From Germanium to Graphene:
On the history of Condensed Matter Physics
AIF - Pisa, February 2014

A survey of Solid State Physics from 20-th to 21-th century:
a science that transformed the world around us

G. Grosso

February 18, 2014

Some considerations on a framework from which to grasp aspects and programs of fundamental and technological research in Condensed Matter Physics (CMP): a necessarily very incomplete account of condensed matter physics at the beginning of the 21th century.

In the history of fundamental science, the area of Solid State Physics represents the widest section of Physics and provides an example of how Physics changes and what Physics can be.

In the 20-th century, research in Solid State Physics had enormous impact both in basic aspects as well in technological applications.

Advances in
- experimental techniques of measurements,
- control of materials structures,
- new theoretical concepts and numerical methods
have been and actually are at the heart of this evolution.

Solid State Physics is at the root of most technologies of today's world and is a most clear evidence of how evolution of technology can be traced to fundamental physics discoveries.

Just an example: Physics in communication industry.......

Eras of physics	Communications technology changes
Era of electromagnetism Electric currents<--> Magnetic fields (Oersted 1820, Faraday and Henry 1825) Electromagnetic eq.s (Maxwell 1864), e.m. waves propagation (Hertz 1880)	First electromagnet (1825) Telegraph systems (Cooke,Wheatstone, Morse 1837) First transcontinental telegraph line (1861) Telephone (Bell 1874-76)
Era of the electron Discovery of the electron (Thomson, 1897) Thermionic emission (Richardson 1901) Wave nature of the electron (Davisson 1927)	Vacuum-tube diode (Fleming 1904)…… Wireless telegraph (Marconi 1896) Low energy electron diffraction (LEED) Radio astronomy (Jansky 1933)
Era of quantum mechanics Bloch, Peierls, Brillouin (1920s), Wilson (1931) Wigner-Seitz (1933)	Kelly at Bell Labs. : Semiconductors for communications (1936). Si,Ge (Shockley Bardeen 1946). Birth of transistor (1947) Digital transmission system (1962) Integrated circuits (Kilby et al. 1958)
Era of quantum optics Laser (Schawlow, Townes 1958), semic. laser (1962), quantun well laser (Dingle, Henry 1976), QCL laser (Capasso 1994)	Low loss silica fibers (1970) ……… Nanotechnology for communications

Source: W. F. Brinkman and D. V. Lang, Rev. Mod. Physics 71 (1999)

A step backward :

At the beginning of the 20th century properties of solid matter were investigated by almost independent disciplines. Only in the 1940s they converged into a unifying framework named ‘‘Solid State Physics’’.
In the sixties it was named ‘‘Condensed Matter Physics’’ and included other matter phases.

In the 20th century the paramount evolution of condensed matter physics was testified by the number of Nobel prize winners in:

- Theoretical and experimental advances
- Instrumentation development
- New materials discoveries
- Chemistry for subjects in material physics

After the second war, **26** Physics Nobel Prizes were awarded to condensed matter physics and associated fields, and **5** Chemistry Nobel Prizes were awarded for subjects in condensed matter physics

http://www.nobelprize.org/nobel_prizes/physics/laureates/
M. L. Cohen, Phys. Rev. Lett. 101, 25000 (2008)

Nobel Prizes related to laser/maser principles and developments in optics

1964 **Charles Hard Townes**, **Nicolay Gennadiyevich Basov** and **Aleksandr Mikhailovich Prokhorov**
"for fundamental work in the field of quantum electronics, which has led to the construction of oscillators and amplifier based on the maser-laser principle"

1971 **Dennis Gabor** "for his invention and development of the holographic method"

1981 **Nicolaas Bloembergen** and **Arthur Leonard Schawlow** "for their contribution to the development of laser spectroscopy"

1997 **Steven Chu**, **Claude Cohen-Tannoudji** and **William D. Phillips** "for development of methods to cool and trap atoms with laser light"

2005 **Roy J. Glauber** "for his contribution to the quantum theory of optical coherence"

2009 **Charles Kuen Kao** "for groundbreaking achievements concerning the transmission of light in fibers for optical communication"
Willard S. Boyle and **George E. Smith** "for the invention of an imaging semiconductor circuit - the CCD sensors

2012 **Serge Haroche** and **David J. Wineland** "for ground-breaking experimental methods that enable measuring and manipulation of individual quantum systems"

Nobel Prizes related to tunneling and electron microscopy

1953 Frits (Frederik) Zernike
"for his demonstration of the phase contrast method, especially for his invention of the phase contrast microscope”

1986 Ernst Ruska
"for his fundamental work in electron optics, and for the design of the first electron microscopy

Nobel Prizes related to developments in device applications

1952 Felix Bloch and **Edward Mills Purcell**
"for their development of new methods for nuclear magnetic precision measurements and discoveries in connection therewith”

1956 William Bradford Shockley, **John Bardeen** and **Walter Houser Brattain** "for their researches on semiconductors and their discovery of the transistor effect”

1973 Leo Esaki and **Ivar Giaever** "for their experimental discoveries regarding tunneling phenomena in semiconductors and superconductors, respectively"

2000 Zhores I. Alferov and **Herbert Kroemer** "for developing semiconductor heterostructures used in high-speed opto-electronics”
and Jack S. Kilby "for his part in the invention of the integrated circuit"

2007 Albert Fert and **Peter Gruenberg**
"for the discovery of Giant Magnetoresistance"

2009 Charles Kuen Kao, and Willard S. Boyle "for groundbreaking achievements concerning the transmission of light in fibers for optical communication"
George E. Smith "for the invention of an imaging semiconductor circuit - the CCD sensor"

Nobel Prizes related to advances in superconductivity and the quantum Hall effect

1972 John Bardeen, Leon Neil Cooper and **John Robert Schrieffer**
"for their jointly developed theory of superconductivity, usually called the BCS-theory"

1973 Leo Esaki and **Ivar Giaever** "for their experimental discoveries regarding tunneling phenomena in semiconductors and superconductors, respectively"

1985 Klaus von Klitzing "for the discovery of the quantized Hall effect"

1987 J. Georg Bednorz and **K. Alexander Mueller**
"for their important break-through in the discovery of superconductivity in ceramic materials"

1998 Robert B. Laughlin, Horst L. Stoermer and **Daniel C. Tsui**
"for their discovery of a new form of quantum fluid with fractionally charged excitations"

2003 Alexei A. Abrikosov, Vitaly L. Ginzburg and **Anthony J. Leggett**
"for pioneering contributions to the theory of superconductors and superfluids"

Nobel Prizes related to low temperature quantum phenomena

1962 Lev Davidovich Landau
"for his pioneering theories for condensed matter, especially liquid helium"

1996 David M. Lee, Douglas D. Osheroff and **Robert C. Richardson**
"for their discovery of superfluidity in helium-3"

2001 Eric A. Cornell, Wolfgang Ketterle and **Carl E. Wieman** "for the achievement of Bose-Einstein condensation in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates"

2003 Alexei A. Abrikosov, Vitaly L. Ginzburg and **Anthony J. Leggett**
"for pioneering contributions to the theory of superconductors and superfluids"

Nobel Prizes related to joint theoretical and experimental discoveries

1998 Robert B. Laughlin, Horst L. Stoermer and **Daniel C. Tsui**
"for their discovery of a new form of quantum fluid with fractionally charged excitations"

Nobel Prizes related to theorists alone

1962 Lev Davidovich Landau
"for his pioneering theories for condensed matter, especially liquid helium"

1972 John Bardeen, Leon Neil Cooper and **John Robert Schrieffer**
"for their jointly developed theory of superconductivity, usually called the BCS-theory"

1977 Philip Warren Anderson, Sir Nevill Francis Mott and **John Hasbrouck van Vleck**
"for their fundamental theoretical investigations of the electronic structure of magnetic and disordered systems"

1982 Kenneth G. Wilson
"for his theory for critical phenomena in connection with phase transitions"

1991 Pierre-Gilles de Gennes
"for discovering that methods developed for studying order phenomena in simple systems can be generalized to more complex forms of matter, in particular to liquid crystals and polymers"

2003 Alexei A. Abrikosov, Vitaly L. Ginzburg and **Anthony J. Leggett**
"for pioneering contributions to the theory of superconductors and superfluids"

Nobel Prizes related to theoretical chemistry

1968 Lars Onsager
"for the discovery of the reciprocal relations bearing his name, which are fundamental for the thermodynamics of irreversible processes"

1998 Walter Kohn, and John A. Pople
"for his development of the density-functional theory"
"for his development of computational methods in quantum chemistry"

Nobel Prizes related to discovery of new materials in physics

1987 J. Georg Bednorz and **K. Alexander Mueller**
"for their important break-through in the discovery of superconductivity in ceramic materials"

2007 Albert Fert and **Peter Gruenberg**
"for the discovery of Giant Magnetoresistance"

2010 Andre Geim and **Konstantin Novoselov**
"for groundbreaking experiments regarding the two-dimensional material graphene"

Nobel Prizes related to discovery of new materials in chemistry

1996 Robert F. Curl Jr., Sir Harold W. Kroto and **Richard E. Smalley**
"for their discovery of fullerenes"

2000 Alan J. Heeger, Alan G. MacDiarmid and **Hideki Shirakawa**
"for the discovery and development of conductive polymers"

2011 Dan Shechtman
"for the discovery of quasicrystals"

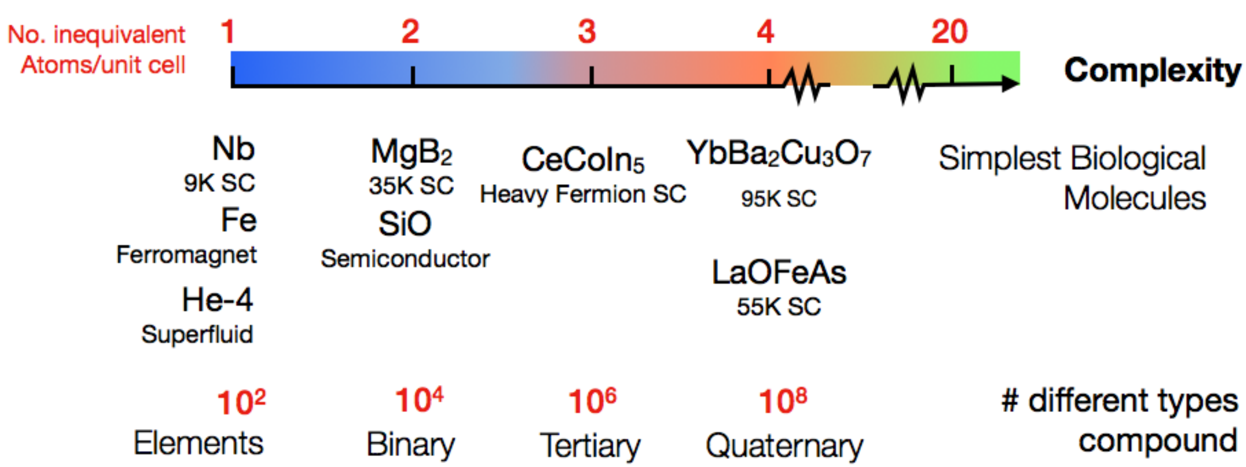
The beauty and difficulty of Condensed Matter Physics originate from

Diversity Interconnections Complexity

Diversity : CMP is a very broad field. In the past it was driven by the curiosity about the natural world an how it responds to light, heat, mechanical forces, etc.. This fundamental understanding grew with the desire to manipulate nature for human needs. Thus very *different* systems, experimental methods, theoretical techniques … are at the fundaments of CMP

Interconnections : CMP has the strongest links, to other branches of physics particularly atomic, molecular, and optical physics, but also to other fields as chemistry, biology, engineering, material science, computer science and global communications.

Complexity : As the number of atoms grows, its complexity as well the potential for new phenomena grows.



P. Coleman
'Introduction to many body theory"(2010)

Addressing CMP, two paradigms can be adopted:

- The atomistic philosophy well suited for isolated atoms, molecules, electronic structure of crystalline solids. Basic question : “what are the microscopic laws of nature ?”

“The general theory of quantum mechanics is now almost complete. The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.”

P.A.M. Dirac (1929)

But… already In 1820, Laplace speculated on determining the consequences of physical laws:

“An intelligent being who, at a given moment, knows all the forces that cause nature to move and the positions of the objects that it is made from, if also it is powerful enough to analyze this data, would have described in the same formula the movements of the largest bodies of the universe and those of the lightest atoms. Although scientific research steadily approaches the abilities of this intelligent being, complete prediction will always remain infinitely far away.”

Theorie Analytique des Probabilites

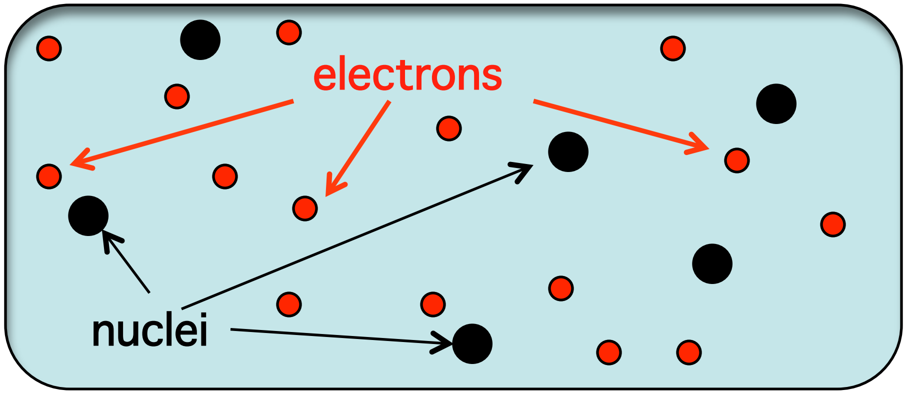
- The philosophy of emergent phenomena (a term from evolutionary biology) which occur when huge numbers of particles assemble. Basic question : "what new principles and laws emerge going from the microscopic to the macroscopic?"

"The behavior of large and complex aggregations of elementary particles, it turns out, is not to be understood in terms of a simple extrapolation of the properties of a few particles. Instead, at each level of complexity entirely new properties appear, and the understanding of the new behaviors requires research which I think is as fundamental in its nature as any other."

