Topological Insulators – in search of new materials for microelectronics/information technology

AKADEMIA GÓRNICZO-HUTNICZA IM. STANISŁAWA STASZICA W KRAKOWIE
AGH UNIVERSITY OF SCIENCE AND TECHNOLOGY

W. Tokarz , A. Kozłowski, M. Dobrzański, I. Miotkowski, Z. Kąkol,

Kraków ,19.11. 2019

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1. Topological Insulators – Conducting Insulators
   - Quantum Hall Effect
   - Topological order
   - Topological Insulators
2. Computation of Materials Properties
   (short introduction to Density Functional Theory)
   - Elementary quantum mechanics
   - Kohn-Sham equations - Kohn-Sham energy functional
   - DFT in practice: The self-consistency loop, implementation
   - Some applications of DFT

Topological Insulators – Conducting Insulators

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TOPOLOGICAL INSULATORS

- topology has nothing to do with the shape,
- insulating state is not the interesting feature.

Topological insulators – group of materials exhibiting a unique physical properties.

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TOPOLOGICAL INSULATORS - materials which:

- do not conduct current through the bulk ,
- carry current along the surface, edges,
- this current has some special properties, resulting from the quantum nature of the material.

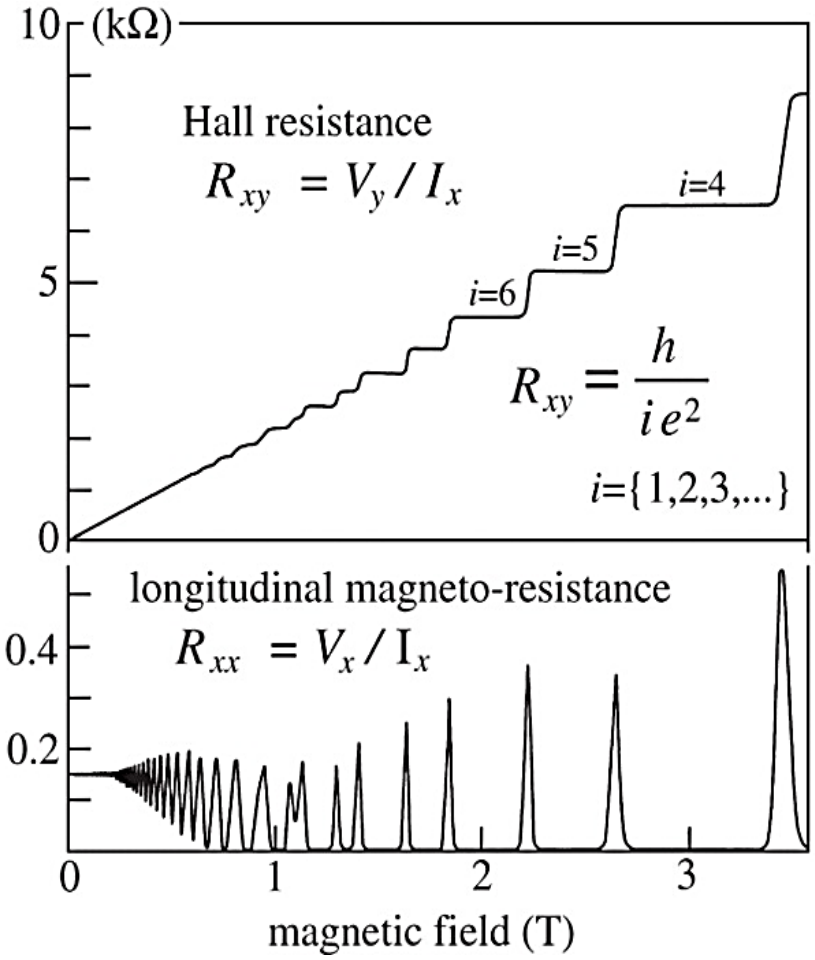
How we can make material where the electrons in the bulk are localized but the ones on the edges are itinerant?

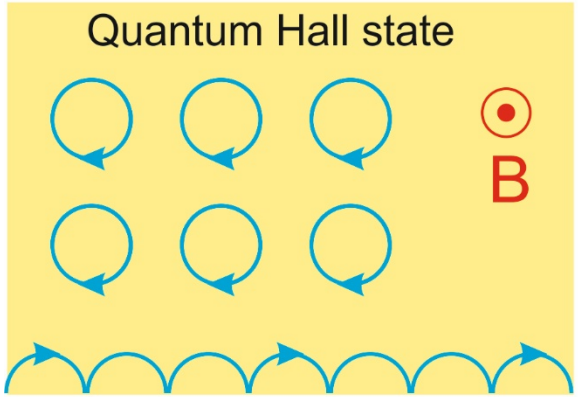
We can do it with magnetic field !

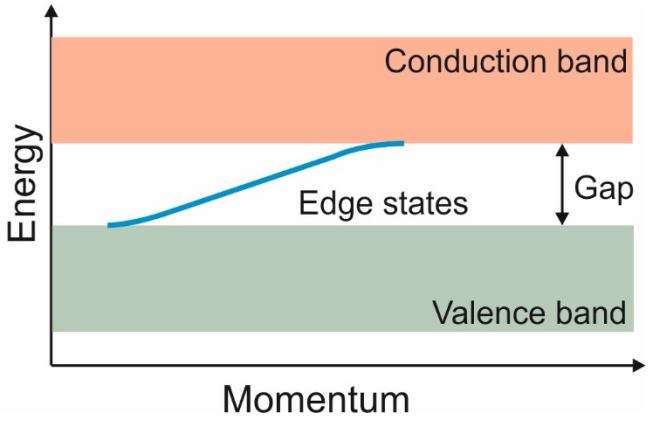
In 1980 von Klitizng found characteristic plateaus in Hall resistance vs magnetic field dependence showing that conductivity at the edge of sample is quantized.

It came as a total surprise to the physics community.

- This effect occurs in layered metals at high magnetic fields,
- Results from the formation of conducting one-dimensional channels that develop at the edges of the sample.







Weis, J. i von Klitzing, K.: 2011, Philosophical Transactions of the Royal Society of London A: Mathematical, Physical and Engineering Sciences 369(1953), 3954

- Each of these edge channels exhibits a quantized conductance that is characteristic of one-dimensional transport,
- The charge carriers in these channels are very resistant to scattering,
- Within the channels, charge carriers can be transported without energy dissipation.

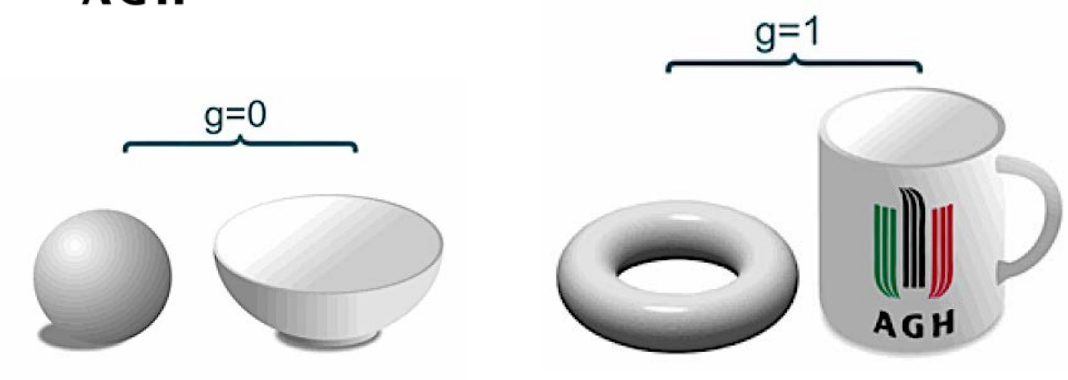
QHE was explained as resulting from topological character of band structure, showing that change in topology can cause metallic surface states to emerge.

