Fundamentals of

Condensed Matter Physics
Solid State Physics
Materials Physics

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Much complexity in Solid State Physics
- Largest discipline in physics

Unifying theory is Quantum Mechanics

Importance of material science in Africa

Abundance of raw materials
- Need to beneficiate, add more value

Excellent mining, geology, minerology
- High tech material science in specific areas, e.g. hard materials, Pt, Fe, Steel, Cu, Au, U, diamonds, etc.
- Turn into mechanized goods for economic development

Need for excellent students, researchers, academics, industrialists
- Create longer-term interest in academic-industrial partnerships

Need a higher level material science research endeavour
- Across all of Africa

Clash of expectations?

Students' Expectations

What do I need to know?

Why do I need to know this?

What is going to be in the examinations?

How can I pass/get a distinction?

My Expectations

I hope and expect that you will understand and appreciate the great accomplishments of Solid State Physics over the past 100 years

You should notice the contributions to the modern technical world in which we live

You will be moved by the sheer beauty of the subject and you will aspire to continue to study the subject into the future (Masters, PhD …)

Aim to become a researcher in Solid State Physics (theoretical, computational, experimental)

Have a successful career, contribute positively to society and the economy, aim to be innovative and entrepreneurial

Ubiquitous nature

New materials for modern technical applications

E.g. Carbon (graphite) fibre in aerospace industry, sports equipment

Many solid state physics experimental techniques have found their way into mainstream society