(P. W. Anderson from "More is Different" , Science 1972)

Both approaches should merge and be adopted together to understand the behavior of condensed matter

CONCEPTUAL GROUNDWORK



$$H_{\rm tot} = T_N + T_e + V_{ee} + V_{eN} + V_{NN}$$
$$= -\sum_I \frac{\hbar^2 \nabla_I^2}{2M_I} - \sum_i \frac{\hbar^2 \nabla_i^2}{2m} + \underbrace{\frac{1}{2}\sum_{i \neq i} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} - \sum_{iI} \frac{z_I e^2}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2}\sum_{I \neq J} \frac{z_I z_J e^2}{|\mathbf{R}_I - \mathbf{R}_J|}},$$

Equazione di Schroedinger

$$\boxed{[T_N(R) + \underbrace{T_e(r) + V(r,\,R)]}_{H_e(r,R)}\Psi(r,\,R) = W\Psi(r,\,R)]}$$

$$\Psi_{\rm trial}(r,\,R) \approx \chi(R)\psi_0(r;\,R)$$

Electronic Problem

$$H_e(r;R) = T_e + V(r,R).$$

$$\boxed{H_e(r;R)\psi_0(r;R) = E_0(R)\psi_0(r;R)}$$

Nuclear Problem

Born-Oppenheimer approximation

$$\boxed{\left[-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial R^2} + E_0(R)\right]\chi(R)} + \cancel{\Lambda_{00}}(R)\chi(R) \boxed{= W\chi(R)}$$

$$E_0(R) = E_0(R_0) + \frac{1}{2}\sum_{IJ}\left(\frac{\partial^2 E_0}{\partial R_I \partial R_J}\right)_0 u_I u_J + \text{higher order terms.}$$

$$\boxed{M_I \ddot{R}_I = -\frac{\partial E_0(\{R_J\})}{\partial R_I}}.$$

Molecular Dynamics

From the many-electron problem

$$H_e \Psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, \ldots, \mathbf{r}_N\sigma_N) = E\Psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, \ldots, \mathbf{r}_N\sigma_N)$$

HARTREE, HARTREE-FOCK, DENSITY FUNCTIONAL THEORY……

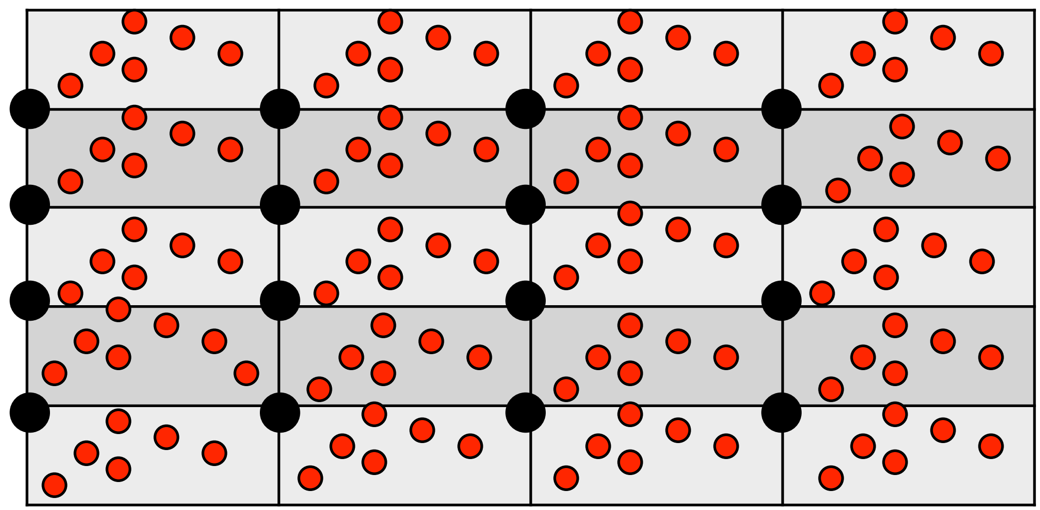
To the one-electron problem

$$\left[\frac{\mathbf{p}^2}{2m} + \mathcal{V}(\mathbf{r})\right]\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

PERIODICITY:

$$\mathcal{V}(\mathbf{r} + \mathbf{t}_n) = \mathcal{V}(\mathbf{r})$$

$$\boxed{\psi(\mathbf{k}, \mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u(\mathbf{k}, \mathbf{r})}$$



$$\boxed{\psi(\mathbf{k}, \mathbf{r} + \mathbf{t}_n)} = e^{i\mathbf{k}\cdot(\mathbf{r}+\mathbf{t}_n)} u(\mathbf{k}, \mathbf{r} + \mathbf{t}_n) = \boxed{e^{i\mathbf{k}\cdot\mathbf{t}_n}\psi(\mathbf{k}, \mathbf{r})}$$

BLOCH THEOREM
BAND STRUCTURE

Interacting atoms model :

Particles: electrons and nuclei
The atomic core electrons are inert, the valence electrons are itinerant or partialli localized)
Interactions: electromagnetic and quantum mechanics

Elementary excitations model :

explanation of the collective excitations induced by probes
Particles (quasiparticles): can be fictitious as phonons, magnons polaritons, excitons.....

Both models are used together to interpret the physics of solids

From GERMANIUM to GRAPHENE

or

From GERMANIUM to GERMANIUM

and

From 2D-GRAPHITE to GRAPHENE

?

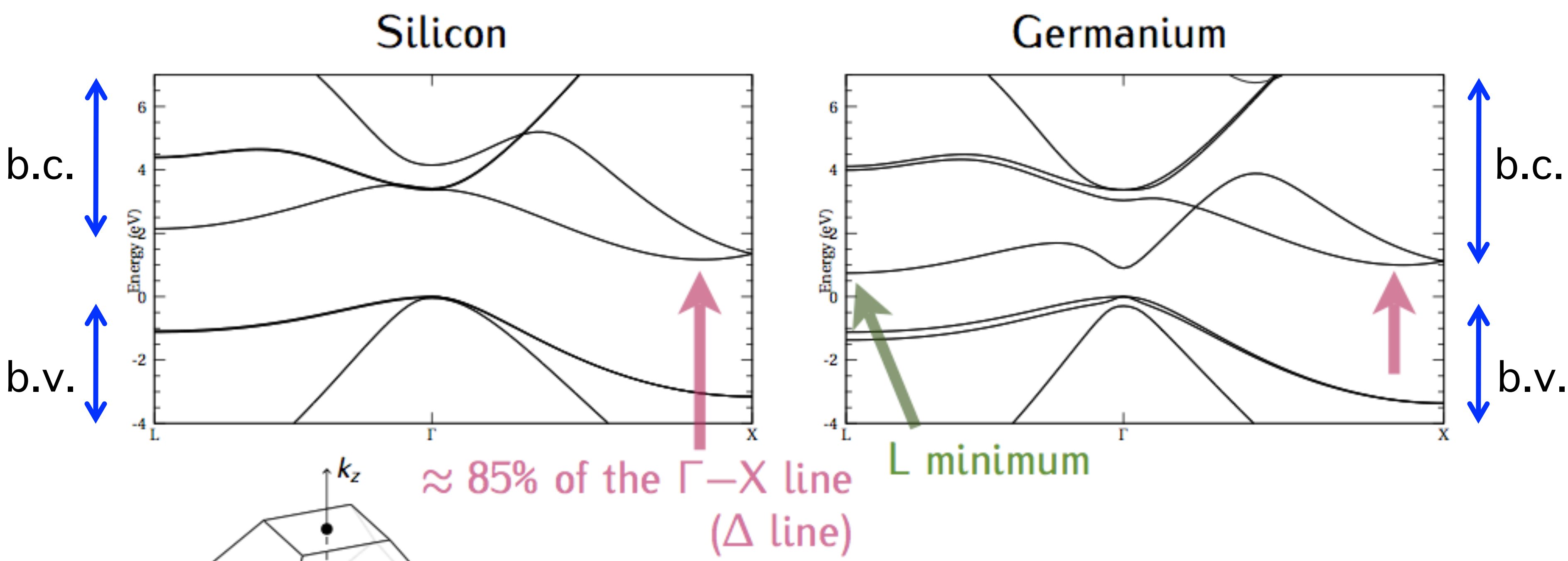
GROUP IV

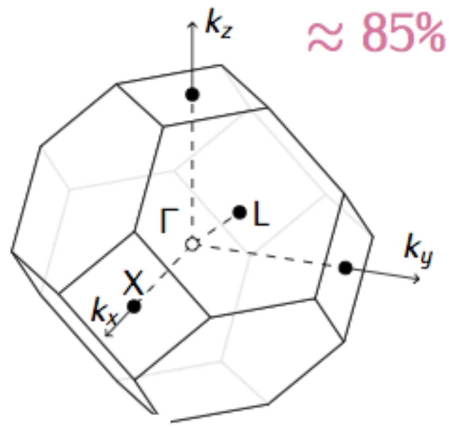
hydrogen 1 H 1.0079																		helium 2 He 4.0026
lithium 3 Li 6.941	beryllium 4 Be 9.0122												boron 5 B 10.811	carbon 6 C 12.011	nitrogen 7 N 14.007	oxygen 8 O 15.999	fluorine 9 F 18.998	neon 10 Ne 20.180
sodium 11 Na 22.990	magnesium 12 Mg 24.305												aluminium 13 Al 26.982	silicon 14 Si 28.086	phosphorus 15 P 30.974	sulfur 16 S 32.065	chlorine 17 Cl 35.453	argon 18 Ar 39.948
potassium 19 K 39.098	calcium 20 Ca 40.078		scandium 21 Sc 44.956	titanium 22 Ti 47.867	vanadium 23 V 50.942	chromium 24 Cr 51.996	manganese 25 Mn 54.938	iron 26 Fe 55.845	cobalt 27 Co 58.933	nickel 28 Ni 58.693	copper 29 Cu 63.546	zinc 30 Zn 65.39	gallium 31 Ga 69.723	germanium 32 Ge 72.61	arsenic 33 As 74.922	selenium 34 Se 78.96	bromine 35 Br 79.904	krypton 36 Kr 83.80
rubidium 37 Rb 85.468	strontium 38 Sr 87.62		yttrium 39 Y 88.906	zirconium 40 Zr 91.224	niobium 41 Nb 92.906	molybdenum 42 Mo 95.94	technetium 43 Tc [98]	ruthenium 44 Ru 101.07	rhodium 45 Rh 102.91	palladium 46 Pd 106.42	silver 47 Ag 107.87	cadmium 48 Cd 112.41	indium 49 In 114.82	tin 50 Sn 118.71	antimony 51 Sb 121.76	tellurium 52 Te 127.60	iodine 53 I 126.90	xenon 54 Xe 131.29
caesium 55 Cs 132.91	barium 56 Ba 137.33	57-70 *	lutetium 71 Lu 174.97	hafnium 72 Hf 178.49	tantalum 73 Ta 180.95	tungsten 74 W 183.84	rhenium 75 Re 186.21	osmium 76 Os 190.23	iridium 77 Ir 192.22	platinum 78 Pt 195.08	gold 79 Au 196.97	mercury 80 Hg 200.59	thallium 81 Tl 204.38	lead 82 Pb 207.2	bismuth 83 Bi 208.98	polonium 84 Po [209]	astatine 85 At [210]	radon 86 Rn [222]
francium 87 Fr [223]	radium 88 Ra [226]	89-102 * *	lawrencium 103 Lr [262]	rutherfordium 104 Rf [261]	dubnium 105 Db [262]	seaborgium 106 Sg [266]	bohrium 107 Bh [264]	hassium 108 Hs [269]	meitnerium 109 Mt [268]	ununnilium 110 Uun [271]	unununium 111 Uuu [272]	ununbium 112 Uub [277]		ununquadium 114 Uuq [289]				

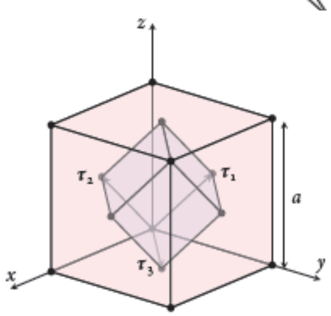
*Lanthanide series	lanthanum 57 La 138.91	cerium 58 Ce 140.12	praseodymium 59 Pr 140.91	neodymium 60 Nd 144.24	promethium 61 Pm [145]	samarium 62 Sm 150.36	europium 63 Eu 151.96	gadolinium 64 Gd 157.25	terbium 65 Tb 158.93	dysprosium 66 Dy 162.50	holmium 67 Ho 164.93	erbium 68 Er 167.26	thulium 69 Tm 168.93	ytterbium 70 Yb 173.04
* *Actinide series	actinium 89 Ac [227]	thorium 90 Th 232.04	protactinium 91 Pa 231.04	uranium 92 U 238.03	neptunium 93 Np [237]	plutonium 94 Pu [244]	americium 95 Am [243]	curium 96 Cm [247]	berkelium 97 Bk [247]	californium 98 Cf [251]	einsteinium 99 Es [252]	fermium 100 Fm [257]	mendelevium 101 Md [258]	nobelium 102 No [259]

Chemistry Resources at BPC: History of the Development of the Periodic Table of Elements - www.bpc.edu

Silicon/Germanium band structures







- Si and Ge have indirect gap: not suited for optical amplification
- Interest in integrating electronics and photonics on the same platform
- Light amplification requires population inversion of Gamma carriers

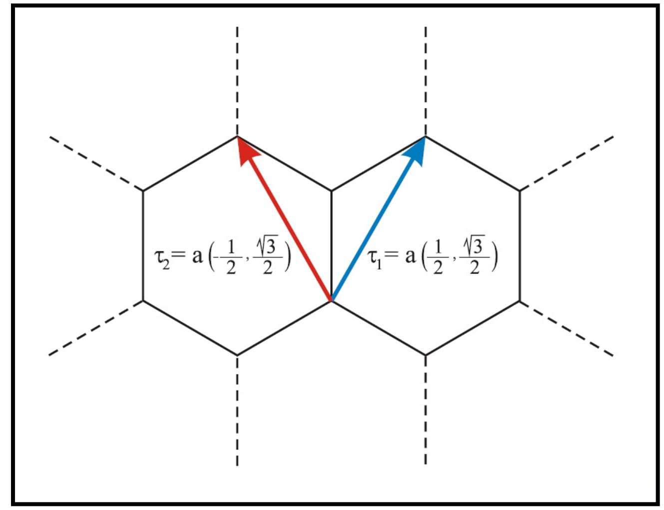
From 2D-GRAPHITE (Wallace 1947) to GRAPHENE (Novoselov et al. 2004) P.R. Wallace “The Band Theory of Graphite” Phys. Rev. 71, 622-634 (1947)

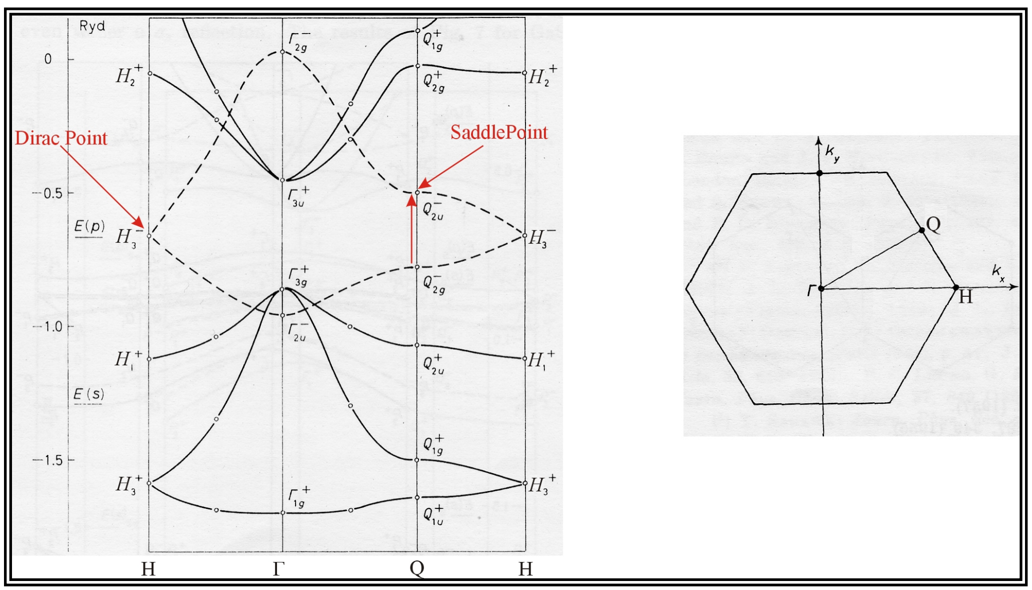
- The structural anisotropy is responsible for peculiar mechanical, electronic, vibrational and optical properties.