For this discovery von Klitzing was awarded Nobel Prize in physics in 1985.

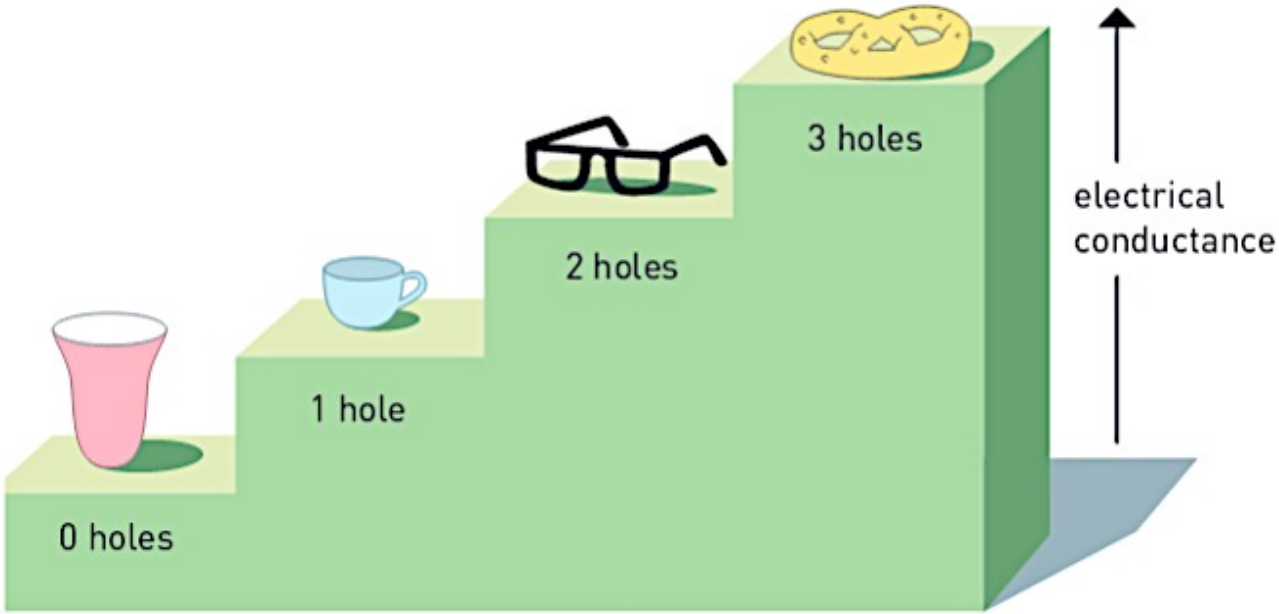
1. What is a topological phase?
   (how does topological order differs from conventional order?)
2. Can we find isolating materials, where edge conducting states are present in the absence of external magnetic field?
3. What is the physical response that characterize a topological insulator?
4. Are topological insulators useful for anything?

- Until 1980, all ordered phases could be understood as “symmetry breaking”,
- Discovery of the QHE has led to a different classification paradigm, based on the notion of topological order,
- The state responsible for the quantum Hall effect does not break any symmetries, but it defines a topological phase.

(in the sense that certain fundamental properties are insensitive to smooth changes in materials parameters and change only when the system passes through a quantum phase transition).



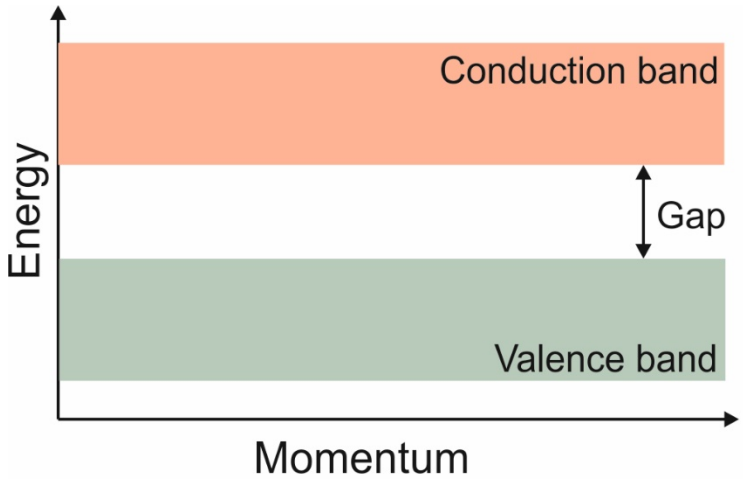
Surfaces with g=0 that cannot be continuously transferred to the surfaces with g=1

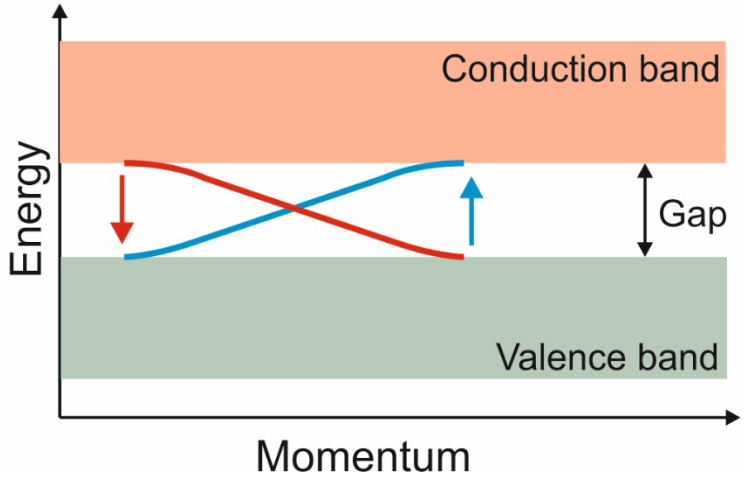


We can calculate the genus, the number distinguishing different topologies, so we can discover what topology our system belongs to.

Space of electronic states can also have different topologies.
And, in equivalence to the normal space, we see nothing strange in their electron local behavior as long as a break in topology does not occur.

Continuous change of electronic interactions is not enough to change ordinary insulator into topological insulator,





But once the topology changes, e.g. when states belonging to two different topologies meet, some strange situation may be found.

Topology of electronic states of ordinary insulator is different from those of topological insulator.

For example, if the insulator of nontrivial topology, is terminated, electronic states of different topologies meet since the vacuum topology is trivial.