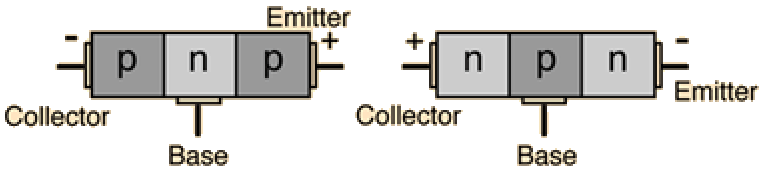
E.g. MRI (NMR), CAT scans

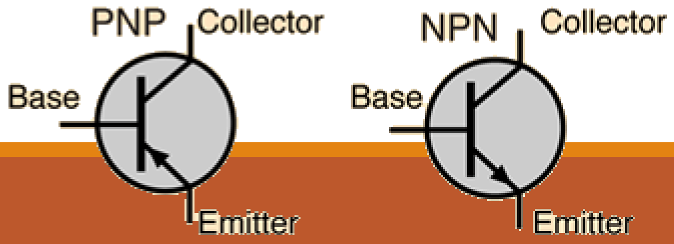
Nobel prizes in physics

Many awarded in areas of Solid State Physics

- studies of electrons

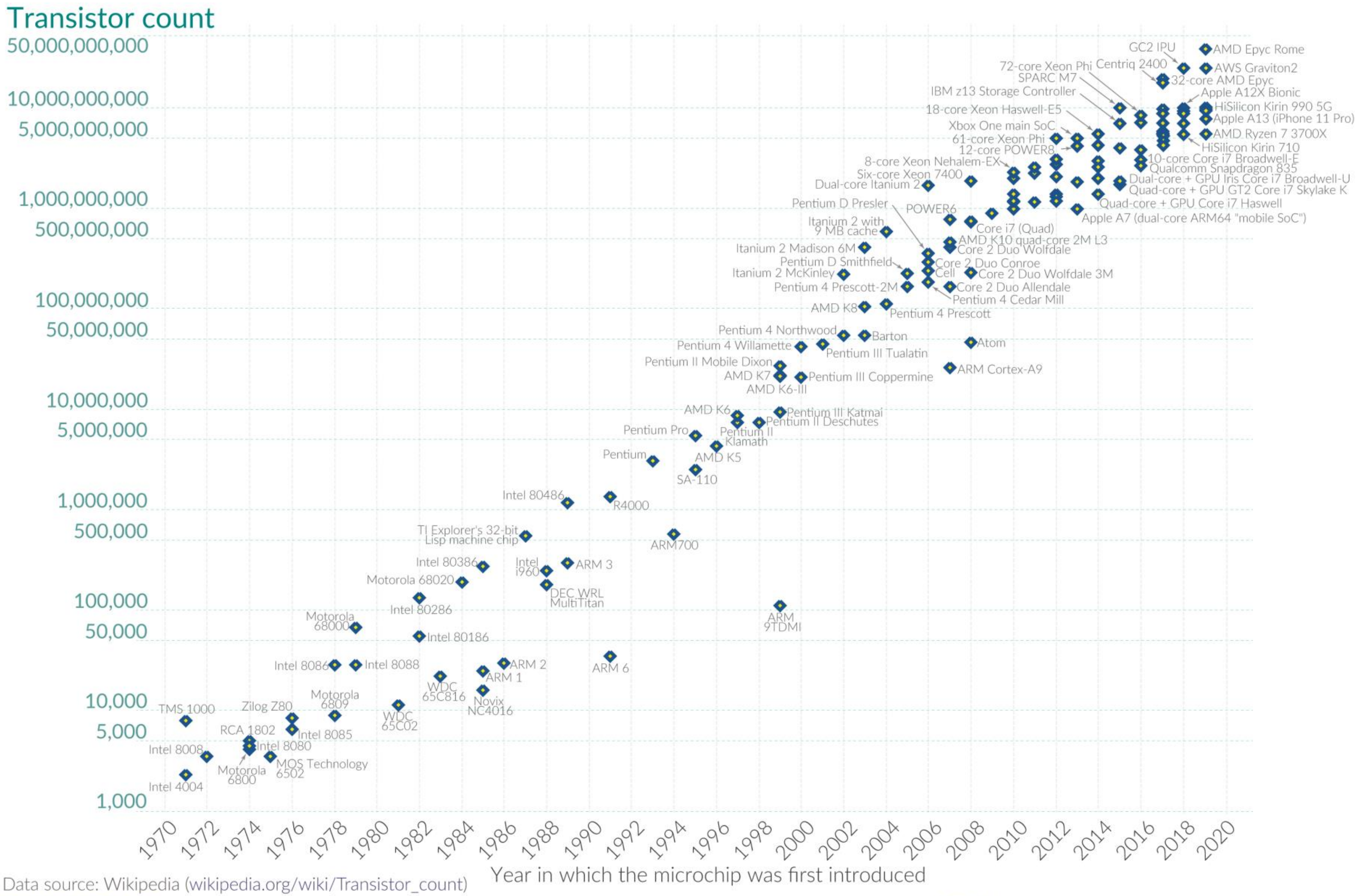
Bardeen, Shockley and Brattain





Moore’s Law: The number of transistors on microchips doubles every two years

Moore's law describes the empirical regularity that the number of transistors on integrated circuits doubles approximately every two years. This advancement is important for other aspects of technological progress in computing – such as processing speed or the price of computers.



Data source: Wikipedia (wikipedia.org/wiki/Transistor_count)

OurWorldinData.org – Research and data to make progress against the world’s largest problems.

What is Solid State Physics?

Study of solid state, condensed matter, material system

Quantum mechanical

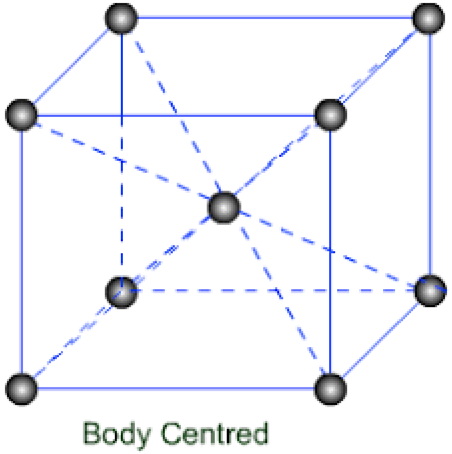