K.S.Novoselov et al. “Electric Field Effect in Atomically Thin Carbon Films” Science 306, 666-669 (2004)

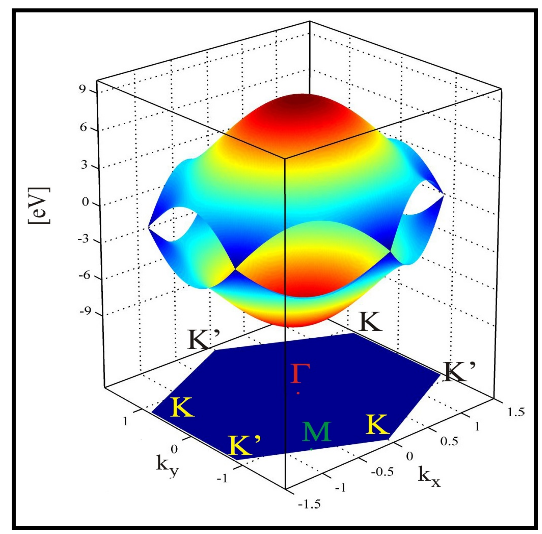
- Experimental realization of monolayers of carbon atoms.
- Striking transport properties of graphene, fully controlled by Dirac points in the low energy region (minimal conductivity, shot noise, Klein tunneling, half-integer quantum Hall, current profiles, valley-valve filtering).

GRAPHENE LATTICE





π−π* ELECTRONIC BAND STRUCTURE

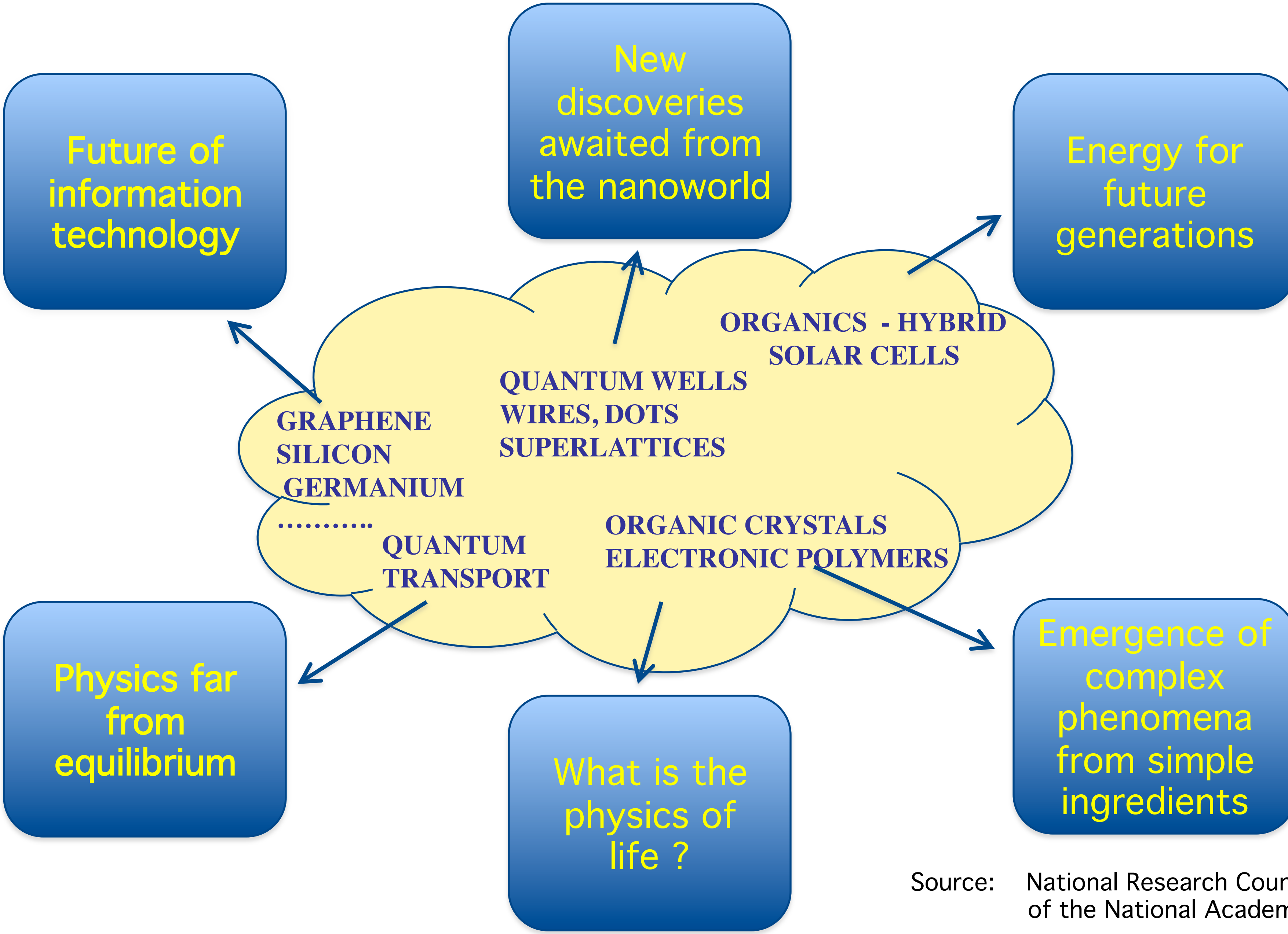


Janus Bifrons in the Vatican Museums

He looks to the past and to the future

Future research frontiers in condensed matter physics

Challanges for CMP in the next decade



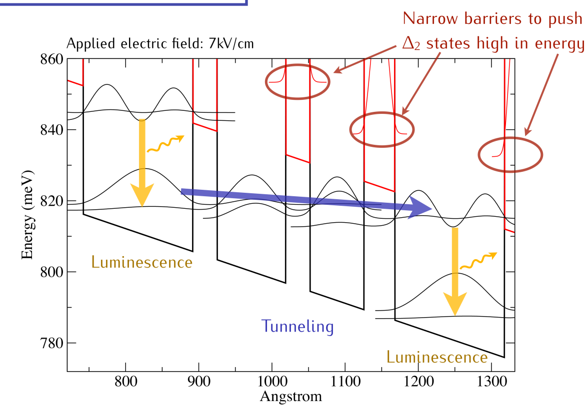
Source: National Research Council of the National Academies

“Methods” oriented scientific themes:
geometrical, electronic, optical and transport properties

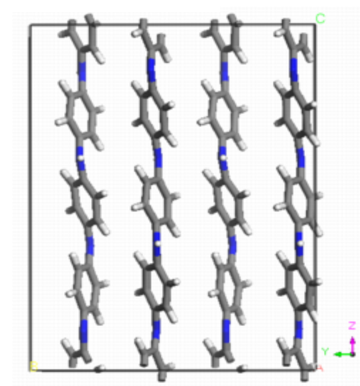
- Ab-initio DFT calculations and Molecular dynamics
- “Real space numerical algorithms for the electronic states in ordered and disordered low dimensional solids
- Density of states, transmittivity, localization length in multichain systems
- Charge transport in mesoscopic systems

"Materials" oriented problems

- Low dimensional physics:
  New materials in nanotechnology:
  new properties, new complexity

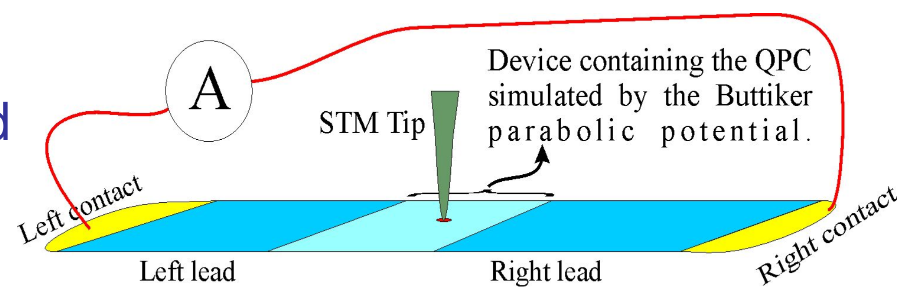


- Organic materials (Conjugated electronic conducting polymers, Molecular crystals)

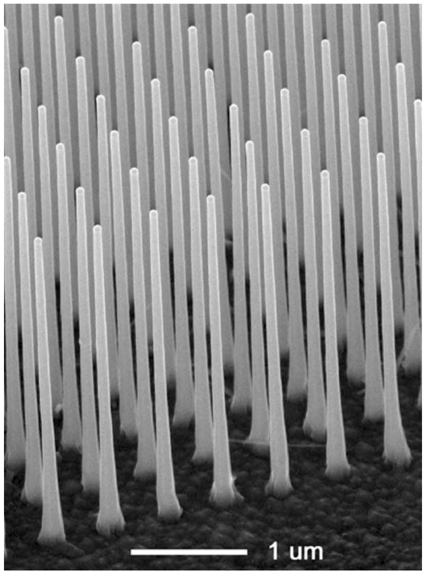


- Complex molecular systems for life science (DNA. Proteins ....)

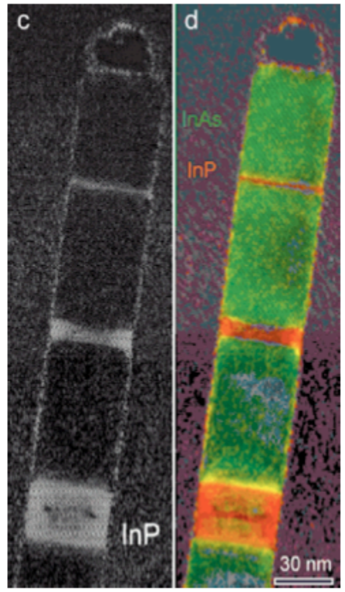
- Quantum transport in nanostructured systems



New materials with nanoscale dimensions
new properties, new complexity



InP nanowire,
L. Samuelson, Lund



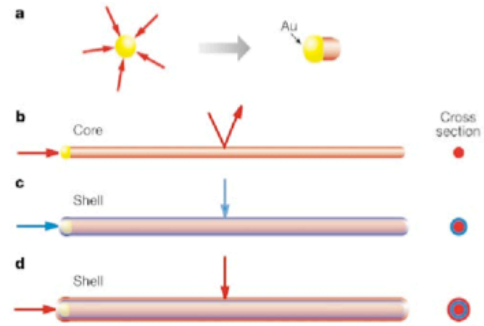
M. Bjork *et al*, Nano Letters 2, 87 (2002)

Diameter: 3-100 nm

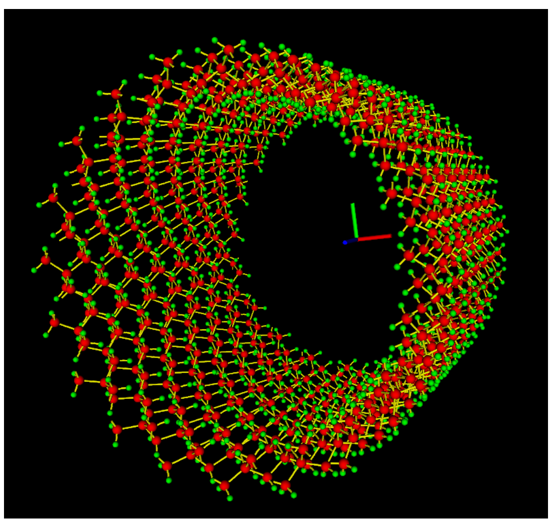
Length: >10 μm

Materials: Si, Ge, GaAs. InAs, InP, ...

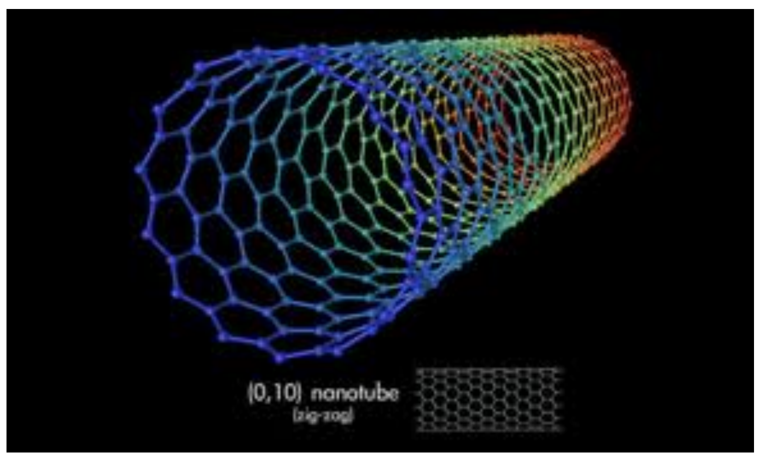
It is possible to realize heterostructures



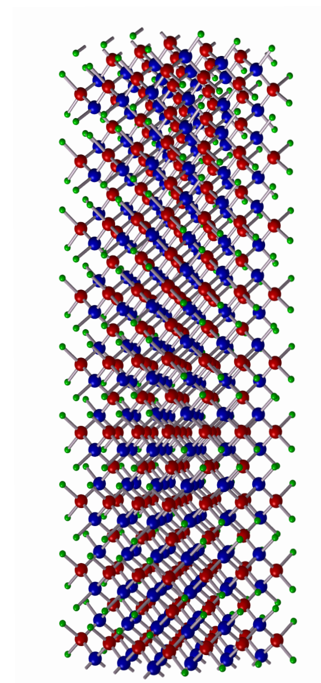
L. J. Lauhon *et al*, Nature 420, 57 (2002)



Silicon Nanotube

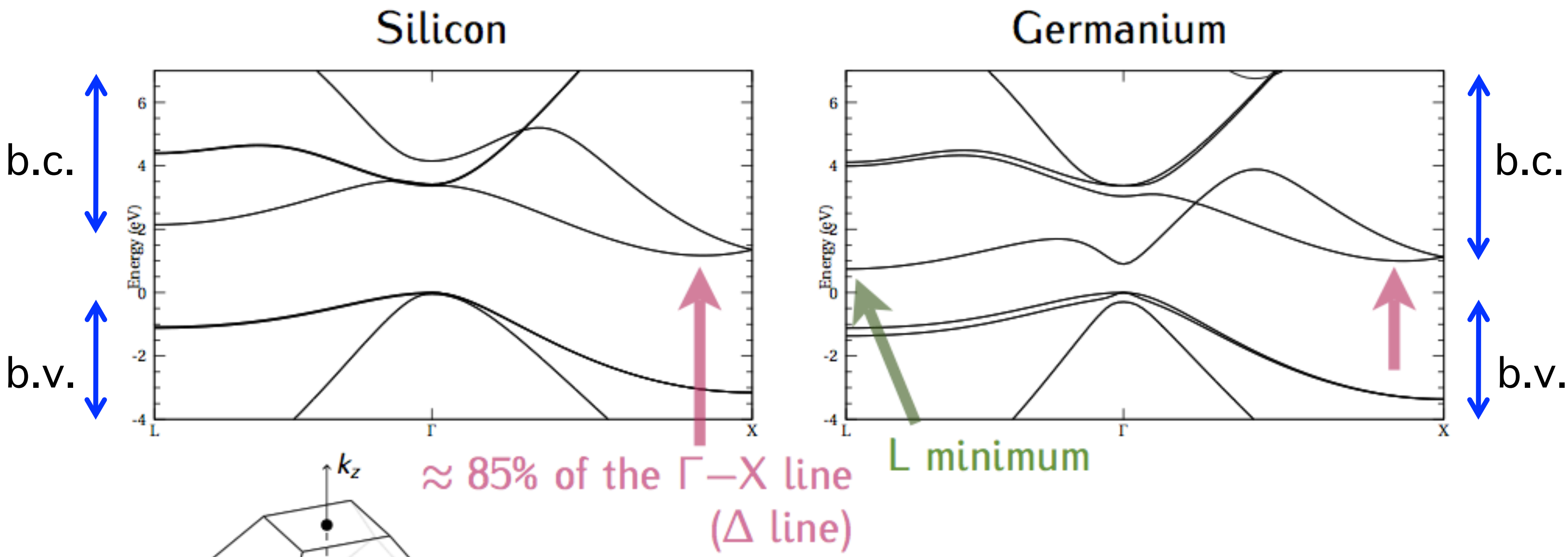


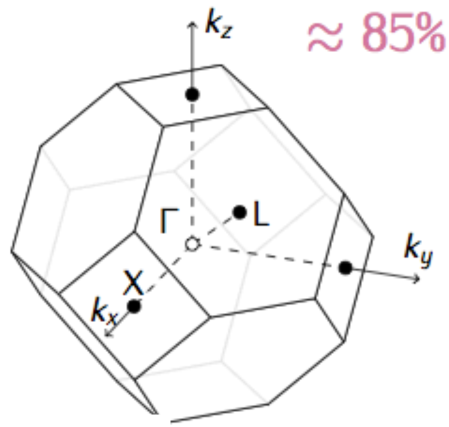
Carbon Nanotube

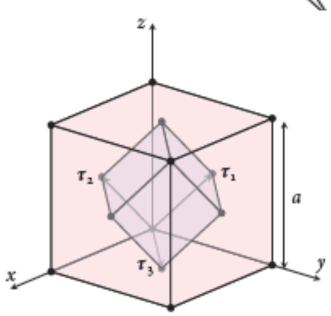


Si/Ge Nanowire

Frontiers in Silicon/Germanium photonics







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- Interest in integrating electronics and photonics on the same platform
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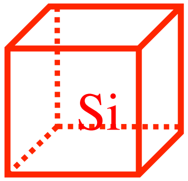
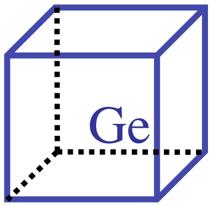
Band structure engineering by STRAIN