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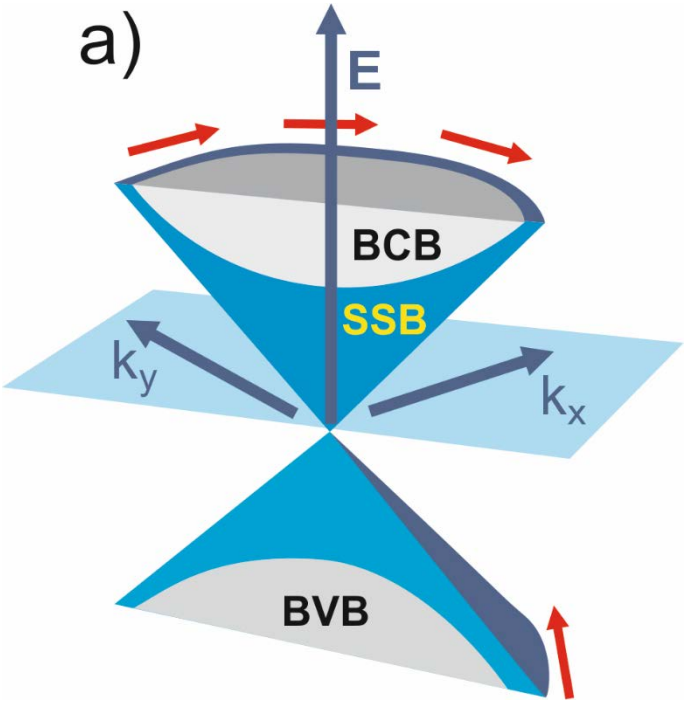
At the end of the first decade of 21st century, this class of materials were found among Bi_2Se_3 and Bi_2Te_3 types of compounds that form 3-dimentional class of topological insulators with the realization of sample-vacum boundary.

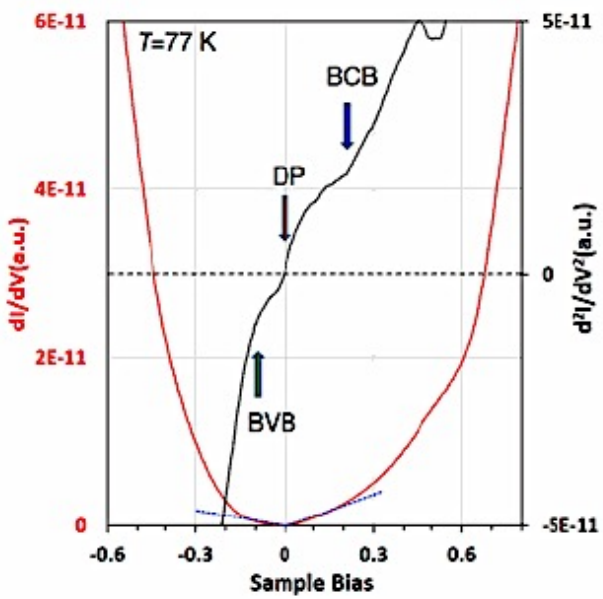
The best recognized feature of this class of materials is the existence of metallic states whenever the TI material breaks its continuity, e.g. on the surface.

Such a situation leads to some electrons on the surface exhibiting a unique physical properties.

Surface, 2D, electronic states are metallic with linear dispersion relation, like in the relativistic case, i.e. in the form of the Dirac cone (as in graphene).

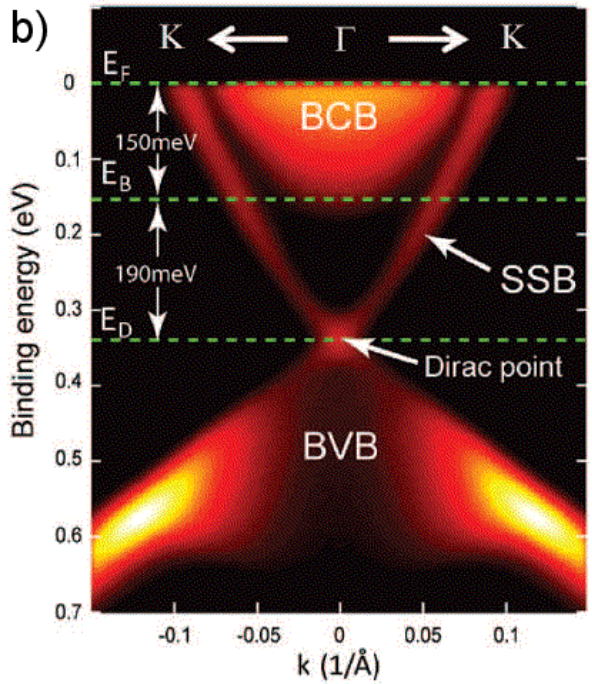


spin-momentum locking indicated by red arrows



Xu et. Al., Nature Physics, 10, (2014) 956

Scanning tunneling spectroscopy (STS)

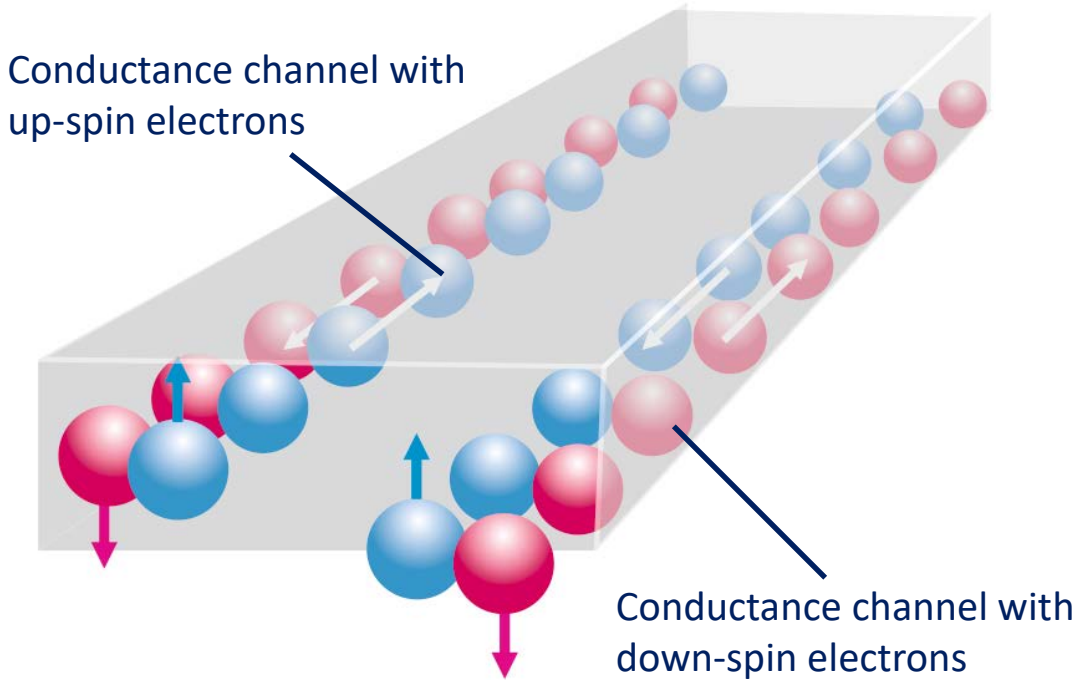


Y. L. Chen et. al., SCIENCE 329 (2010) 659

Angle-resolved photoemission spectroscopy (ARPES)

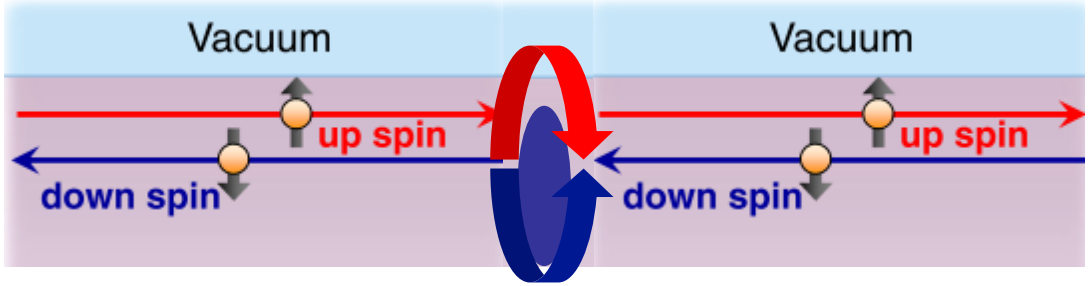
Since this surface links two spaces of different topologies, the surface metallicity is protected: no action can ruin metallic Dirac properties.