Primarily at the atomic, electronic level

For intellectual curiosity (fundamental research), but also for technical contributions to modern civilization (applied research)

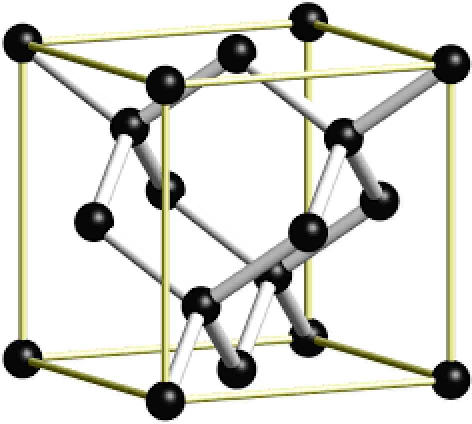
Stone age (2.5million years ago), bronze age, iron age …. opto-electronic age

Electron only discovered in 1897

iron ore

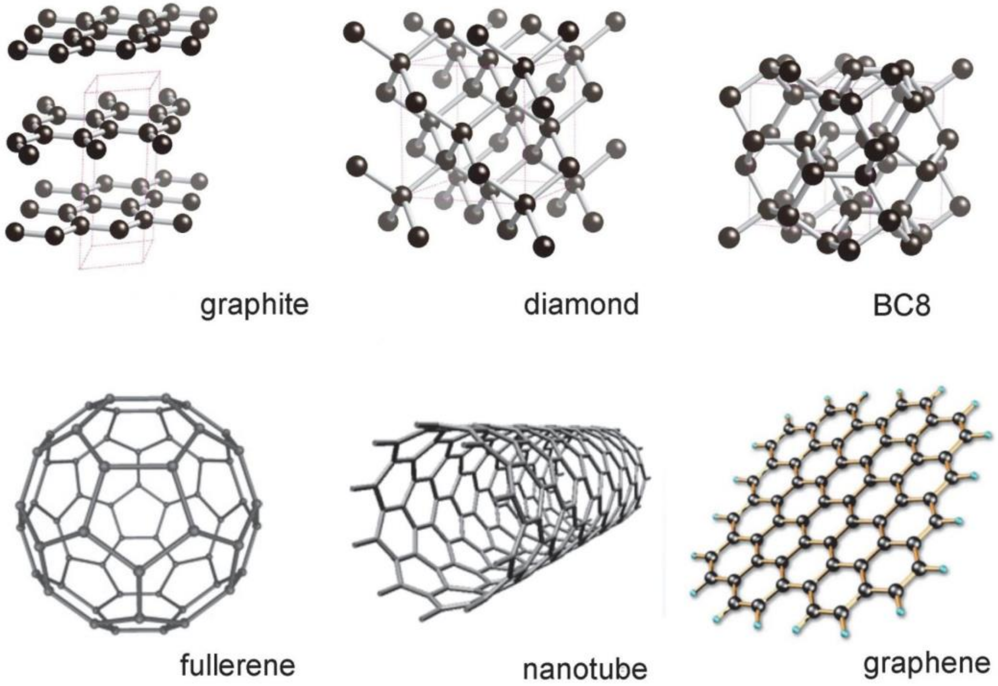


rough diamond



cut and polished diamond

graphite



Carbon-based elemental systems

Silicon Carbide

Carbon-based compound system

- Different structures: cubic, hexagonal
- Strong material: high elastic constants, high melting temperature
  - Used as cutting tool, abrasives, powders for technical ceramics
  - Car brakes, armoured vests
  - Heat shielding, ceramics in NASA space vehicles
  - Nuclear cladding
- Bang gap material
  - LED’s, semiconductor devices, high temperature applications
- High refelectivity
  - Telescope mirrors, e.g. Herschel Space Telescope