$a_0 = 5.431$ A

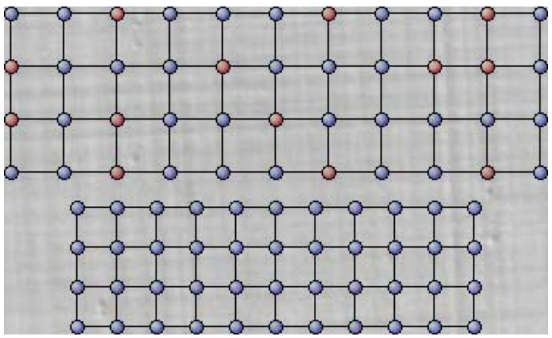


$a_0 = 5.657$ A

~ 4% mismatch of the lattice constants

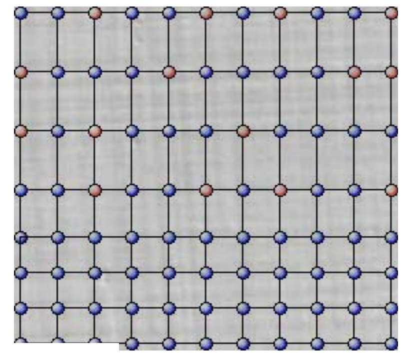
matching condition:

$$a_{\parallel}^{x} = a_{\parallel}^{y} = a_{0}^{y}$$



$Si_{1-x}Ge_x$ active layer

Relaxed Si substrate



x

y

- Renewed interest in SiGe also due to:
  - recent advances in SiGe epitaxy (also in the Ge-rich regime) which is difficult also due to the unavoidable strain
  - recent developments of a Ge-on-Si laser (MIT)

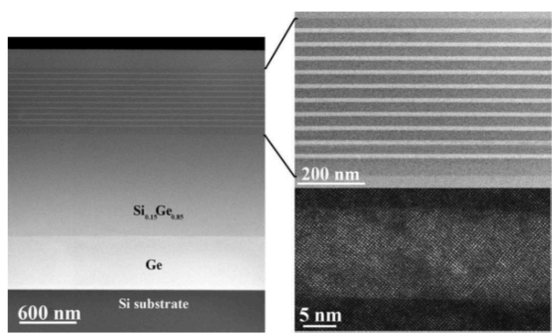
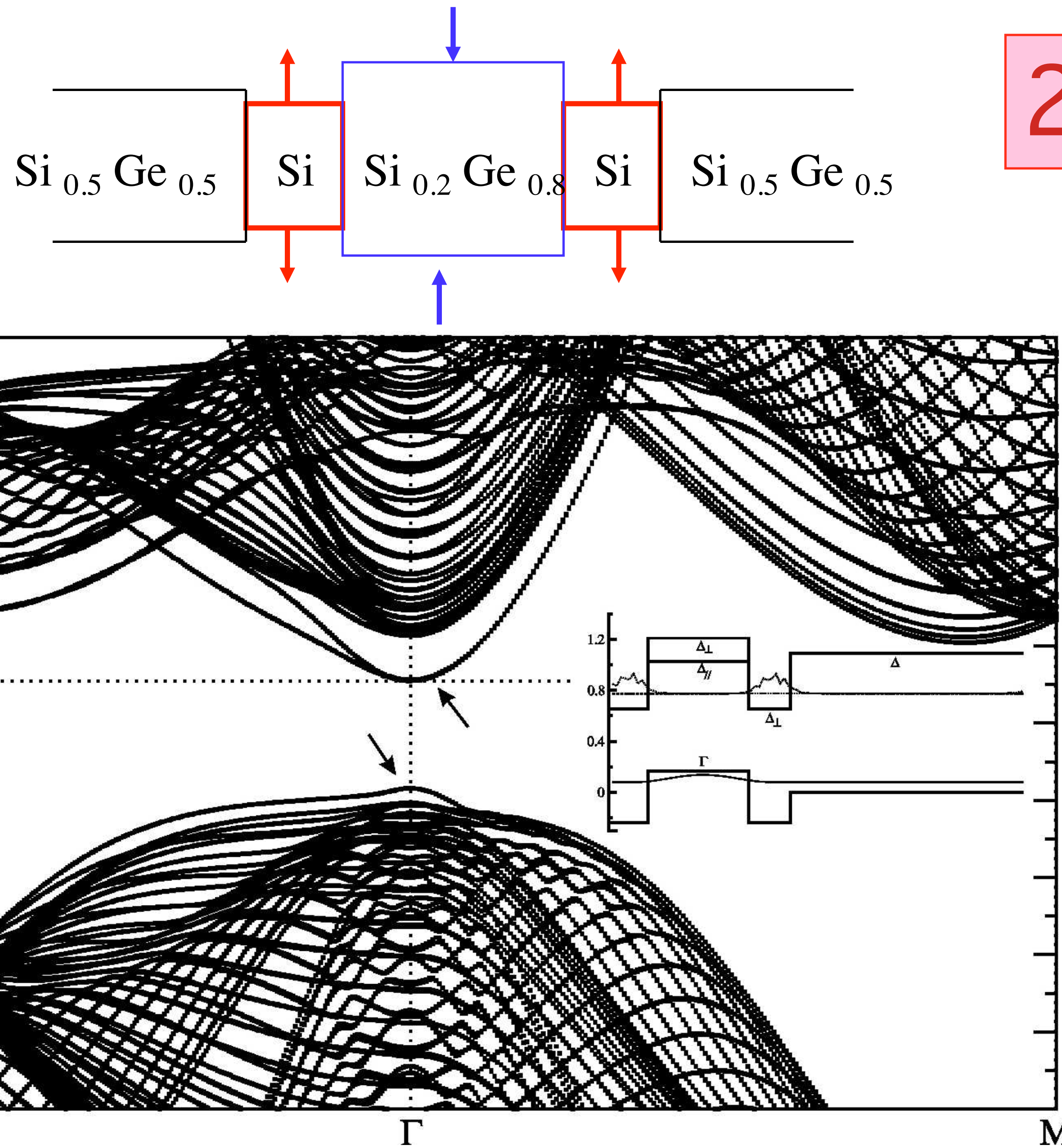


Image from Y. Busby, GP et al., Phys. Rev. B 82, 205317 (2010)