Additionally, spin is confined to momentum: spin-momentum states exist, where spin is perpendicular to the momentum vector.

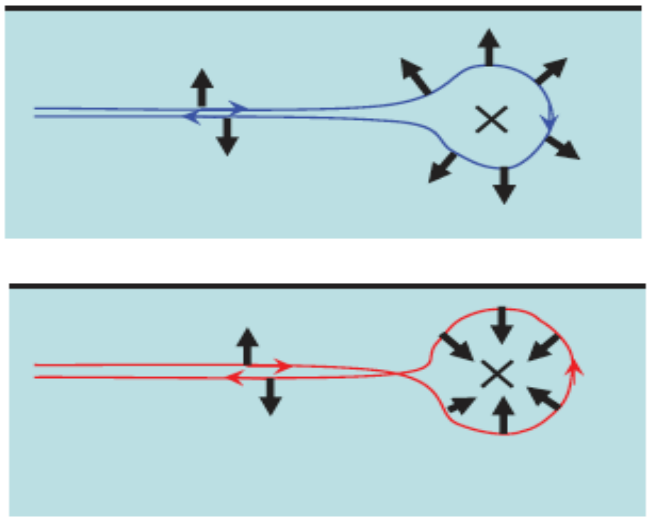


This results in the remarkable property: surface electrons can not be back-scattered, i.e. they are robust against perturbations.

- |ks> states can not be scattered to, non-existing, |-ks> states



- quantum interference cancels out |ks> to |-k-s> scattering, as long as the perturbations are not magnetic.



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Potential applications

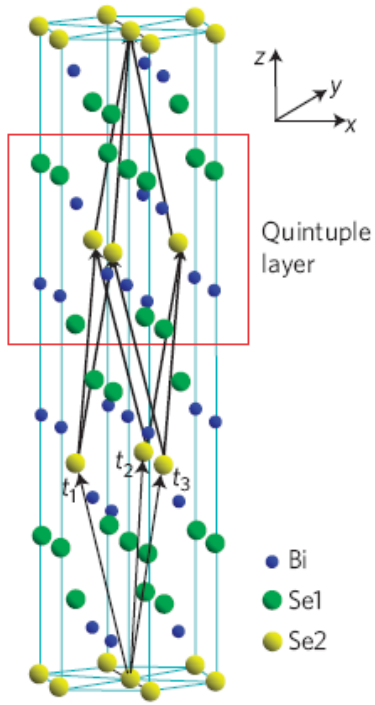
TI may revolutionize modern electronic devices.

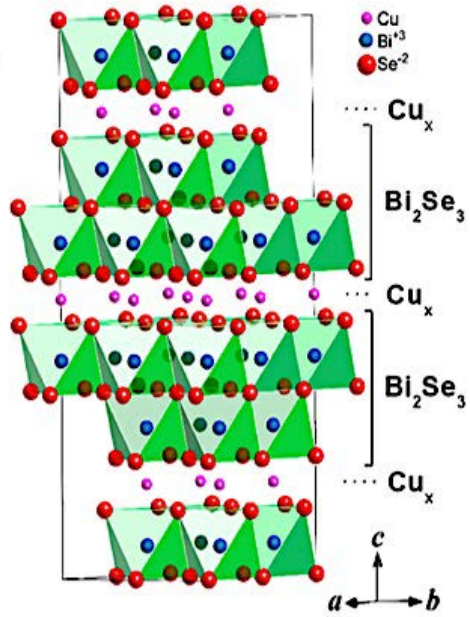
Since, surface states are largely protected, this fact can be utilized in spintronic applications and in devices carrying quantum information where avoiding decoherence is of outmost importance.

This fact may have a tremendous effect on the stability of spintronic devices and quantum computers.

Potential applications

- New thermoelectric materials,
- New class of superconductors (FeTeSe, CuBiTe),
- New class of semimagnetic semiconductors.



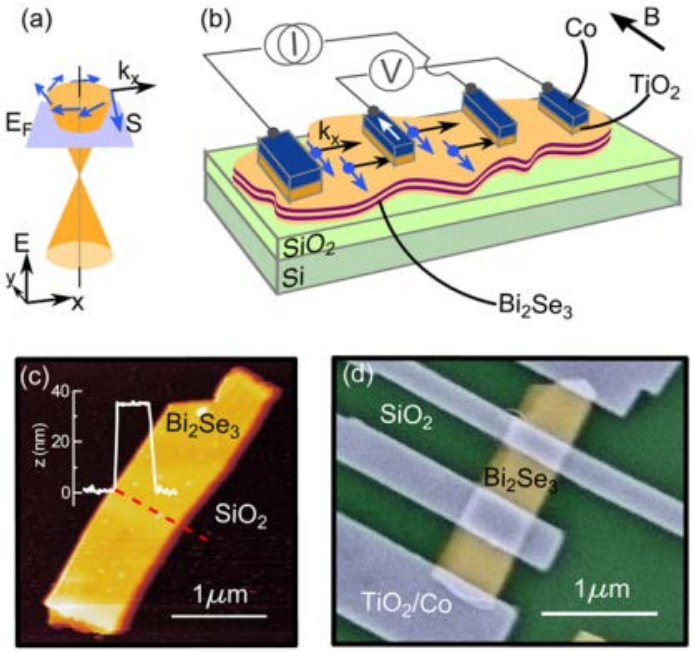


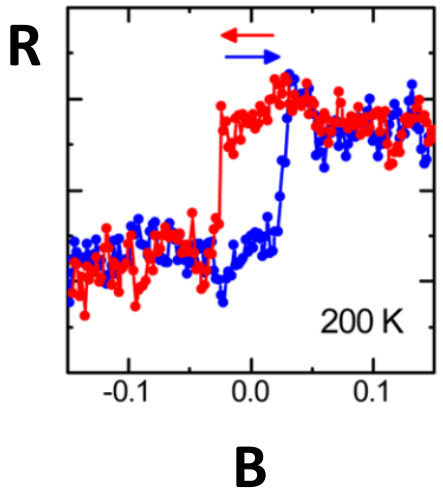
Superconducting

Potential applications - example

Tunneling spin valve

Current (electrons) going in one direction has defined spin direction.
As a result magnetoresistance R depends on the direction of magnetic field.





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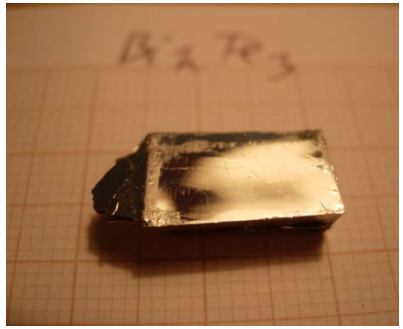
Our Research Project Objectives

From the point of view of potential applications it natural to ask to what extent such a material may be altered by:

- magnetic impurities,
- introducing electrodes,
- changing its shape and size,

to make microelectronic devices, before its unique properties are lost.

Material preparation



All known facts suggest that the outmost precaution of TI materials treatment may not be necessary, but, at the same time, may uncontrollably change carrier concentration. Therefore, ...

