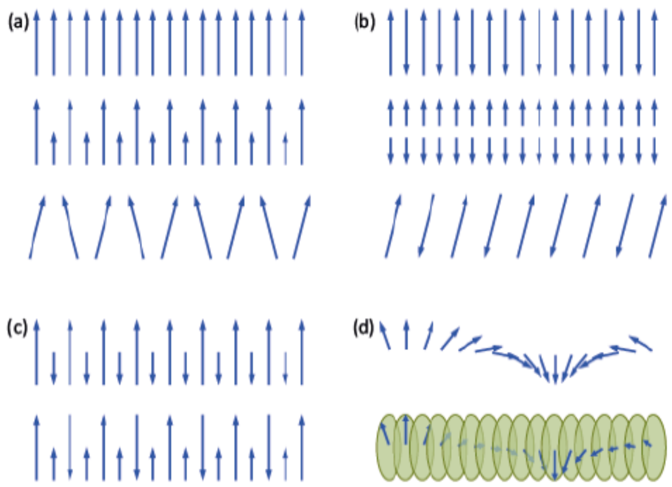
1) **Atomic origin of magnetism**
   - Hund´s rules
   - Crysal Field
   - 3d and 4f elements
   - Magnetic susceptibilities

2) **Magnetic order, Magnetic insulators**
   - Magnetic interactions (dipole, exchange)
   - para-, ferro,- diamagnetism
   - Heisenberg Model
   - Goodenough-Kanamori rules

3) **Magnetic order in metals**
   - Pauli susceptibility
   - Stoner Instability
   - RKKY interaction

4) **Determination of the magnetic structures**
   - neutrons and x-ray scattering


The Triple Axis Neutron Spectrometer (circa 1957) invented by Bertram N. Brockhouse



Some good literature