Metallic alloys

Stainless steel – Fe + Cr + other trace elements

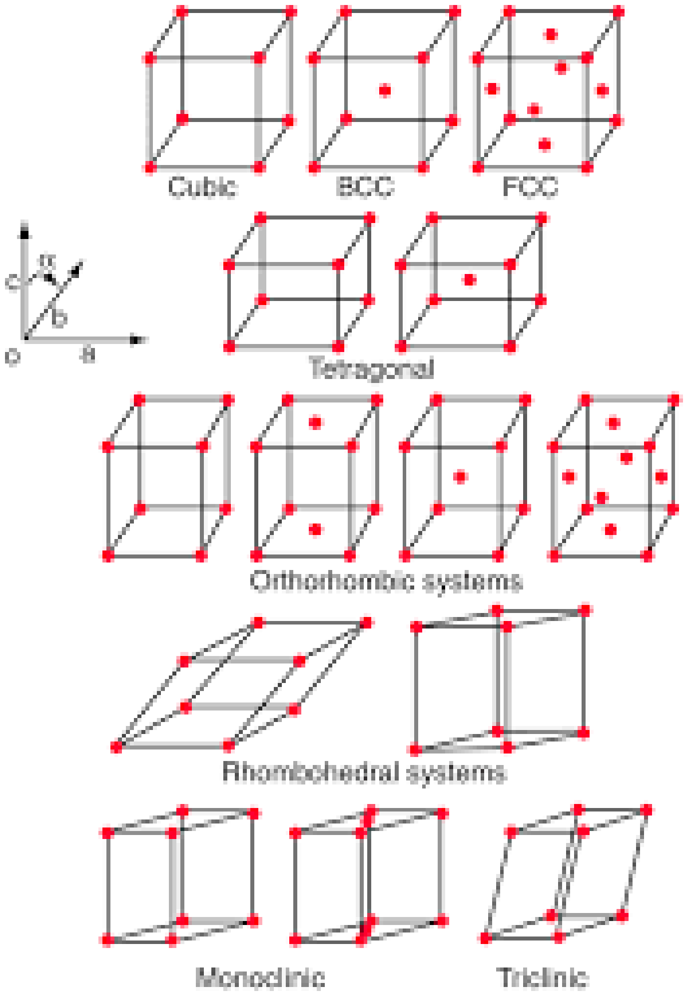
Aluminium alloys – Al + Cu, Mn, Mg, Cr

- for aircraft structure

Nickel alloys – Ni + Co, Cr, Al, Ti, Fe, Mo, etc

- for turbines

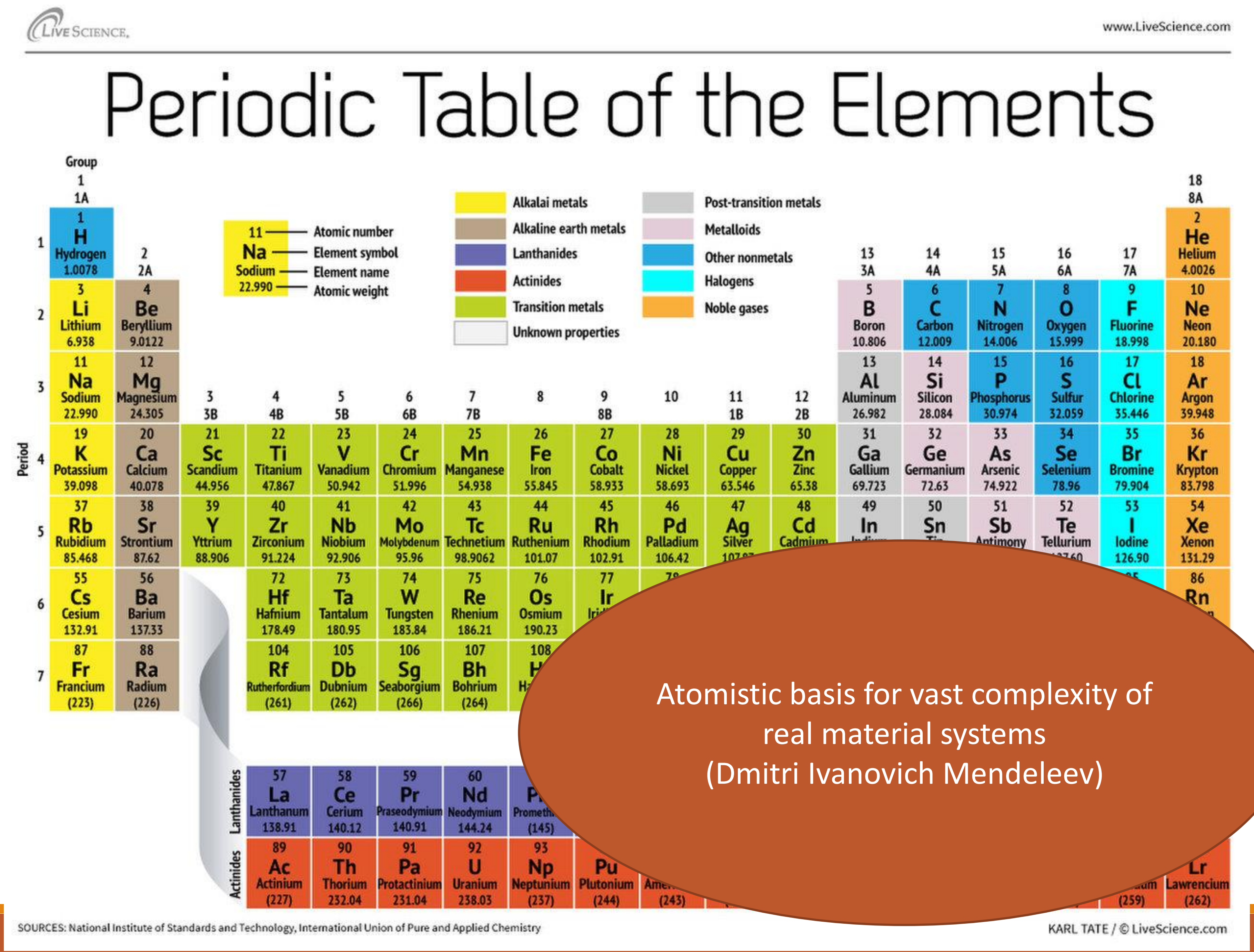
Binary and ternary systems



Structure and composition gives rise to an infinite number of different possible material systems, each with its unique set of characteristics and properties

Why only 118 elements?

Where have the elements come from?



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Periodic Table of the Elements

11 — Atomic number
Na — Element symbol
Sodium — Element name
22.990 — Atomic weight

- 🟨 Alkalai metals
- 🟫 Alkaline earth metals
- 🟪 Lanthanides
- 🟥 Actinides
- 🟩 Transition metals
- ⬜ Unknown properties
- ⬜ Post-transition metals
- ⬜ Metalloids
- 🟦 Other nonmetals
- 🟦 Halogens
- 🟧 Noble gases

Period	Group 1 1A	2 2A	3 3B	4 4B	5 5B	6 6B	7 7B	8	9 8B	10	11 1B	12 2B	13 3A	14 4A	15 5A	16 6A	17 7A	18 8A
1	1 H Hydrogen 1.0078																	2 He Helium 4.0026
2	3 Li Lithium 6.938	4 Be Beryllium 9.0122											5 B Boron 10.806	6 C Carbon 12.009	7 N Nitrogen 14.006	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180
3	11 Na Sodium 22.990	12 Mg Magnesium 24.305											13 Al Aluminum 26.982	14 Si Silicon 28.084	15 P Phosphorus 30.974	16 S Sulfur 32.059	17 Cl Chlorine 35.446	18 Ar Argon 39.948
4	19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.867	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.845	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.63	33 As Arsenic 74.922	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 83.798
5	37 Rb Rubidium 85.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.96	43 Tc Technetium 98.9062	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.91	46 Pd Palladium 106.42	47 Ag Silver	48 Cd Cadmium	49 In	50 Sn	51 Sb Antimony	52 Te Tellurium	53 I Iodine 126.90	54 Xe Xenon 131.29
6	55 Cs Cesium 132.91	56 Ba Barium 137.33		72 Hf Hafnium 178.49	73 Ta Tantalum 180.95	74 W Tungsten 183.84	75 Re Rhenium 186.21	76 Os Osmium 190.23	77 Ir	78								86 Rn
7	87 Fr Francium (223)	88 Ra Radium (226)		104 Rf Rutherfordium (261)	105 Db Dubnium (262)	106 Sg Seaborgium (266)	107 Bh Bohrium (264)	108 H										

Lanthanides	57 La Lanthanum 138.91	58 Ce Cerium 140.12	59 Pr Praseodymium 140.91	60 Nd Neodymium 144.24	P Prometh (145)										
Actinides	89 Ac Actinium (227)	90 Th Thorium 232.04	91 Pa Protactinium 231.04	92 U Uranium 238.03	93 Np Neptunium (237)	Pu Plutonium (244)	Ame (243)							um (259)	Lr Lawrencium (262)

SOURCES: National Institute of Standards and Technology, International Union of Pure and Applied Chemistry