- All our measurement were performed on high quality single crystals synthesized via the Bridgman method.
- All starting materials, namely the 5N Bi, 5N Te and 5N Se, were deoxidized and purified further by multiple vacuum distillations until they reach 7N purity.

- The discovery of topological insulators has sparked extensive investigations of new materials with nontrivial topological order i.e. where change of topological order results in metallic or even superconducting states that are protected against dopants, defects, and impurities.

- The dissipationless spin current that exists in the topological surface state in equilibrium is expected to be useful for low energy consumption spintronic devices and attracts strong interest from the innovative technology industry.

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PHYSICS

Nobel for 2D exotic matter

Physics award goes to theorists who used topology to explain strange phenomena.

BY ELIZABETH GIBNEY AND DAVIDE CASTELVECCHI

KUNGL. VETENSKAPS-AKADEMIEN
THE ROYAL SWEDISH ACADEMY OF SCIENCES

4 OCTOBER 2016

Physics prizewinners Michael Kosterlitz (left), David Thouless (centre) and Duncan Haldane (right).

ΕΗΤΙΚΥΑ/RONI REKOMAA/REUTERS; TRINITY HALL, UNIV. CAMBRIDGE; DOMINIC REUTER/REUTERS

confined to thin films, chilled to near absolute zero and subjected to a strong magnetic field, they flow in an orderly way with conductivity that increases in steps with an increasing magnetic field. Thouless viewed the problem through the concept of topology, which

atoms could show topological properties that result in half spins at either end. Because this quantum property depends on the collective action of the whole chain, rather than on any individual particle, similar phenomena are now being explored as robust ways to encode

2016 award goes to physicist who used topology to explain strange phenomena.

Scientific Background on the Nobel Prize in Physics 2016

TOPOLOGICAL PHASE TRANSITIONS AND TOPOLOGICAL PHASES OF MATTER

compiled by the Class for Physics of the Royal Swedish Academy of Sciences

VL Berezinskii - has identified the role played by topological defects; his work led to the discovery of the **Berezinskii–Kosterlitz–Thouless transition**.

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Computation of Materials Properties

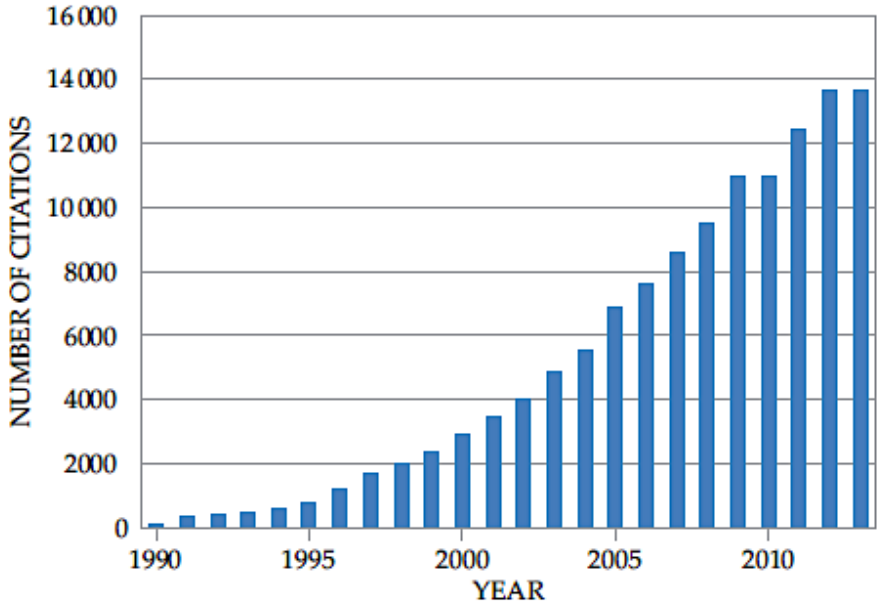
- short introduction to **D**ensity **F**unctional **T**heory

- DFT is presently the most successful and the most popular method to compute the electronic structure of matter
- It works for atoms, molecules, solids, liquids and plasmas
- DFT provides both the scientific justification and the basis for understanding the meaning behind the algorithms used in the computer codes

The Density Functional Theory was introduced in two papers:

- Inhomogeneous Electron Gas, P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964).
- Self Consistent Equations Including Exchange and Correlation Effects, W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965).

Walter Kohn receiving Nobel Prize (1998)



The number of annual citations to one or both of the foundational of density functional theory (DFT). Both papers are among the most highly cited in the history of Physical Review (Data from the Web of Science.)

In quantum mechanics, the physical state of an electron is described by a wave function. The quantum mechanical wave function contains, in principle, all the information about a given system.

- The ultimate goal of most approaches in solid state physics and quantum chemistry is the solution of the time-independent, non-relativistic Schrödinger equation

$$\hat{H}\psi_i = E_i\psi_i \qquad \left(\hat{T}+\hat{V}\right)\psi_i = E_i\psi_i$$

- For the simple case we can solve the Schrödinger equation exactly to get the wave function of the system ψ_i

- Then we can determine the energy states of the system E_i

- The wave function is a mathematical expression (not measurable)
- Born interpretation - the square modulus of the wavefunction, $|\psi_i|^2$, at any given point is proportional to the probability of finding the particle at that point. (The quantity $|\psi_i|^2$ is thus a probability density.)

electron density $$n(r) = \sum_i |\psi_i(r)|^2$$

The Schrödinger equation $\hat{H}\psi_i = E_i\psi_i$

Kinetic energy: ions electrons

$$\hat{H} = -\sum_n \frac{\hat{\boldsymbol{p}}_n^2}{2M} - \sum_i \frac{\hat{\boldsymbol{p}}_i^2}{2m_e} +$$

$$+\frac{1}{4\pi\varepsilon_0}\frac{1}{2}\sum_{n\neq m}\frac{Z_n Z_m e^2}{|\boldsymbol{R}_n - \boldsymbol{R}_m|} + \frac{1}{4\pi\varepsilon_0}\frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|} - \frac{1}{4\pi\varepsilon_0}\sum_{i,n}\frac{Z_n e^2}{|\boldsymbol{r}_i - \boldsymbol{R}_n|}$$

Potential energy: ions electrons electrons - ions

$$\hat{H} = \hat{T}_R + \hat{V}_R + \hat{T}_r + \hat{V}_r + \hat{V}_{r,R}$$

$$\psi_i(\boldsymbol{r}_1, \boldsymbol{r}_2, ..., \boldsymbol{R}_1, \boldsymbol{R}_2, ...; t)$$

It is impossible to solve the Schrödinger equation for a N-body system

we must use some approximations

DFT is a method of obtaining an approximate solution to the Schrödinger equation of a manybody system

Born-Oppenheimer approximation:

- motion of ions and electrons can be separated
- ions are fixed in space

The ions kinetic energy is zero and their potential energy is constant.

The Hamiltonian for electrons reduces to :

$$\hat{H}_e = -\sum_i \frac{\hat{\boldsymbol{p}}_i^2}{2m_e} + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|r_i - r_j|} - \sum_{i,n}\frac{Z_n e^2}{|r_i - R_n|} = \boxed{\hat{T}_r + \hat{V}_r} + \boxed{\hat{V}_{r,R}}$$

electron — electrons - ions

The total energy is then the sum of electron energy and the constant nuclear repulsion.

$$\hat{H}_e = \hat{T}_r + \hat{V}_r + \boxed{\hat{V}_{r,R}}$$

electrons - ions

the only term that distinguishes
one material (e.g. alloy) from another

determines the wavefunction, which in turn
determines the electron density $n(r)$ and the
total energy. The energy is thus a functional of $\hat{V}_{r,R}$

Kohn proposed a radical inversion of that thinking !