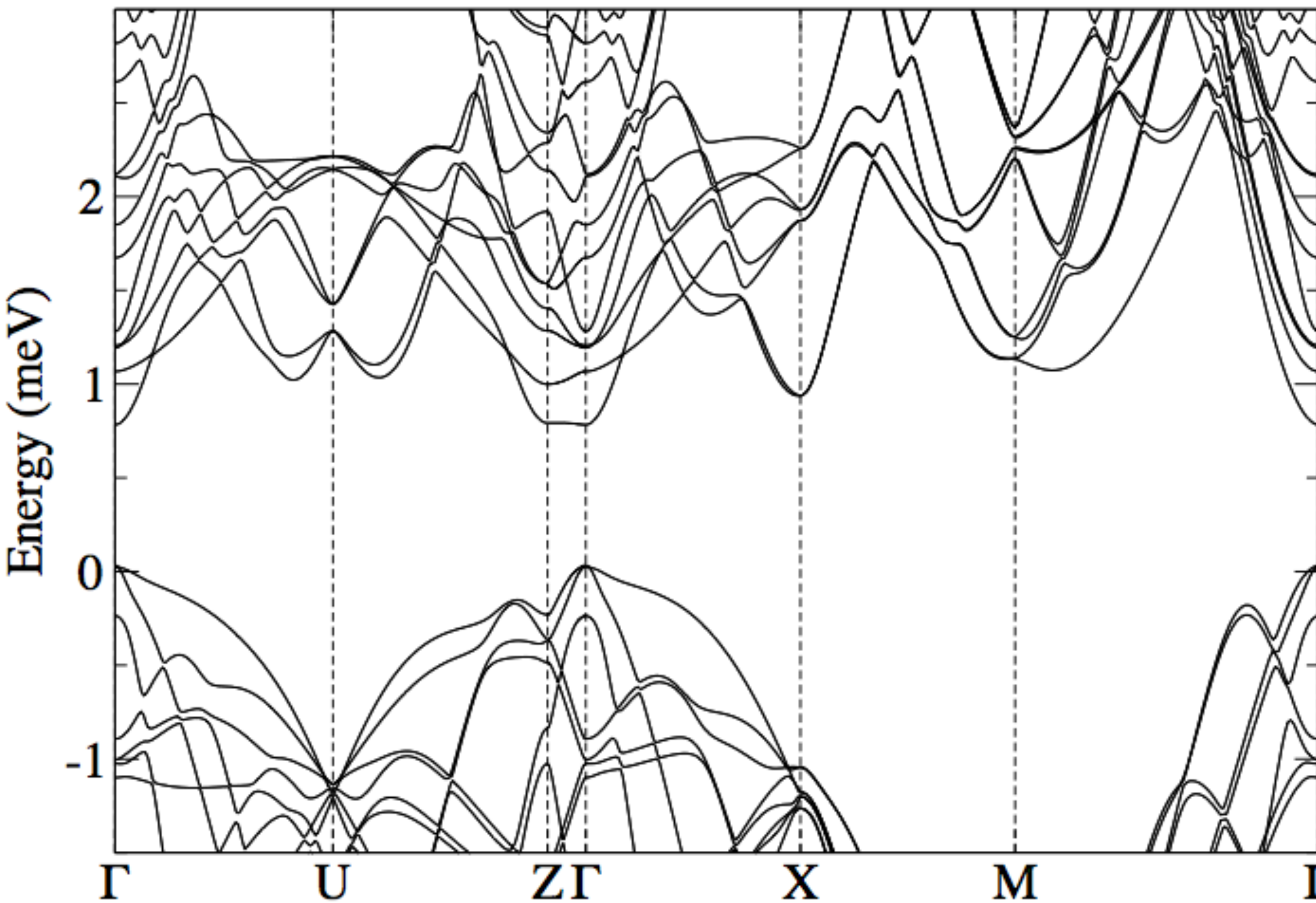
2D



J. Appl. Phys. 100,093506 (2006)

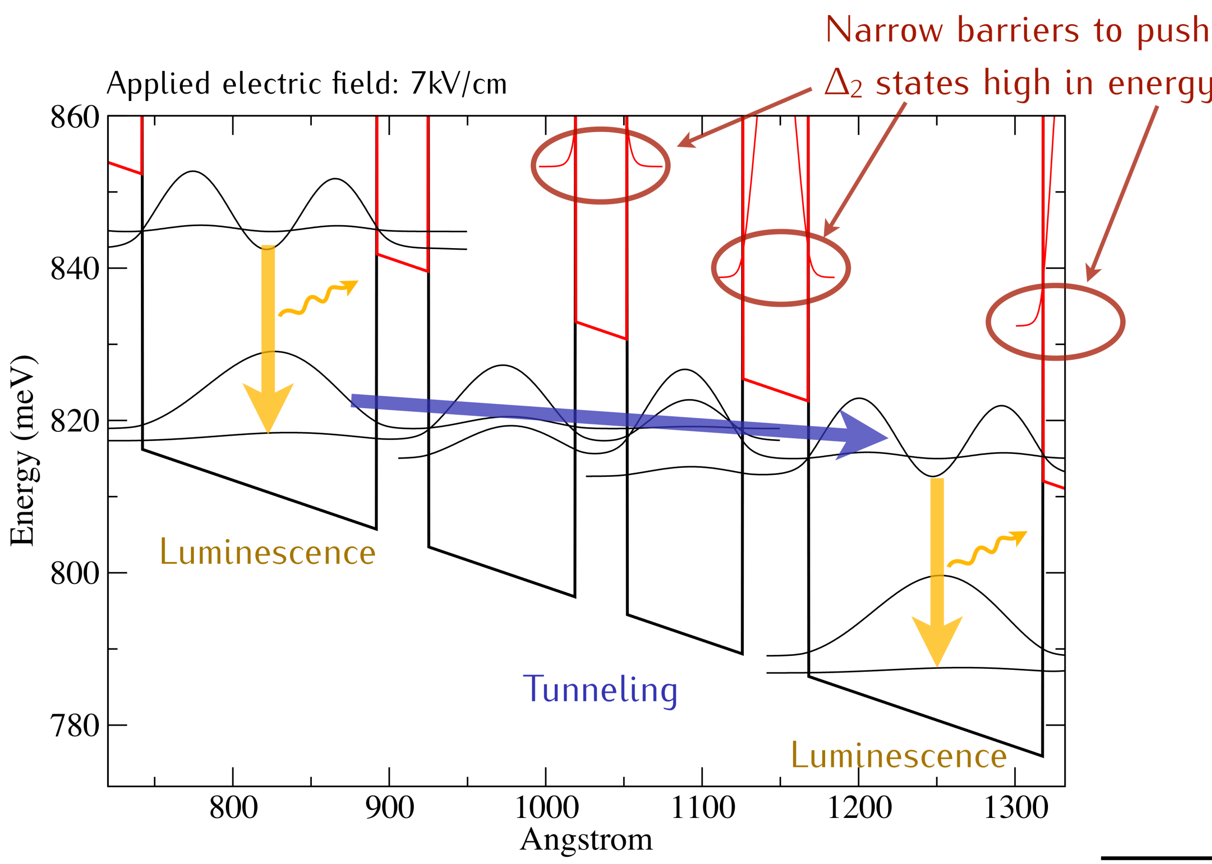
Si_2Ge_{14} Superlattice

2D

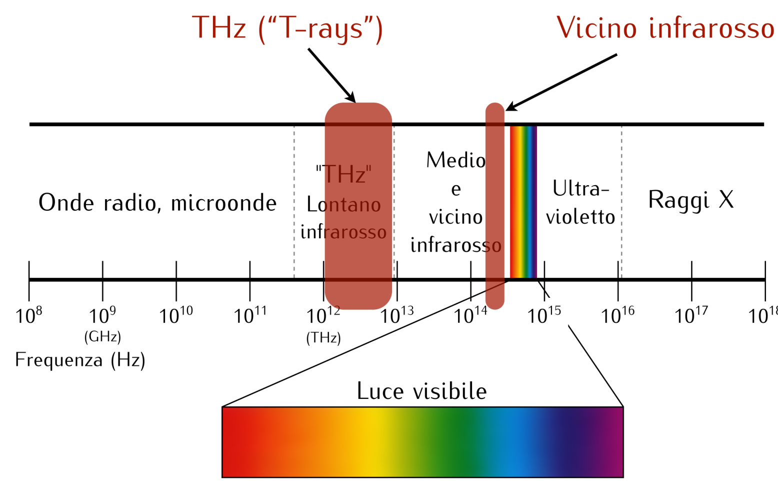


Multiple Quantum Wells for terahertz radiation

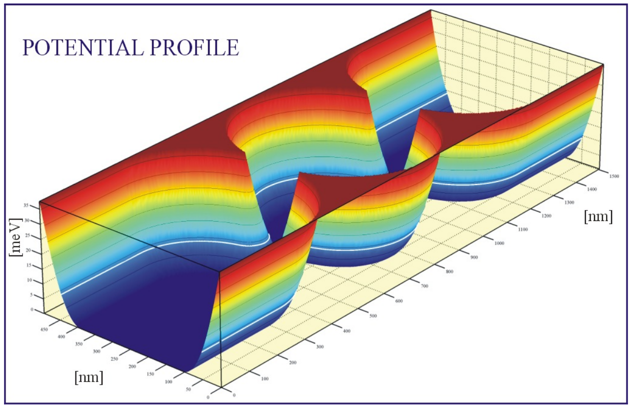
2D



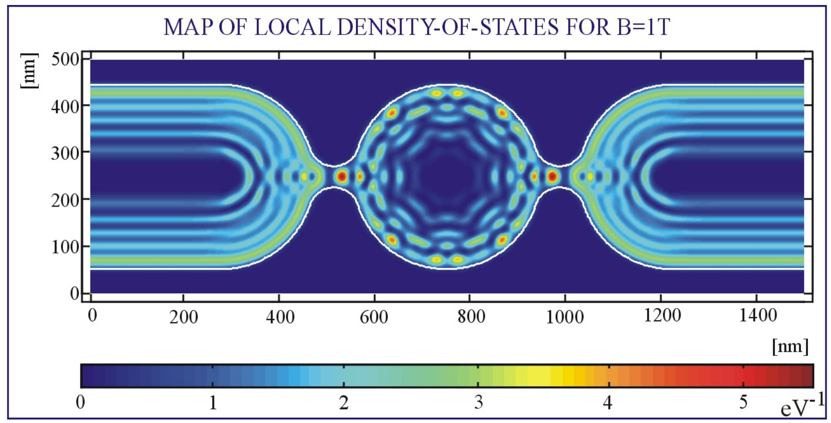
Si/Ge - based materials
Conduction Interband
transitions

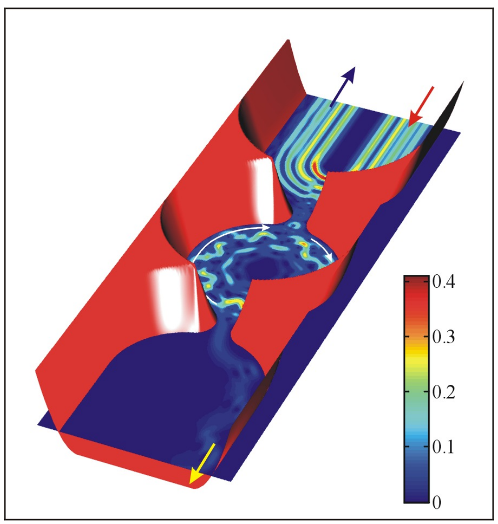


Quantum electronic conduction in nanostructures



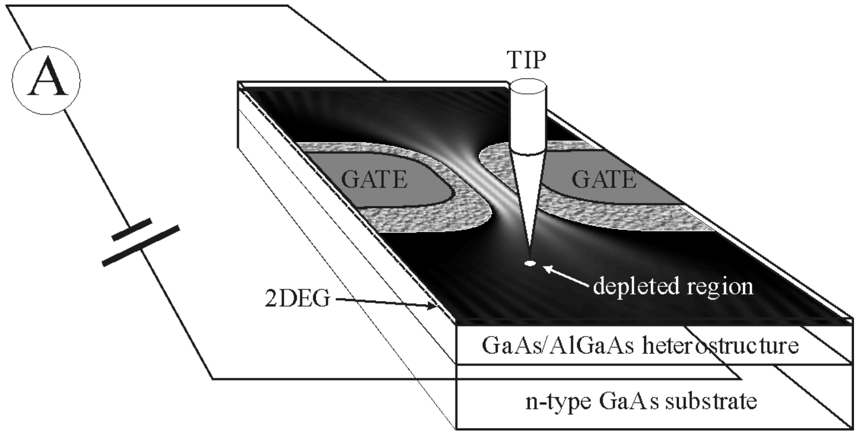
Currents imaging

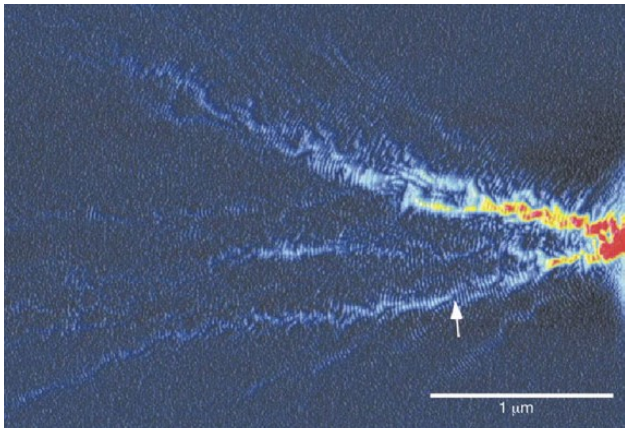




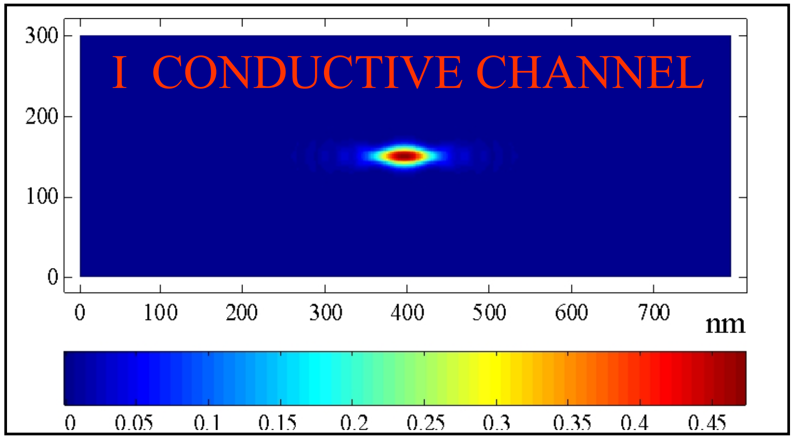
Nanotechnology **18**, 055403 (2007)

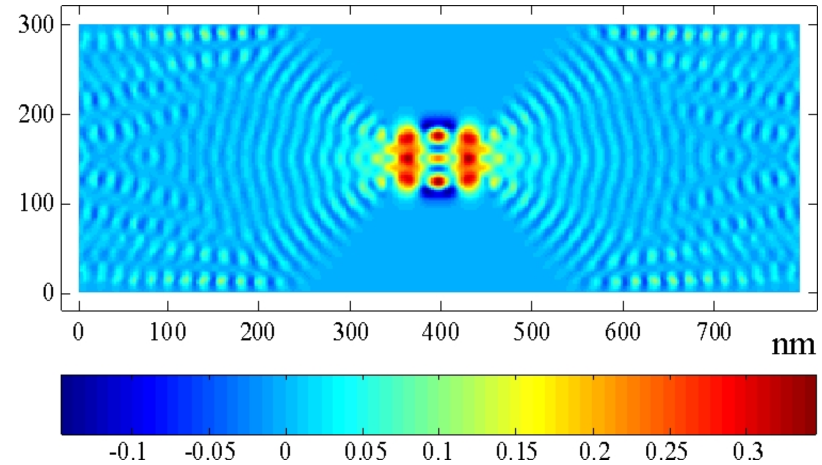
Charge transport :Microscopic Currents Imaging

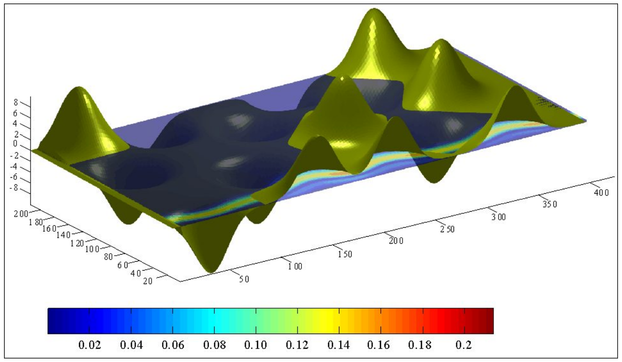




Topinka *et al*., Nature 410, 183 (2001).

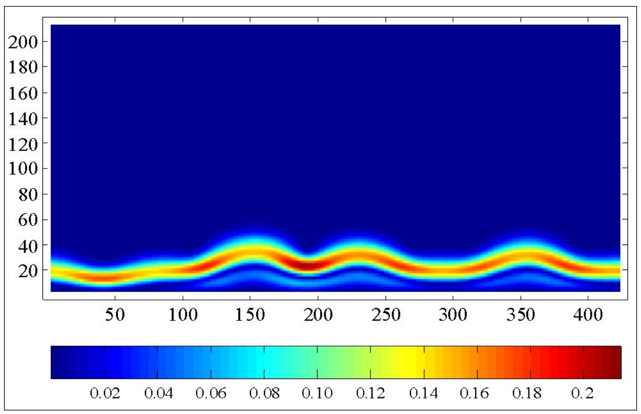




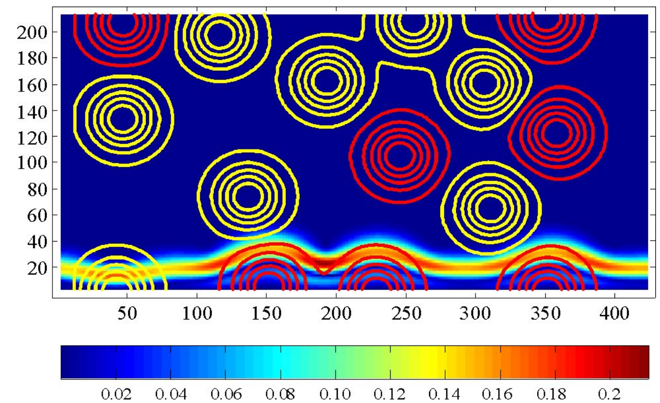


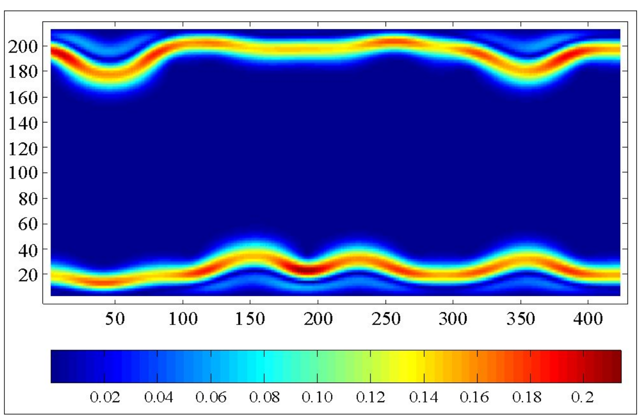
Quantum Hall regime

In Chiral regime the obstacles do not change the total net current through the device. Quantization of conductances is exact.