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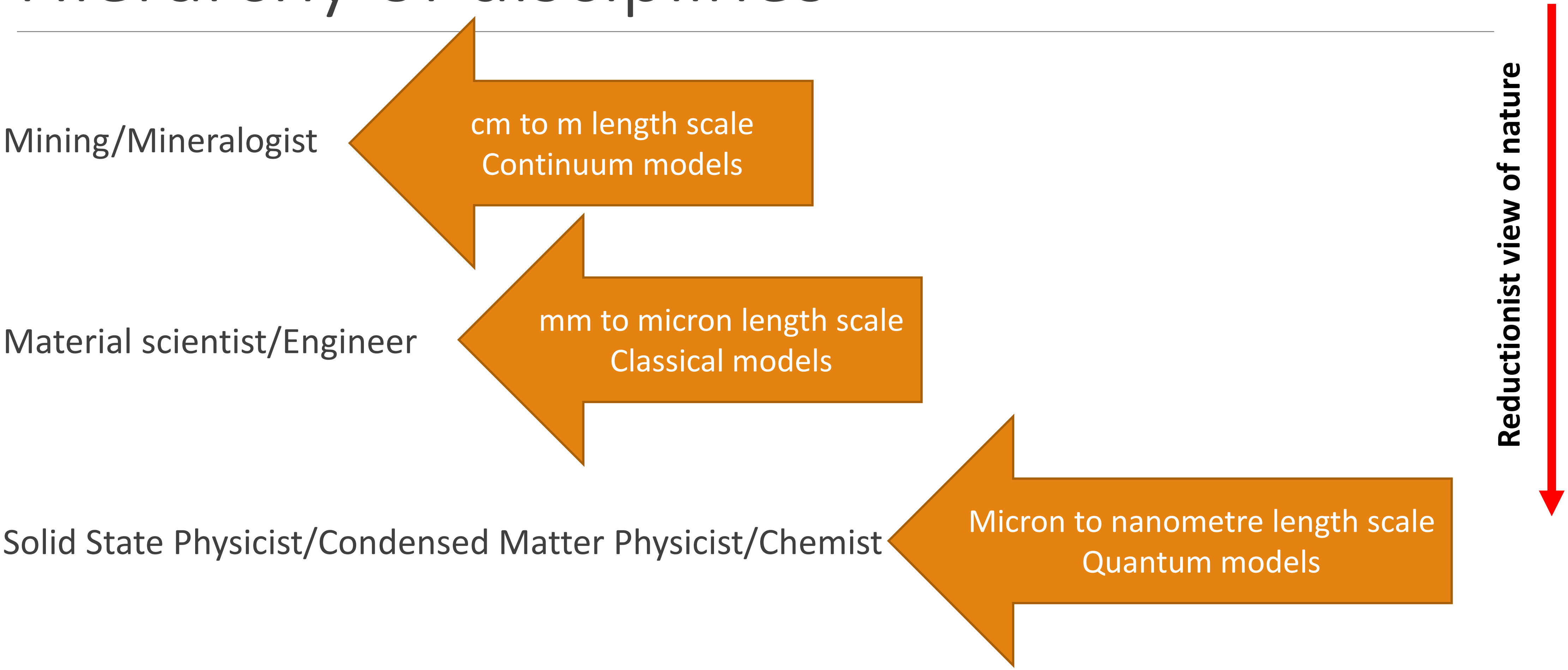
Atomistic basis for vast complexity of real material systems
(Dmitri Ivanovich Mendeleev)

Hierarchy of disciplines



Reductionist view of nature

Mining/Mineralogist

cm to m length scale
Continuum models

Material scientist/Engineer

mm to micron length scale
Classical models

Solid State Physicist/Condensed Matter Physicist/Chemist

Micron to nanometre length scale
Quantum models

Nuclear physics, particle physics, string theory, etc.

Physics looks at ideal systems

What are the essential interactions?

What are the main causes and the main effects?

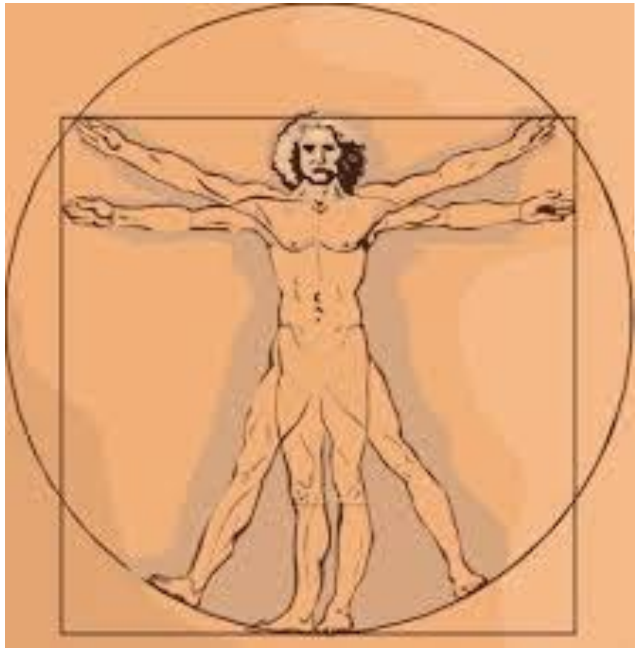
How can we simplify the problem?

How can we model the system using physical principles, and fundamental physical laws?

How can we measure and/or calculate the phenomenon or property of interest?

From complexity comes reduction

… but from reduction can we get complexity?



Can we understand the complexities of life from a reductionist view of the universe?

Understanding Solid State Physics from a theoretical, computational and experimental point of view gives one an excellent basis for understanding many of the quantitative disciplines such as chemistry, biology, engineering, etc

Provides basic ingredients for understanding life more fundamentally

Some key issues to consider

Many body effects (the whole is greater than the sum of the individual parts)

Phase transitions (e.g. ice vs water, graphite vs diamond)

Effects of temperature, pressure, EM waves, other external stimuli and conditions (evolution)

Equilibrium systems versus non-equilibrium systems

Emergence of effective theories (classical mechanics vs quantum mechanics, e.g. motion of a cricket ball)

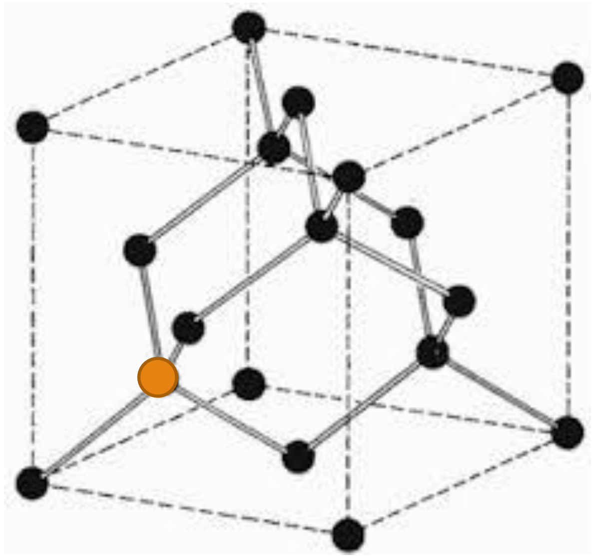
Statistical physics (physics of ensembles)