Is it possible that the total energy depends only on the electron density $n(r)$?

If it were true, knowledge of $n(r)$ was sufficient to determine the external potential,
the many-particle wavefunction, and all the ground-state properties

P. C. Hohenberg, W. Kohn, L. J. Sham, Adv. Quantum Chem. 21, 7 (1990)

1st theorem

For any electronic system in an external potential V_{ext}, this potential is determined uniquely, to within a constant, by the ground state density $n_0(r)$

All properties of the system are completely determined only by the ground state density

- $n(r)$ is a non-negative function of only the three spatial variables
- $n(r)$ is an observable and can be measured experimentally, e.g. by X-ray diffraction

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2nd theorem

Universal functional of the energy $E[n(r)]$ can be defined in terms of the density $n(r)$, which is valid for any external potential $V_{ext}(r)$

The universal functional contains the individual contributions of kinetic energy , classical Coulomb interaction , and the non-classical exchange correlation energy $E_{xc}[n(r)]$

Electron correlation, refers to all the effects that are missed when the electrons are treated as independent.

- An essential feature of the theory is the exchange correlation energy $E_{xc}[n(r)]$.
- It maps the electron density function $n(r)$ to the scalar energy E_{xc} associated with all exchange and correlation effects.
- An approximation to $E_{xc}[n(r)]$ is needed for practical work, and Kohn and Sham proposed useful approach.

Replace the original many-body problem with an auxiliary non-interacting reference system with the same density as the real, interacting one!

The exchange and correlation energy E_{XC} contains everything that is unknown.

$$\left(-\frac{\hat{\boldsymbol{p}}_i^2}{2m_e} + V_{ext}(r) + V_{Coul}(r) + V_{XC}(r) \right) \psi_i(r) = E_i \, \psi_i(r)$$

kinetic energy non-interacting particles

potential from the nuclei

classical Coulomb energy

exchange and correlation

KS eigenenergy

KS WF

effective potential $V_{eff}(\boldsymbol{r})$

$\psi_i(r)$ is the *i*-th single-electron wavefunction of a noninteracting electron system with the same density, $n(r)$ as the interacting electron system of interest.

Real interacting system:

External potential $V_{ext}(r)$

$V_{ij} = e^2/r_{ij}$

$\psi(r_1, r_2, \ldots\ldots); E[n(r)]$

Non-interacting system:

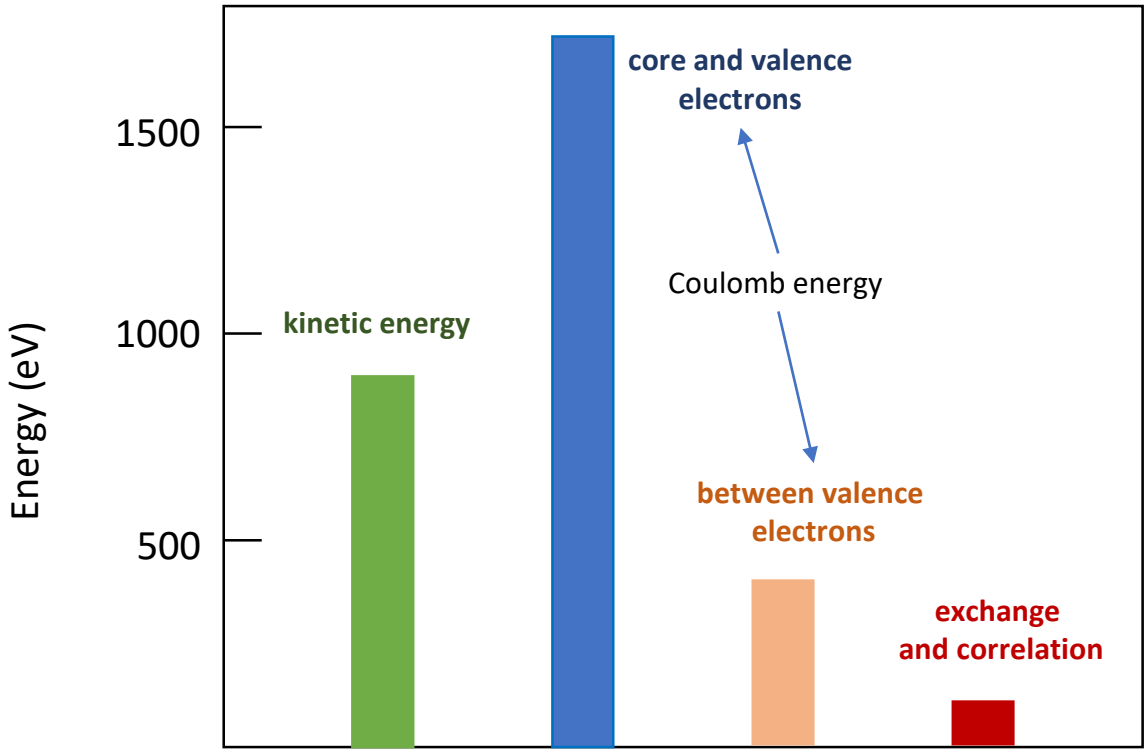
Effective potential $V_{eff}(r)$

$V_{ij} = 0$

$\psi_i(r) \rightarrow n_{eff}(r)$

Minimize $E[n(r)]$ with $n_{eff}(r)$ by varying $V_{eff}(r)$

3*N*-dimensional problem is reduced to a 3-dimensional one



Relative magnitudes of contributions to total valence energy of Mn atom

R. O. Jones, O. Gunnarsson, Reviews of Modern Physics, Vol. 61, No. 3, 1989

Unfortunately, $E_{xc}[n(r)]$, is unknown.

So Kohn and Sham proposed a local density approximation (LDA) for $E_{xc}[n(r)]$, in which electrons move on a positive background charge distribution (time averaged electron density) such that the total ensemble is neutral.

- LDA calculations yielded ground-state properties of solids to within 1–10% of their experimental value
- This accuracy that LDA delivers was insufficient for most applications in chemistry

In the 1980s new approximation for $E_{xc}[n(r)]$ - called generalized gradient approximation (GGA) were introduced.

It used not only the information about the density at a particular point but also information about the gradient of the charge density, in order to account for the non-homogeneity of the true electron density.

GGA outperformed the LDA when applied to atoms, solids, and surfaces.

Both the Coulomb energy and the exchange-correlation energy depend on the density $n(r)$, which in turn depends on the ψ_i , which are the solution of the Schrödinger equation (that we search for!).

This means that we are dealing with a self-consistency problem: the solutions ψ_i determine the original equation (V_{eff}), and the equation cannot be written down and solved before its solution is known.

An iterative procedure is the solution.