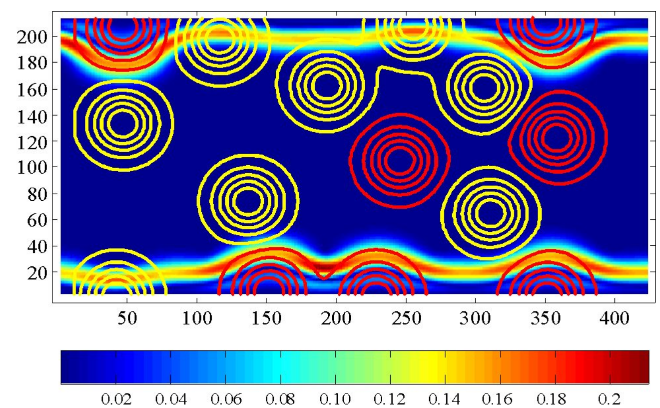


Transport



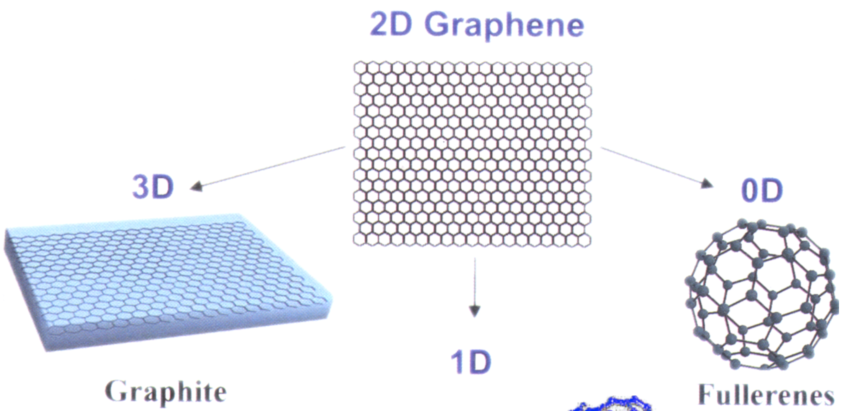


Persistent

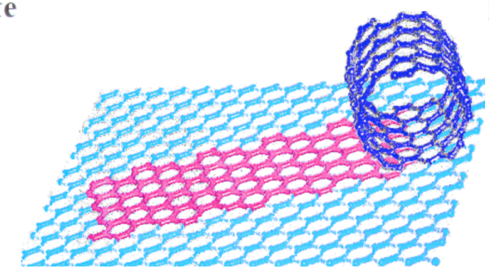


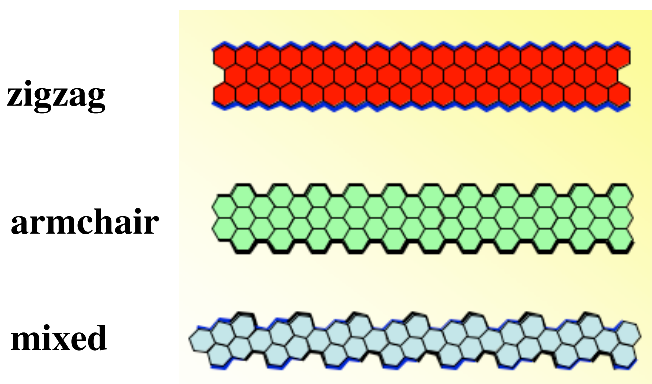
The new carbon era

From 2D-GRAPHITE to GRAPHENE

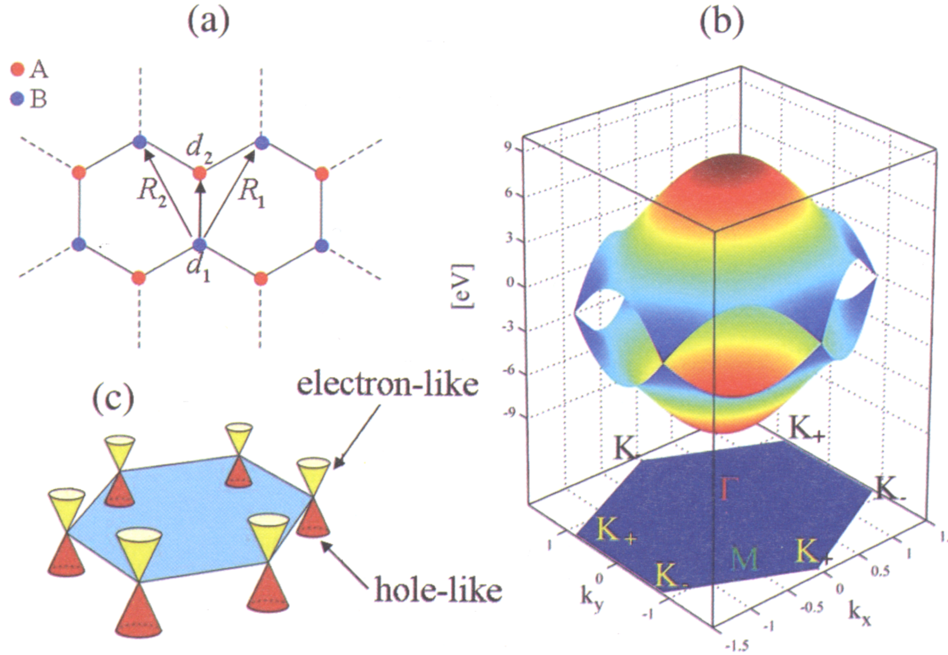


Nanotube





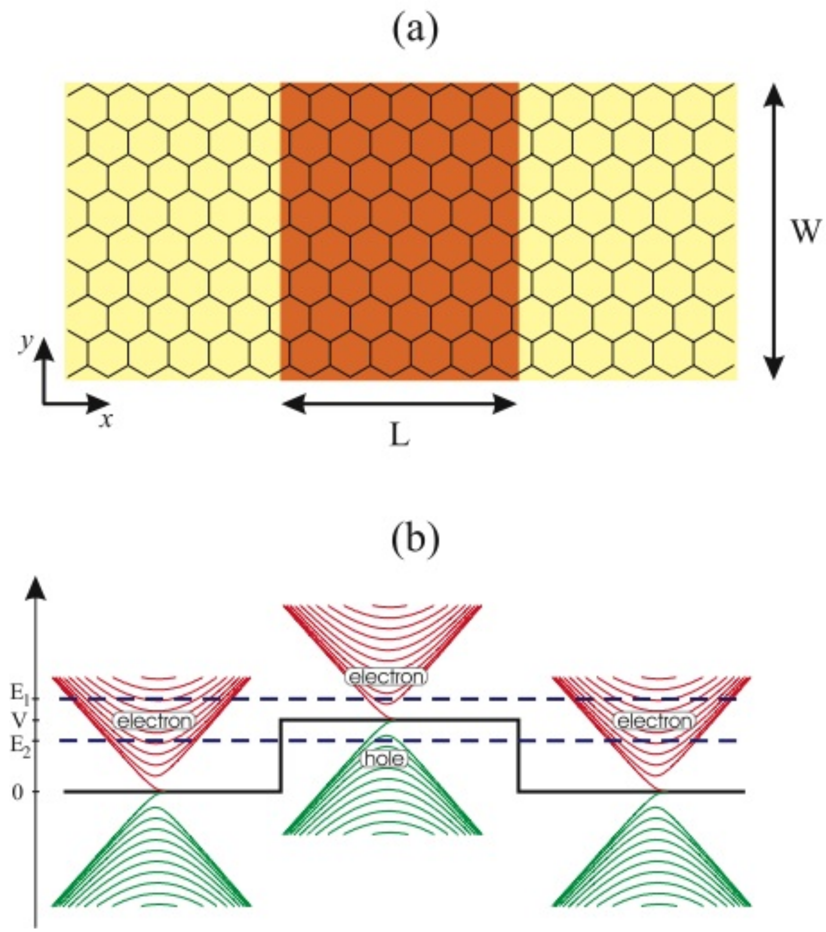
Nanoribbons

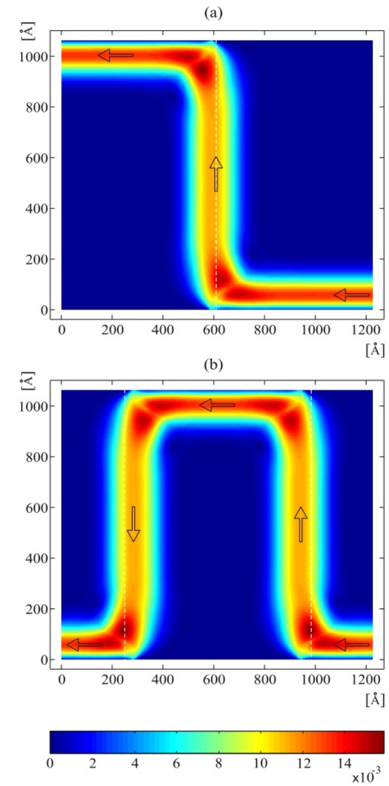


fundamental physics and **technological** issues that involve **graphene**:

Dirac electrons, Klein tunneling in a solid state system
Half-integer quantum Hall effect, Berry phase
Massive electrons in graphene multilayers
High room temperature mobility
Optical conductivity and optical transparency
Screening effects and collective excitations
Electronic and magnetic properties of **graphene ribbons**
Gap opening ………..

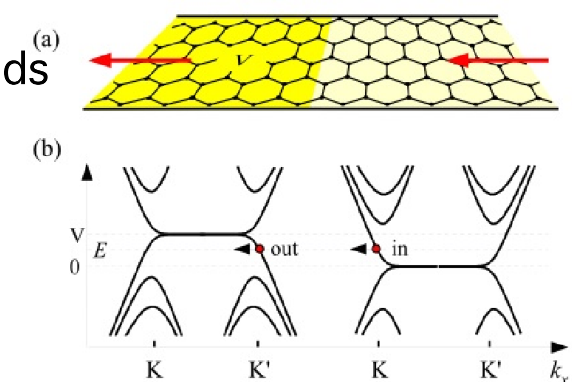
Variation of the potential energy across the ribbon for the injected electrons

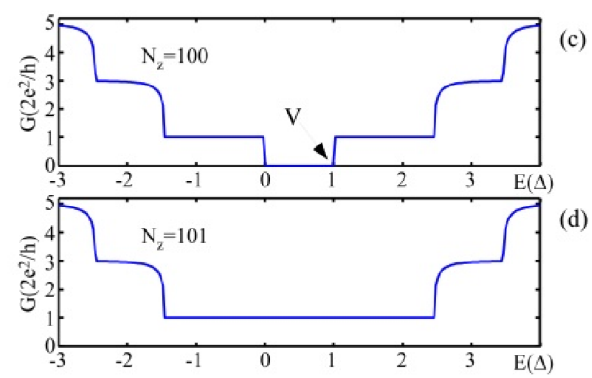




Current distribution
In the presence of H

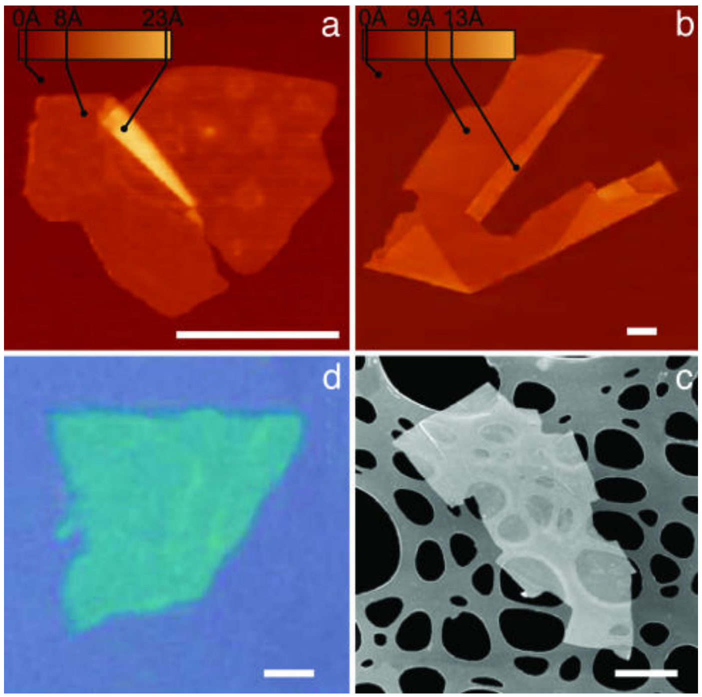
(a, b) Scheme of the energy bands
(c) Differential conductance for
N = 100 carbon chains.
(d) Differential conductance for
N = 101 carbon chains.





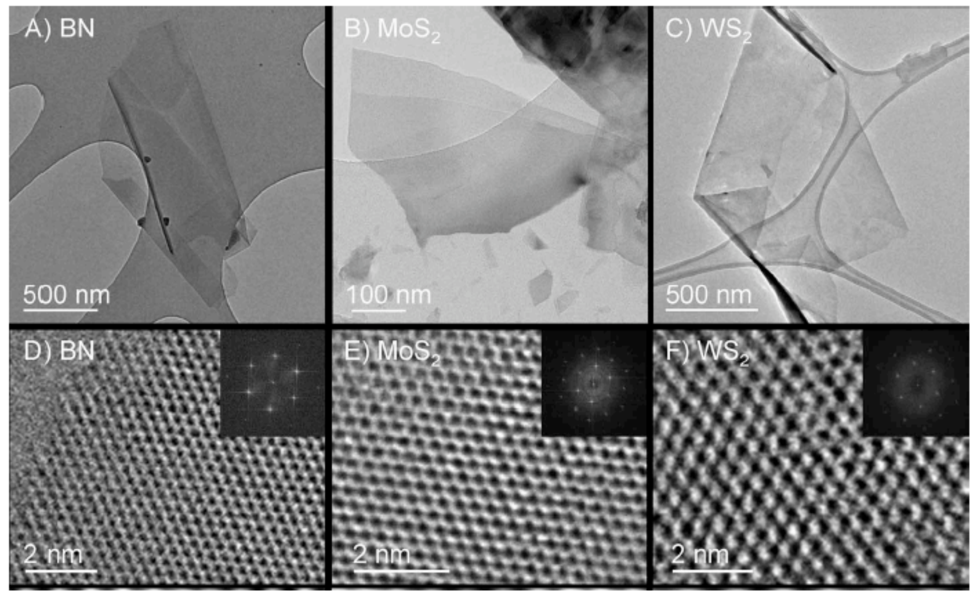
Two dimensional nanosheets exfoliated from layered materials are just behind the corner

MoS_2, WS_2, $MoSe_2$, $MoTe_2$, $TaSe_2$ $NbSe_2$, $NiTe_2$ BN, Bi_2Te_3, $Bi_2Sr_2CaCu_2O_x$



AFM and SEM images of single-layer crystallites of $NbSe_2$ (a), graphite (*b*), $Bi_2Sr_2CaCu_2O_x$ (c), MoS_2 (d)

K. S. Novoselov et al., Proc. Natl. Acad. Sci. U.S.A. 102, 10451 (2005)



TEM images of BN, MoS2 ans WS2

J. N. Coleman et al. Science 331,568 (2011)

Blended with suspensions of other nanomaterials or polymer solutions give rise to new hybrid materials with specific properties

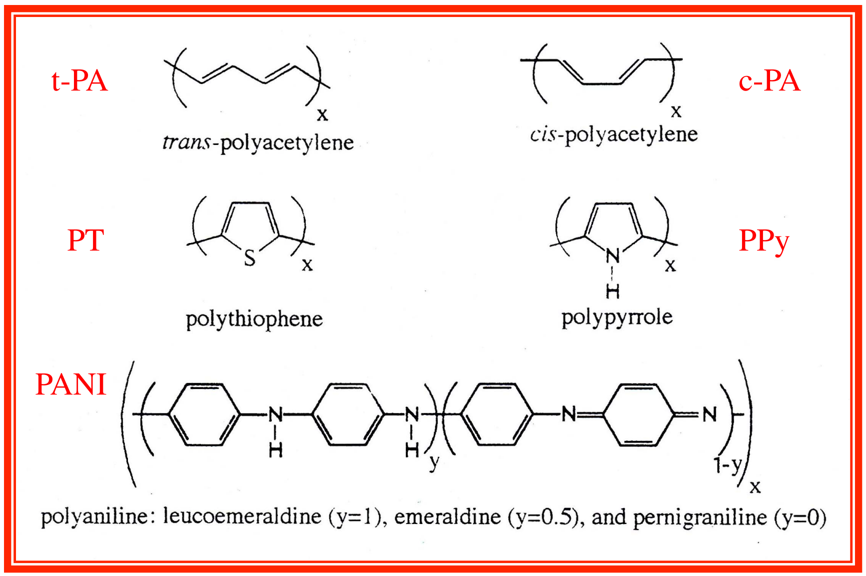
Organic crystals, conducting polymers, biological systems

Conjugated Conducting Polymers (Electronic polymers)

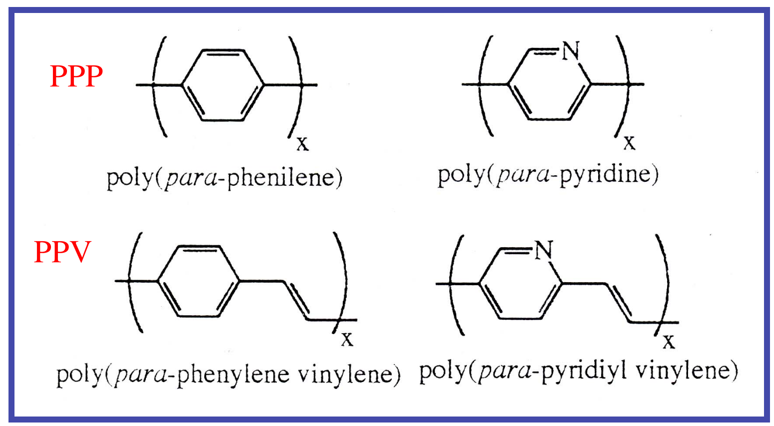
- Electronic polymers are quasi-one dimensional semiconductors (E_G=1 ÷ 3 eV) that can be transformed into metals upon doping

- The unique electronic properties of conjugated polymers derive from the presence of π - electrons with wavefunctions delocalized over long portions of the polymer chain when the molecular structure of the backbone is almost planar.