Relativity (spin and hence magnetism is inherently a relativistic phenomenon)

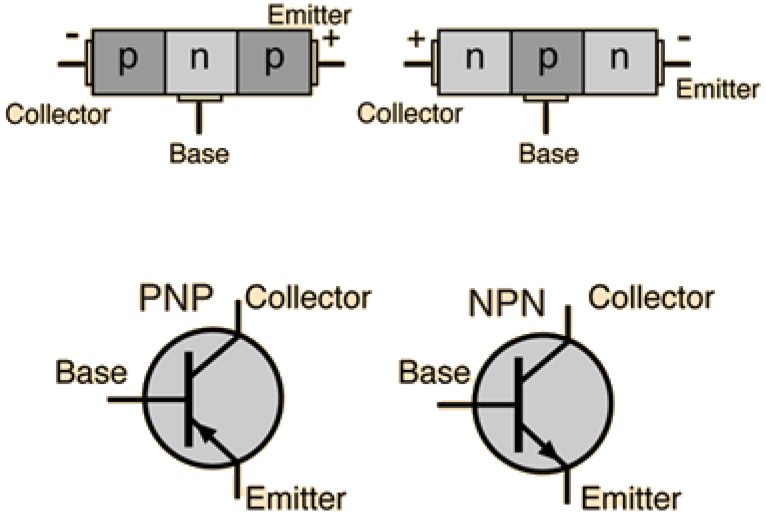
- Periodic crystal structures, e.g. diamond, hexagonal, BCC, FCC, etc.
- Groups of the periodic table, e.g. lanthanides, actinides, alkali metals, alkali earth metals, transition metals, noble gases, noble metals
- Alloys and compound systems, e.g. SiC, GaAs, NaCl; Stainless steel, Al-based alloys, Ni-based alloys

- Defective systems often with useful new properties, e.g. point defects (vacancies, substitutional impurities, interstitial impurities, defect complexes), line defects (stacking faults, dislocations); Doped materials are critically important for semiconductor devices, also for alloying of metals

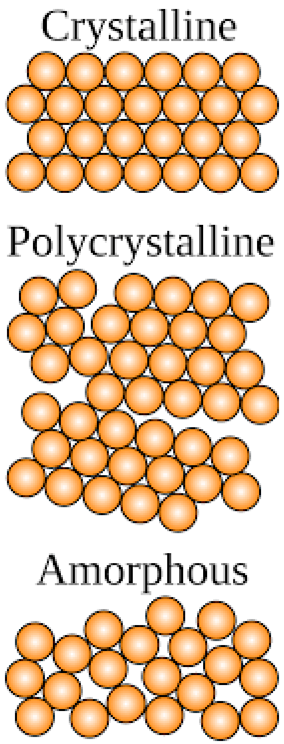
Silicon in diamond structure



Al	**Z=13**
Si	**Z=14**
P	**Z=15**



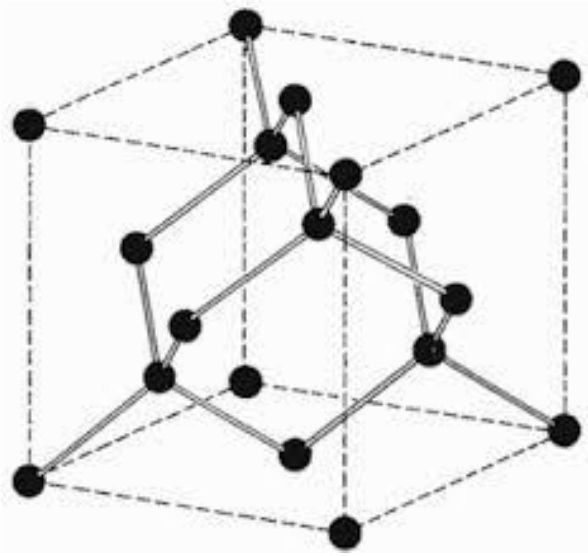
- Amorphous, polycrystalline and ceramic systems, although not periodic, have useful properties and applications, e.g. lighter and harder materials, polycrystalline Si for photovoltaic cells

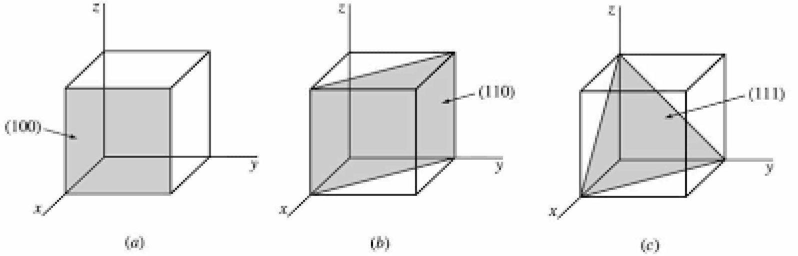


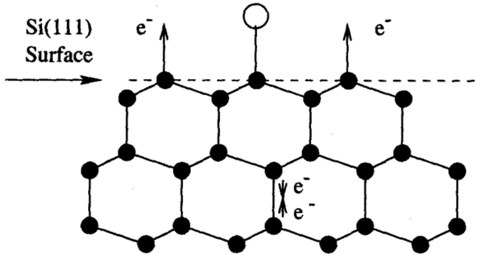
Polycrystalline silicon solar panel

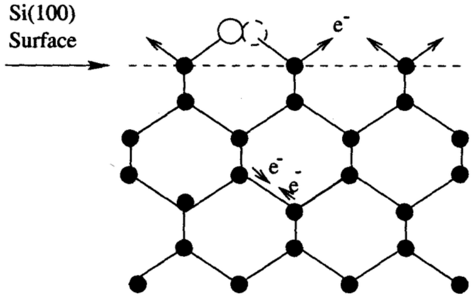
- Surfaces, e.g. (111) surface, which enables one to consider catalysis and surface reactivity