DFT in practice: The self-consistency loop

Start with initial guess (usually superposition of atomic densities k=1)

$n^{(k)}(r)$

Evaluate effective potential

$$V_{eff}(r) = V_{ext}(r) + V_{Coul}(r) + V_{XC}\left[n^{(k)}(r)\right]$$

Solve KS equations (for given potential)

$$\left(-\frac{\hat{\boldsymbol{p}}_i^2}{2m_e} + V_{eff}\left[n^{(k)}(r)\right]\right)\psi_i(r) = E_i\,\psi_i(r)$$

Evaluate (construct) actual density

$$n(r) = \sum_i |\psi_i(r)|^2$$

Consistent?

$$\left\| n^{(k)}(r) - n(r) \right\|_2 < \delta$$

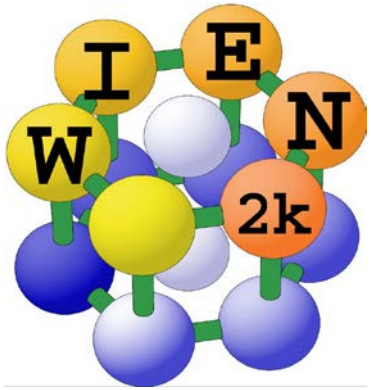
Yes

No

$k \to k+1$

Compute energy, forces, stresses …

Commercial DFT software allow nonexperts with modest computational resources to perform calculations with great accuracy for many, if not all, systems of interest.



The program package WIEN2k allows to perform electronic structure calculations of solids using density functional theory (DFT).

Wien2k is used worldwide by about 2600 groups

See www.wien2k.at

Molecular Physics
Vol. 108, Nos. 21–23, 10 November–10 December 2010, 3147–3166

INVITED ARTICLE

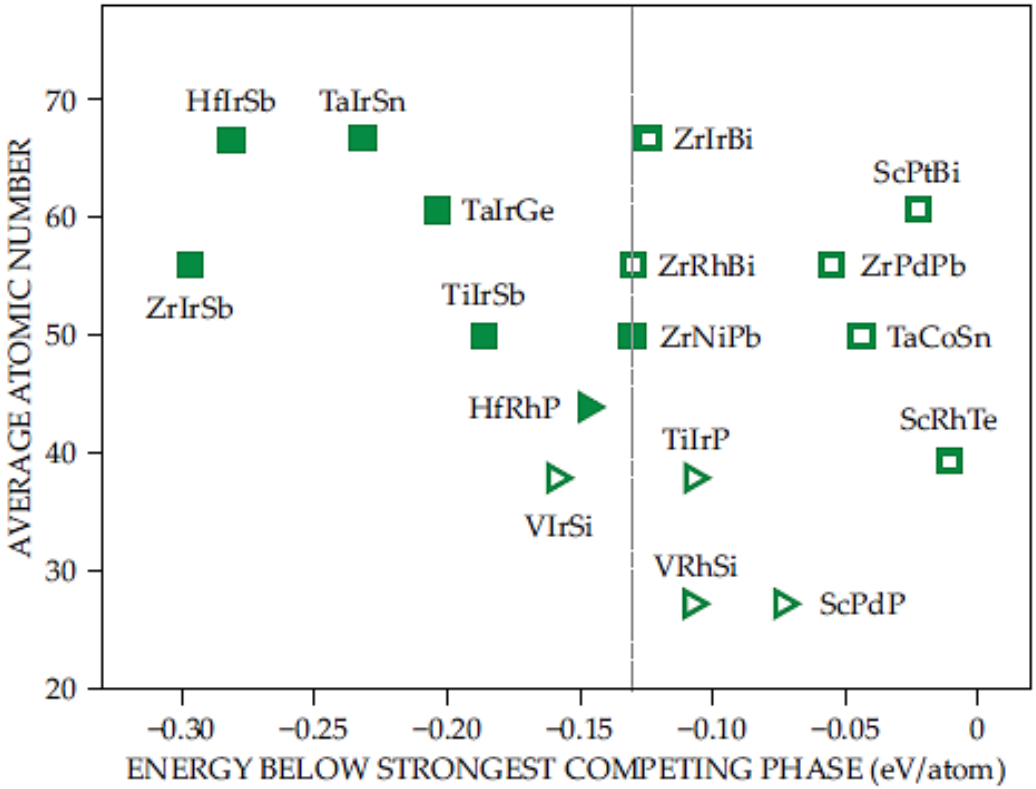
Electronic structure of solids with WIEN2k

Karlheinz Schwarz[a]*, Peter Blaha[a] and S.B. Trickey[b]

[a]*Institute of Materials Chemistry, Vienna University of Technology, Vienna, Austria;*
[b]*Quantum Theory Project, University of Florida, Gainesville, Fl, USA*

(Received 5 May 2010; final version received 24 June 2010)

Structure prediction and phase stability



R. Gautier et al., Nat. Chem. 7, 308 (2015), „Prediction and accelerated laboratory discovery of previously unknown 18-electron ABX compounds”

Previously unknown ternary compounds were predicted by DFT to be thermodynamically stable and were later synthesized by experiment.

- cubic
- noncubic

→ single phase

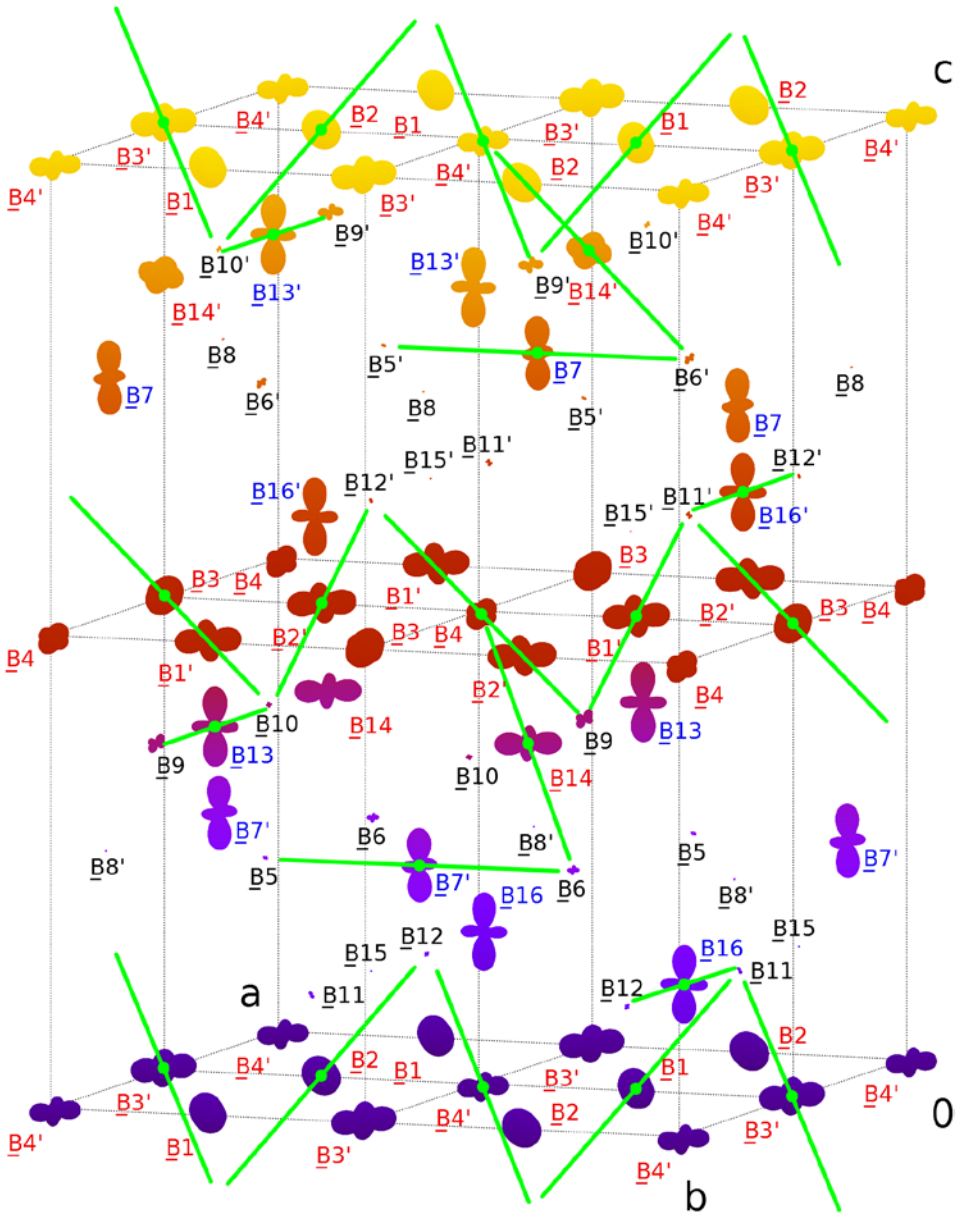
- cubic
- noncubic

→ multiphase

DFT calculations also predicted the correct optical properties for the compounds.