- The carbon atoms are not fourfold but three-fold coordinated

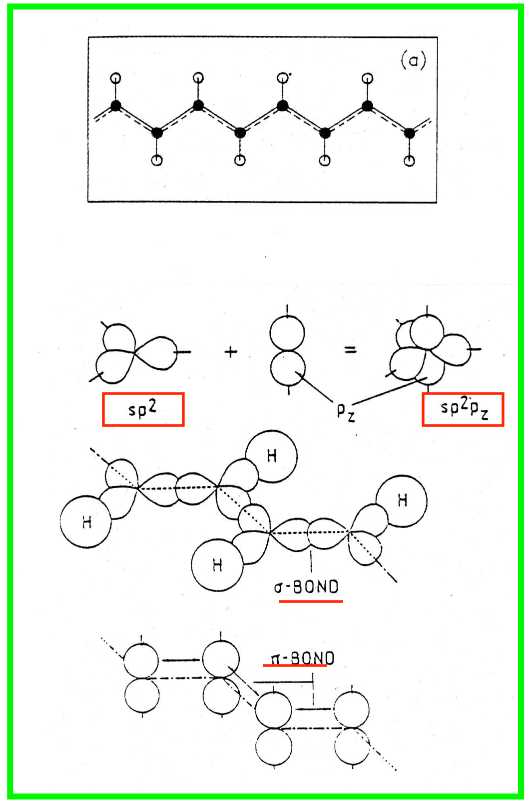


Most studied in the conducting state



Most studied in the semiconducting state π bonds

Conjugated polymers have in common a succession of conjugated i.e. alternate single and double bonds with σ orbitals in the plane of the polymer and one π orbital per atom perpendicular to the plane; e.g trans-polyacetilene



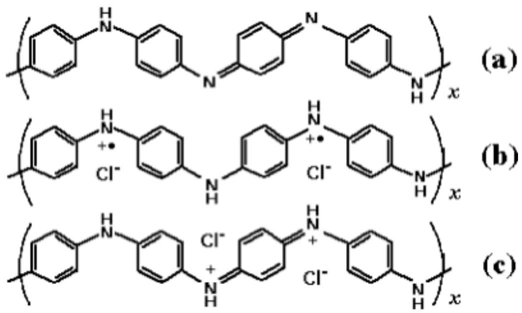
Doping

In conjugated polymers doping means charge transfer:
oxidation (p-type doping)
reduction (n-type doping)
Insertion of counter-ions in the vicinity of the polymer

Heavily doped polymers are conventional metals (disappearance of the gap, Pauli-like susceptibility); however often static conductivity decreases decreasing temperature

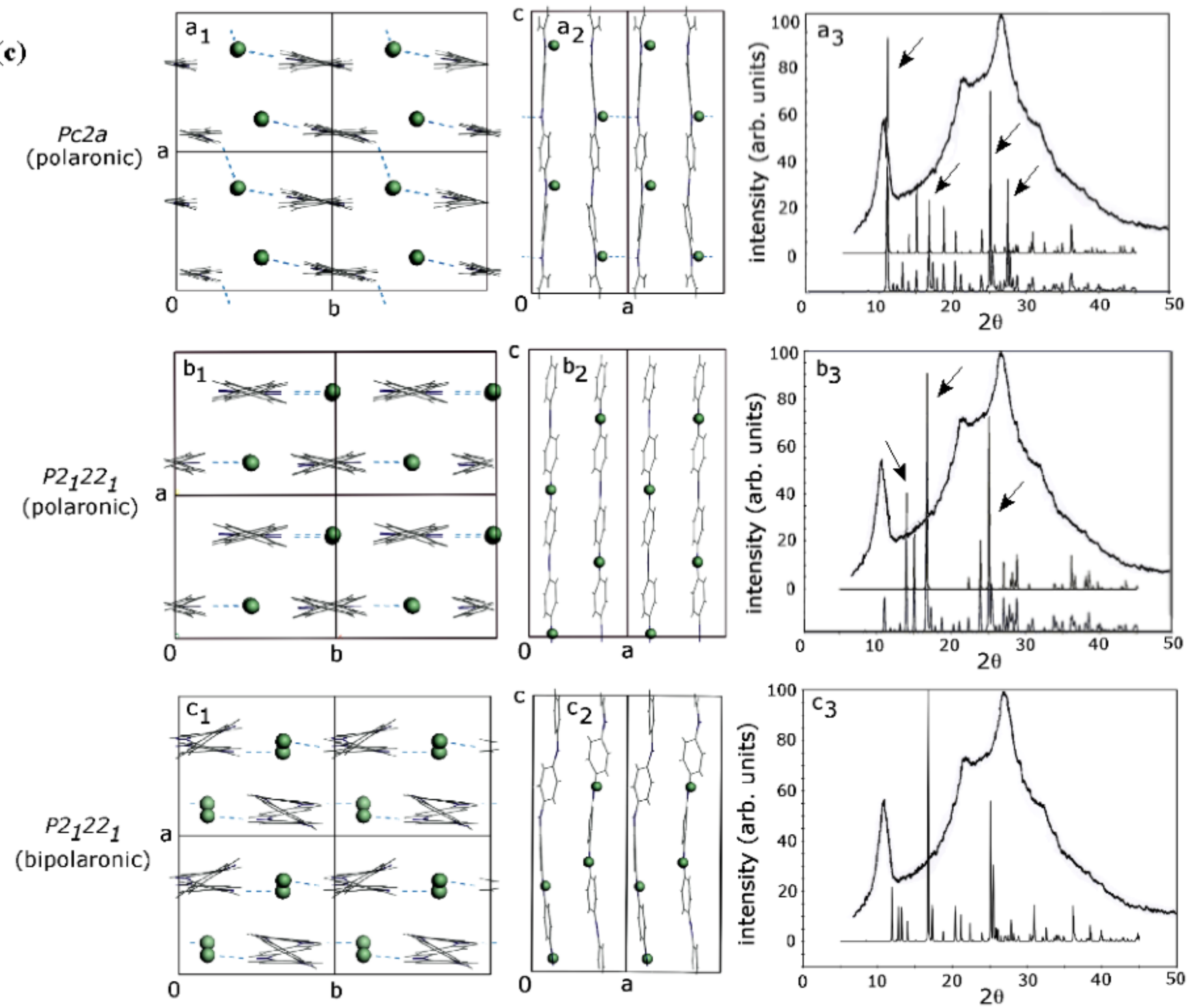
OPEN PROBLEMS

- Intrinsic **nature** of the metallic state and **mechanisms** of charge conduction
- central role of **disorder**, **localization** of states
- **anisotropy** and **dimensionality**



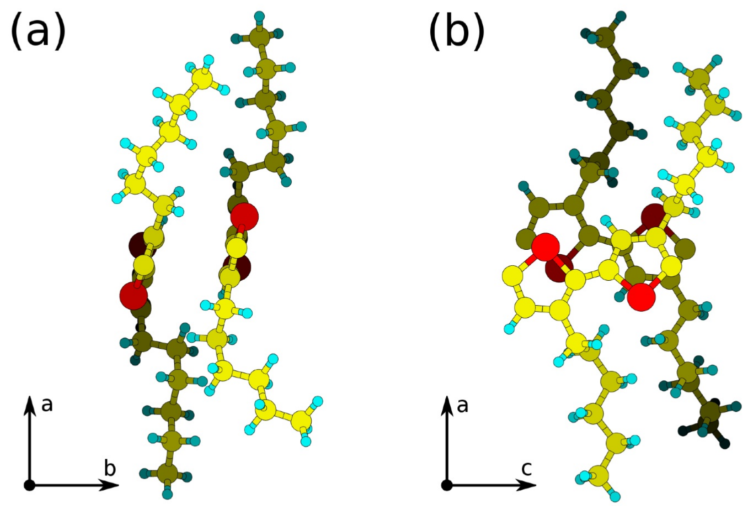
HCl-doped Emeraldine:

From insulator to conductor

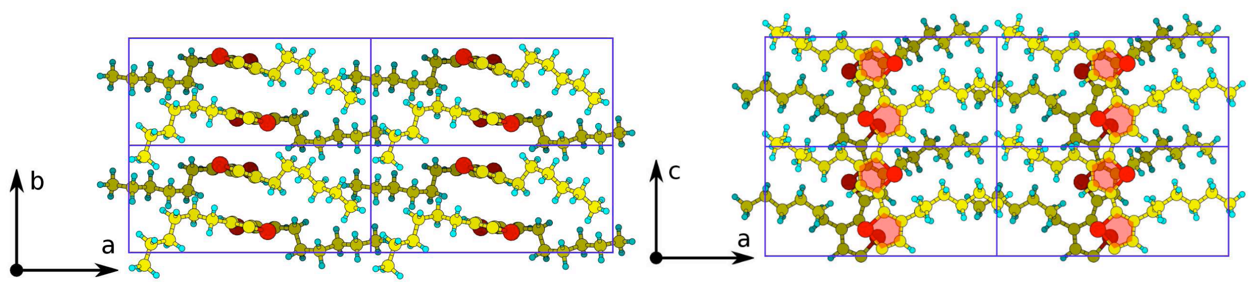


Phys. Rev. B **74**, 033103 (2006)

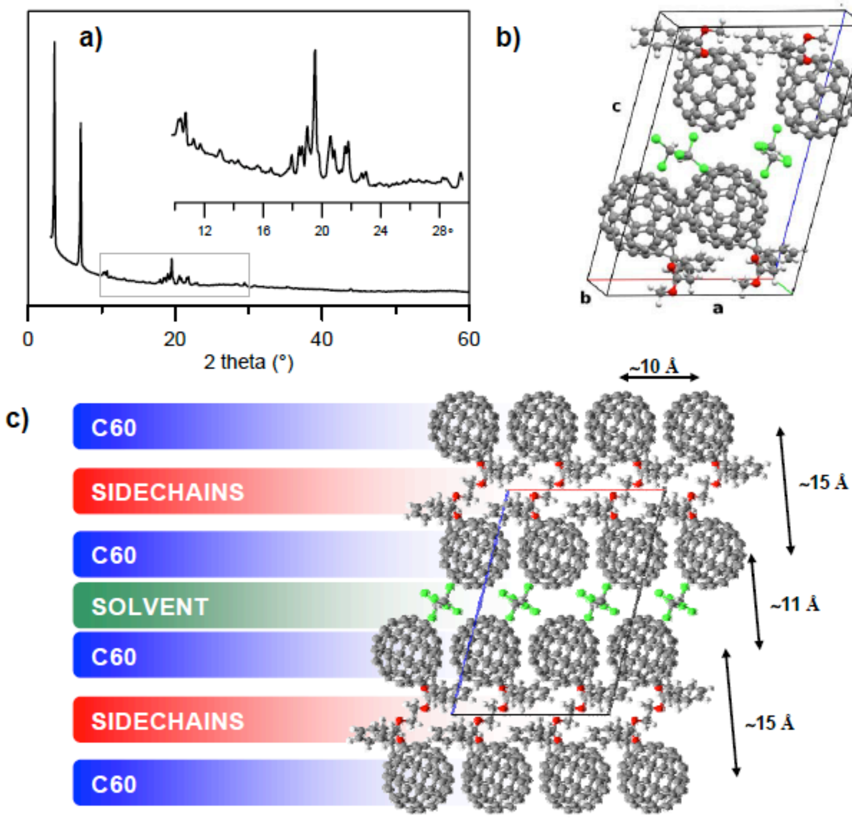
One important issue is the morphology of individual polymeric chains:
Structural studies (XPS) have shown presence of inhomogeneous disorder with nearly crystalline regions within the polymer films and regions where interchain correlations are very short range



Geometrical arrangement and electronic band structure of P3HT chains in the orthorhombic primitive cell,as obtained from KS-DFT-vdW structural optimization



Packing of primitive cells of the crystalline rr-HT-P3HT polymer.



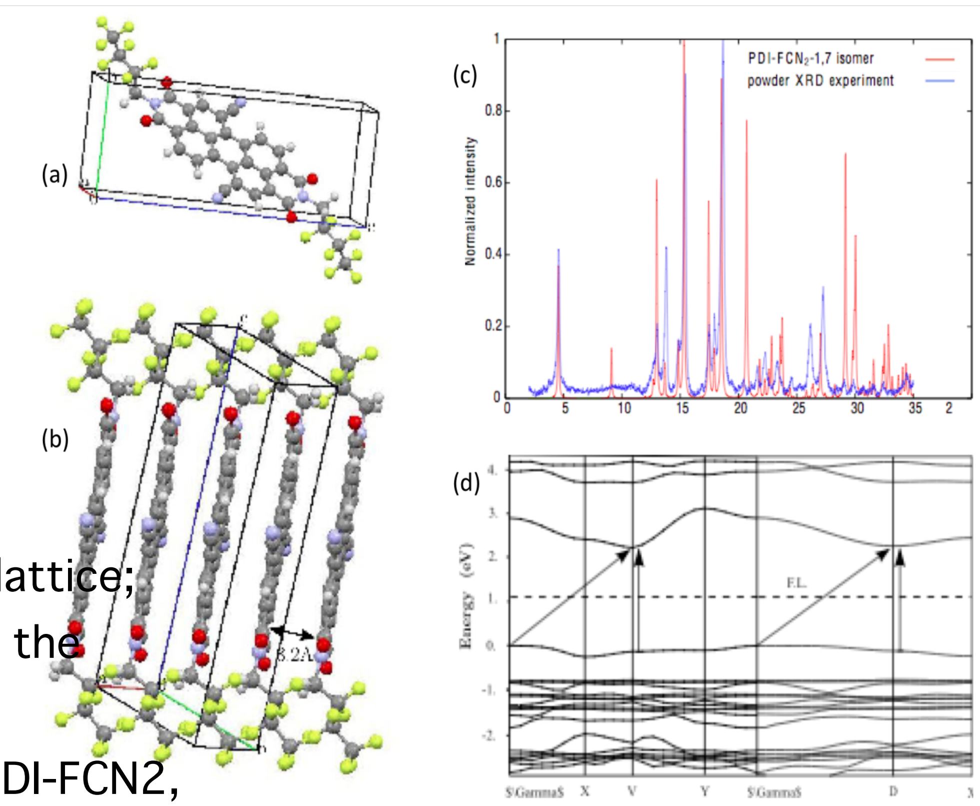
a) XRD pattern of crystalline PCBM

b) Monoclinic primitive cell obtained by modeling.

c) Corresponding PCBM molecular packing.

ORGANIC CRYSTALS
for solar cells

ORGANIC CRYSTALS
for Field Effect Transistors OFET



(a)Primitive cell of the triclinic PDI-FCN2 lattice;

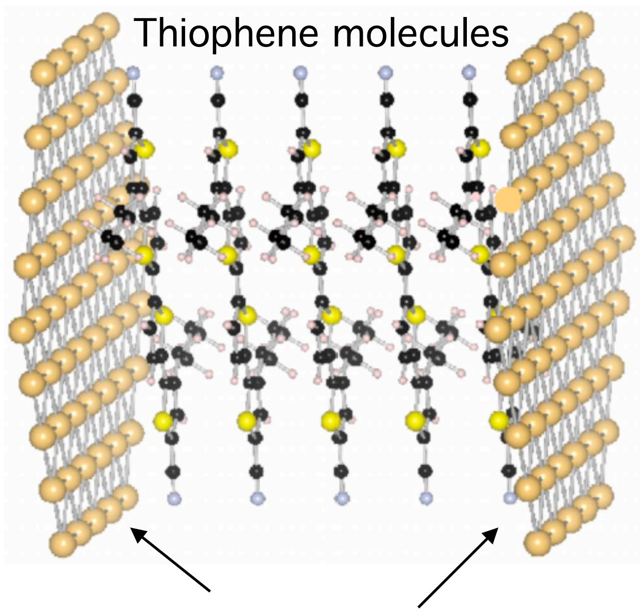
(b) packing of the PDI-FCN2 molecules in the crystalline structures;

(c) powder XRD spectrum of crystalline PDI-FCN2,

(d) DFT band structure.