cut and polished diamond





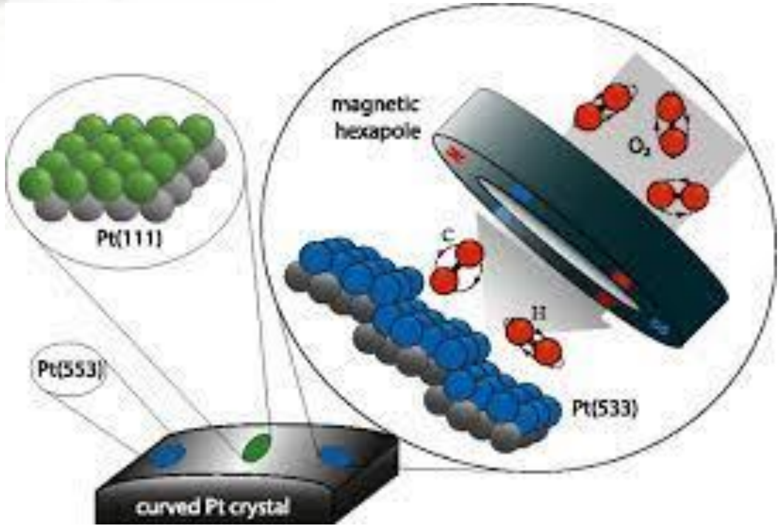




A catalytic converter

Pt as catalyst

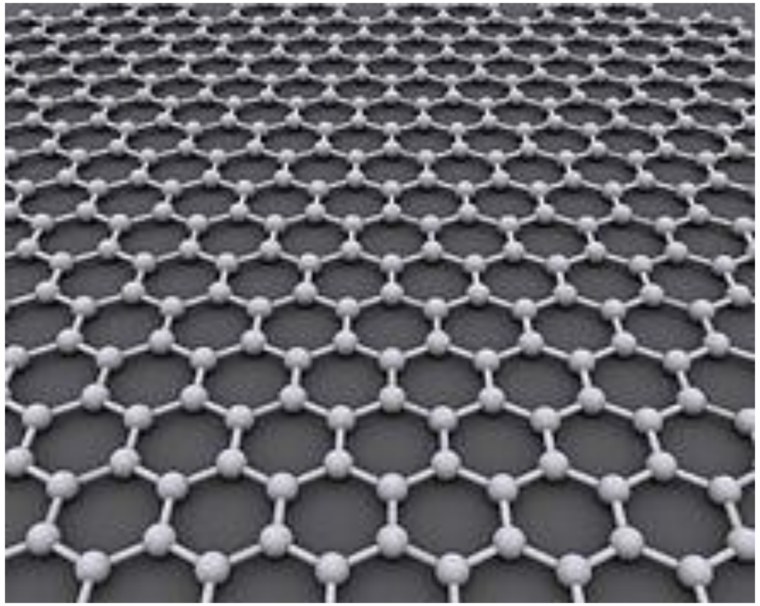
- **oxidize hydrocarbons to water and CO_2**
- **convert carbon monoxide CO to CO_2.**



- Interfaces, e.g. in quantum well structures, transistors, solid state lasers
- Thin films and multi-layers e.g., photovoltaic cells, giant magneto-resistance for recording
- 2D systems e.g., graphene

Quantum well

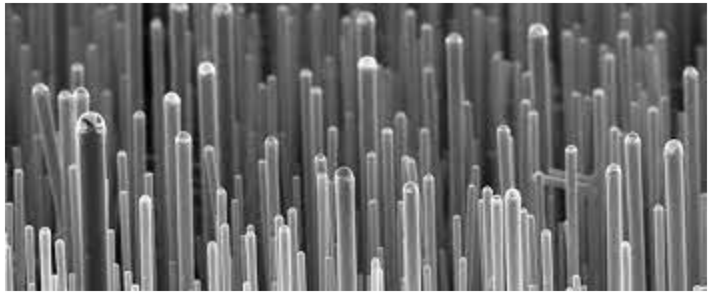
Human-made materials
- Not readily found in nature



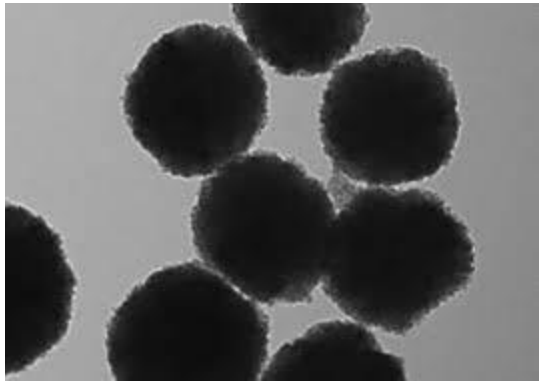
Graphene = single layer of graphite

- Nanosystems often straddle classical and quantum mechanics, and this is giving rise to new phenomena with exciting new applications
- At this length scale, the theoretical and experimental methodologies and instrumentation are applicable also to biological systems.

e.g. quantum wells, quantum dots, quantum wires exhibit new phenomena compared with the bulk