DFT: applications in solid state physics

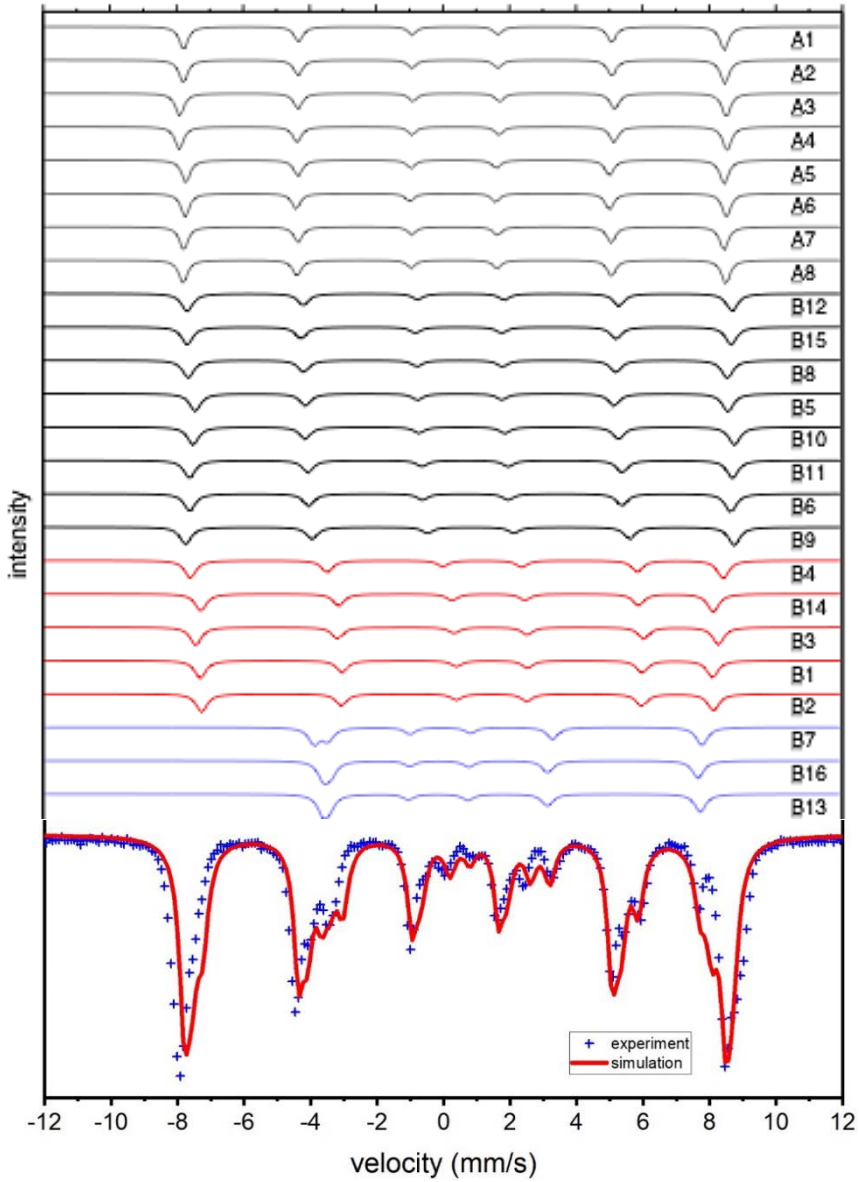
Visualization of the Electric Field Gradient tensors at Fe(B - octahedral) sites in the elementary cell



DFT: applications in solid state physics

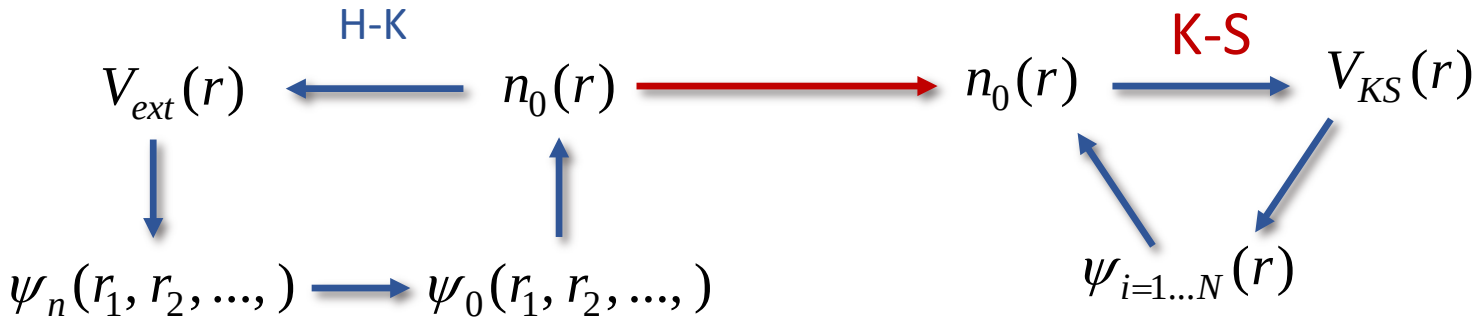
Simulation of a zero-field ^{57}Fe Mössbauer spectrum;
comparison with experimental data

All features visible in experimental Mössbauer spectrum can be explained by the ab initio calculated electronic structure



1. Hohenberg-Kohn theorems
   - All properties determined by electron density
   - A functional can be defined the minimum of which yields the ground energy state

2. Kohn-Sham equations
   - Replace fully interacting system with set of fictitious effective single-particle problems
   - The exchange-correlation functional plays a key role
   - Can be solve iteratively



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Density functional theory (DFT)

3. … yields total energies, forces, and electronic structure, allows computing e.g.,
   - Structural relaxation and phase stability
   - Energy differences (input for thermodynamics, kinetics …)
   - Phonon dispersions (mechanical stability)
   - Property prediction and screening
   - Band structures

Density functional theory (DFT)

4. … provides a reasonable balance between computational efficiency and accuracy (scales N^3 or better, thousands of electrons, hundreds of atoms)

5. … has limitations e.g., with respect to
   - Band gaps and optical properties
   - Strongly correlated systems

Topological Insulators – in search of new materials for microelectronics/information technology

AKADEMIA GÓRNICZO-HUTNICZA IM. STANISŁAWA STASZICA W KRAKOWIE
AGH UNIVERSITY OF SCIENCE AND TECHNOLOGY

W. Tokarz , A. Kozłowski, M. Dobrzański, I. Miotkowski, Z. Kąkol,

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