From inorganic Quantum Wires to Conducting Polymers to Molecule - based electronics

Can a molecule act as an interconnect in a conducting Nanojunction? Toward the ultimate limit of miniaturization

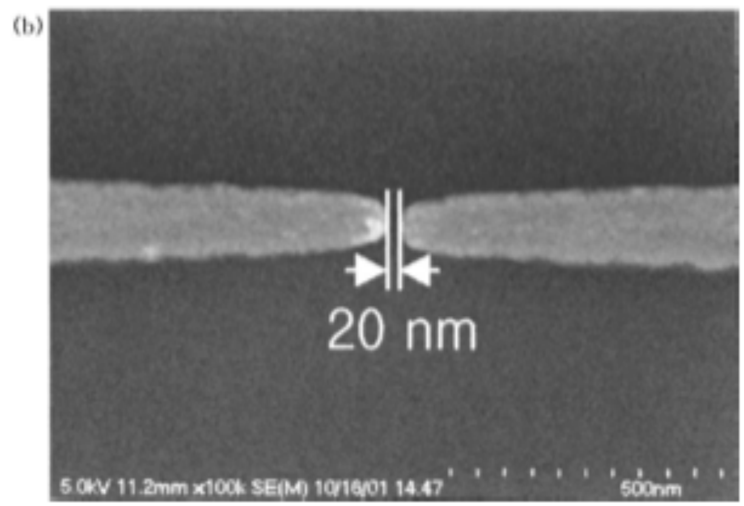


K. Morawetz et al. PRB 79, 085405 (2009)

DNA as a biological molecular wire

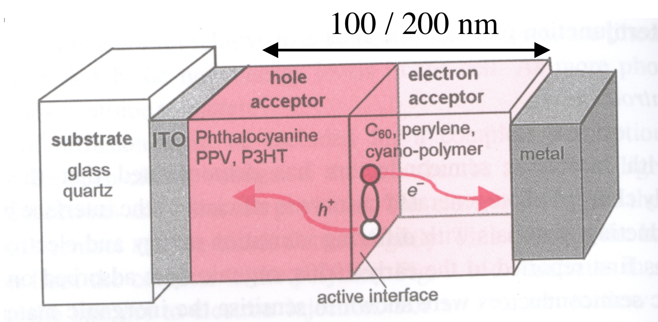
R. G. Enders et al.
Rev.Mod. Phys. 76,195 (2004)

M. Zwolak et al.
Rev. Mod. Phys. 80, 141(2008)



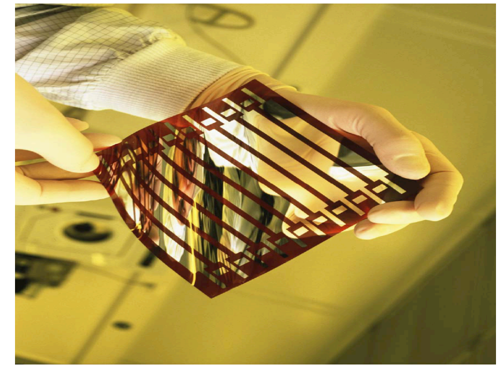
Materials for solar energy conversion

All- Organic Solar cells



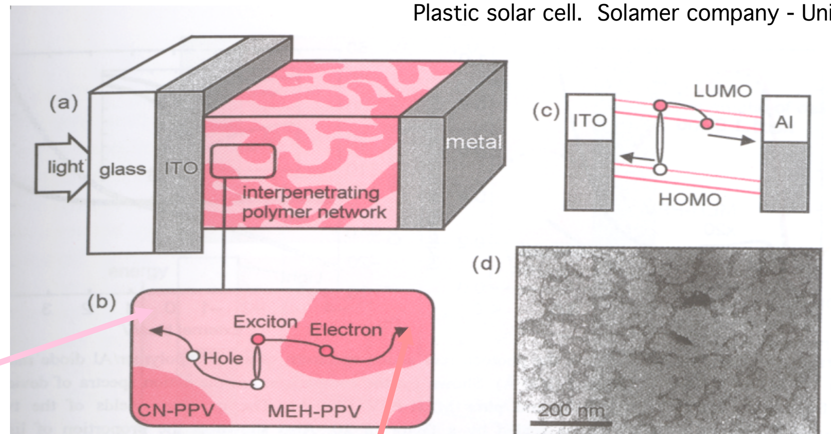
D. Uglietti, Univ. Geneva)

Organic Hetero
-Junction n-p Cell



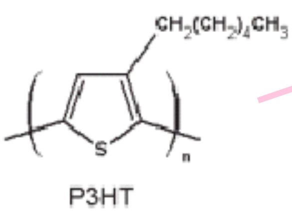
Plastic solar cell. Solamer company - Univ. Chicago

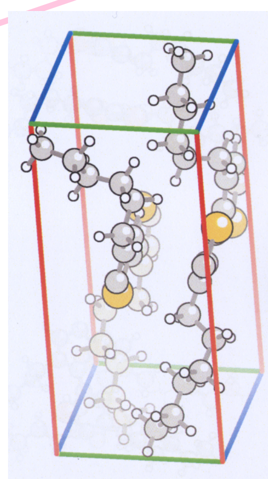
The Bulk Hetero
-Junction

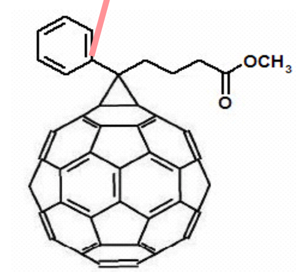


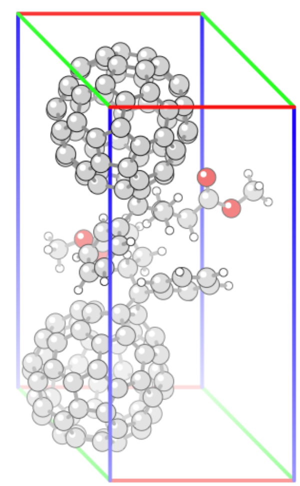
Morphology must be optimised !

Example: The P3HT - PCBM system









Conductive polymer

electron donor

Hole transport material

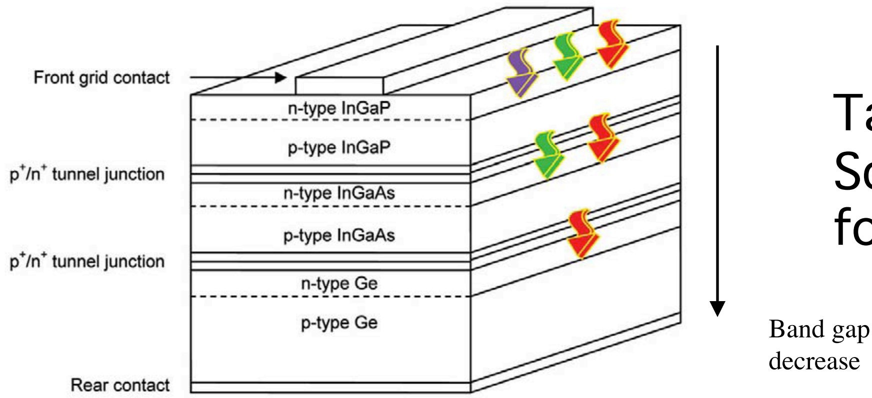
R. Colle et al., Phys. Stat. Sol. (2011)

C_{60} derivative PCBM

electron acceptor

Electron transport material

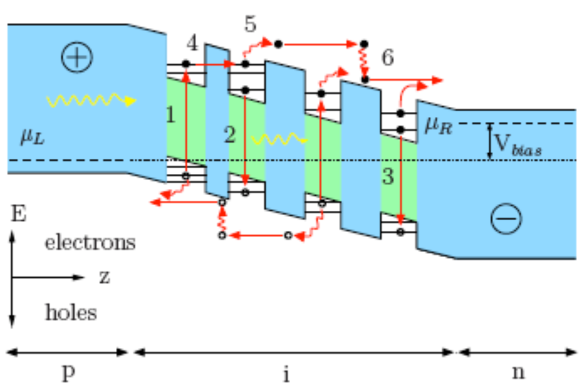
Inorganic photovoltaics



Tandem or multicolor cells:
Schematic of a three band gap solar cell for photon selectivity

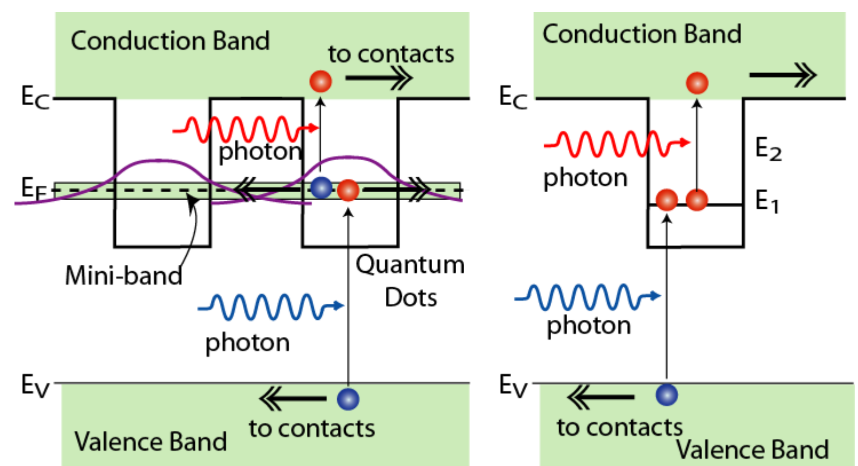
G. Conibeer, Materials today, 42,10 (2007)

Third generation photovoltaics:
Quantum wells, Quantum dots Solar cell



U. Aheberard et al., PRB 77,125343 (2008)

1 - photogeneration
2 - rad. recombination
3 - non rad.recombination
4 - tunneling
5 - thermal escape
6 - relaxation by optical phonons



N. S. Lewis, Science, 315, 798 (2007)

And more ….

NON CRYSTALLINE SYSTEMS

HIGH TEMPERATURE SUPERCONDUCTIVITY

SPINTRONICS

PHOTONICS

PLASMONICS

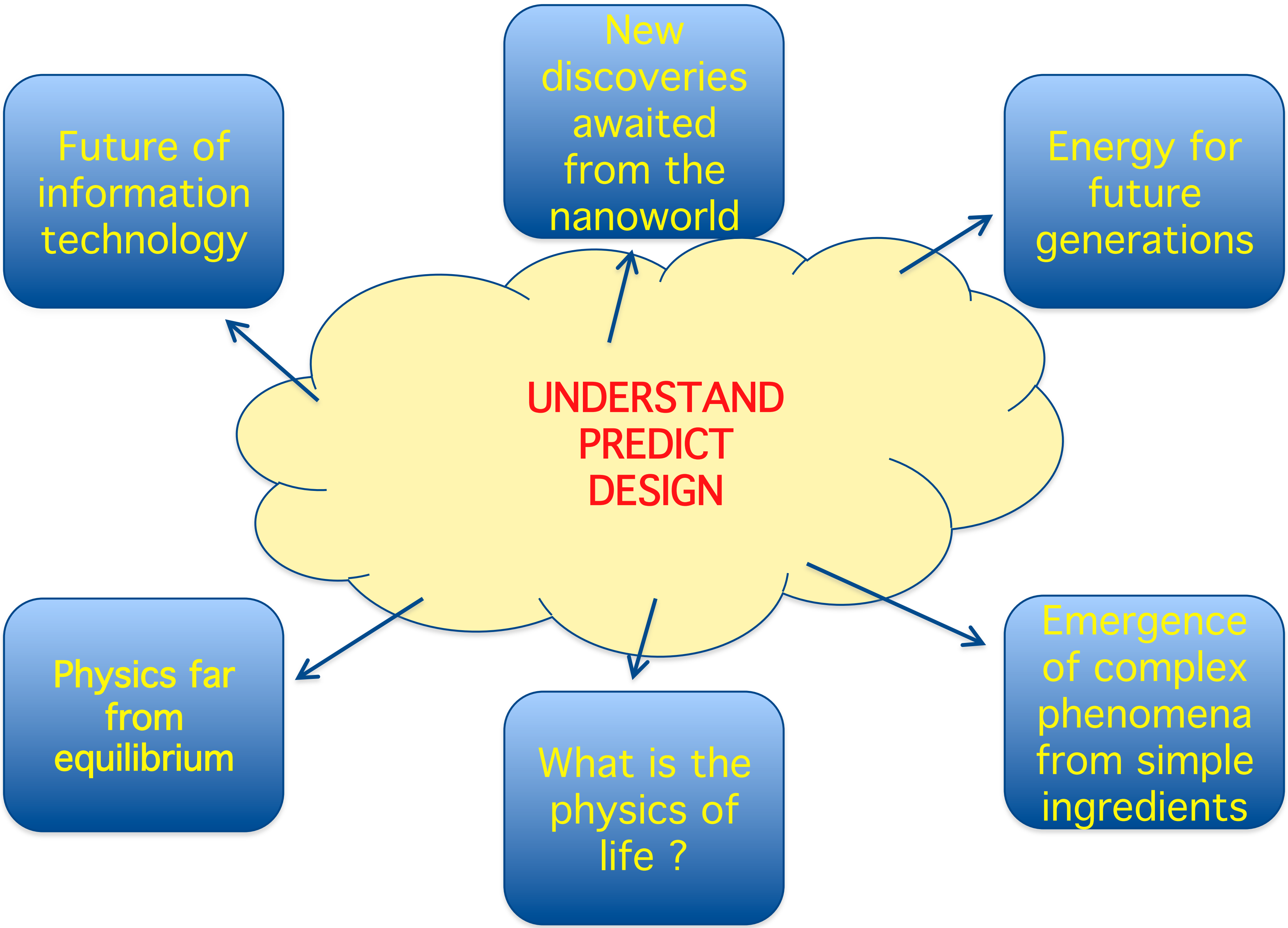
STRONGLY CORRELATED SYSTEMS

MAGNETISM IN NANOSTRUCTURES

THERMOELECTRICS

……………..
……………..

Mission


New discoveries awaited from the nanoworld
Future of information technology
Energy for future generations
UNDERSTAND
PREDICT
DESIGN
Physics far from equilibrium
What is the physics of life ?
Emergence of complex phenomena from simple ingredients

Predictions for the next years is rather hard in the field of CMD. Theory and numerical simulations will take a large role in predicting and understanding basic and technological challenges .

There is no doubt that in the next future

- synthesis of new materials,
- more sophisticated experimental probes,
- emergence of new phenomena
- but also needs of the society in different areas as energy,health and security....

will drive theoreticians and experimentalists of CMD in a land where boundaries of traditional disciplines are intertwined.

A final consideration:

"*The 20th century was a period of remarkable fundamental and technological progress in CMP. Continued federal and private investments led to considerable advances in the basic understanding of condensed-matter phenomena.*

Years and often decades later, these advances led in turn to the invention of devices that now form the basis of much of our technological society, including the transistor, the integrated circuit, the laser, magnetic resonance imaging, liquid-crystal displays, and, more recently, high-efficiency solid-state lighting.

U.S. leadership in nurturing invention, from initial scientific discoveries to commercial technological products, has contributed significantly to this nation's economic strength. In particular, the industrial development of many of these technologies has led to current U.S. leadership in computing and global communications.

Although the relationship is difficult to measure quantitatively, there is a consensus among economists that advances in technology have been the main driver of economic growth over the past 60 years."

Source: National Research Council
of the National Academies