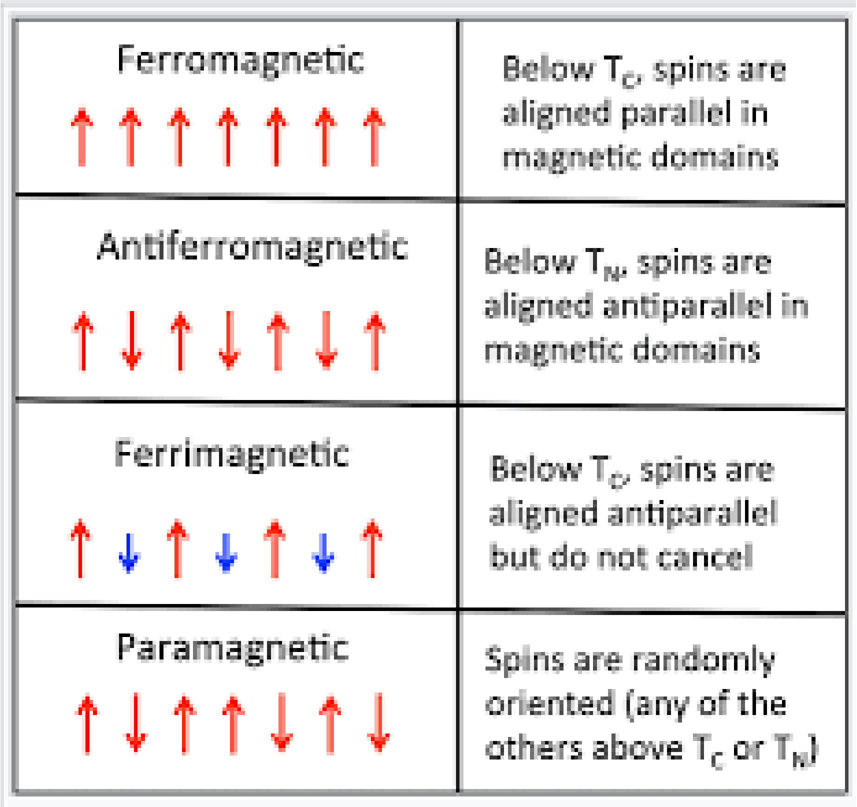


Silicon nanowires



Gold nanoparticles

- Electronic or magnetic properties, e.g. metals, semiconductors, insulators, semimetals, superconductors (conventional, high temperature), heavy fermions, magnetic materials (ferrimagnetism, ferromagnetism, antiferromagnetism, Curie paramagetism, Paul paramagnetism, diamagnetism)



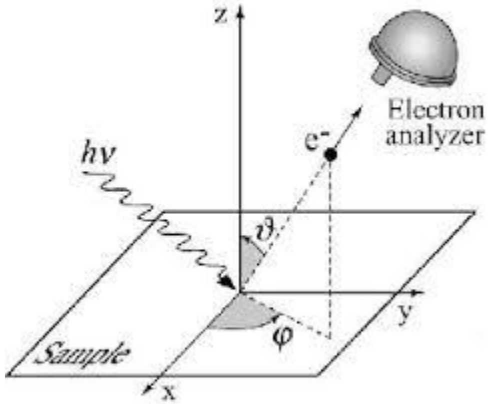
Ferromagnetic ↑ ↑ ↑ ↑ ↑ ↑ ↑	Below T_C, spins are aligned parallel in magnetic domains
Antiferromagnetic ↑ ↓ ↑ ↓ ↑ ↓ ↑	Below T_N, spins are aligned antiparallel in magnetic domains
Ferrimagnetic ↑ ↓ ↑ ↓ ↑ ↓ ↑	Below T_C, spins are aligned antiparallel but do not cancel
Paramagnetic ↑ ↓ ↑ ↑ ↓ ↑ ↓	Spins are randomly oriented (any of the others above T_C or T_N)

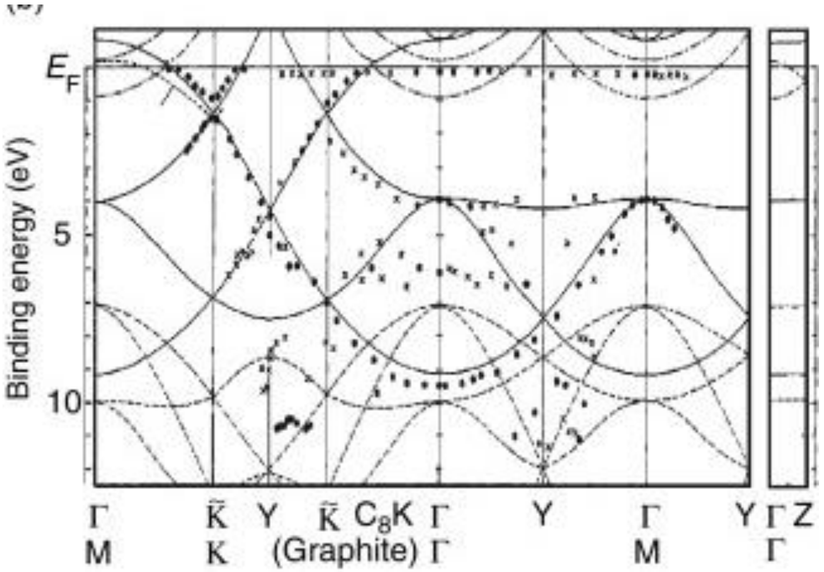
- Variety of properties, e.g. transport properties (electrical and thermal conductivity), crystal phase structure and transitions especially under conditions of temperature and pressure, hardness (brittle, ductile, malleable), elastic properties (bulk modulus, shear modulus, Young’s modulus, Poisson ratio), lustre, optical properties (refractive index, absorption coefficient, reflectivity, transmission coefficient, dielectric function)

Blue-green light is absorbed, its complementary colour, red-orange, is reflected.

Hence copper appears a red-orange colour.

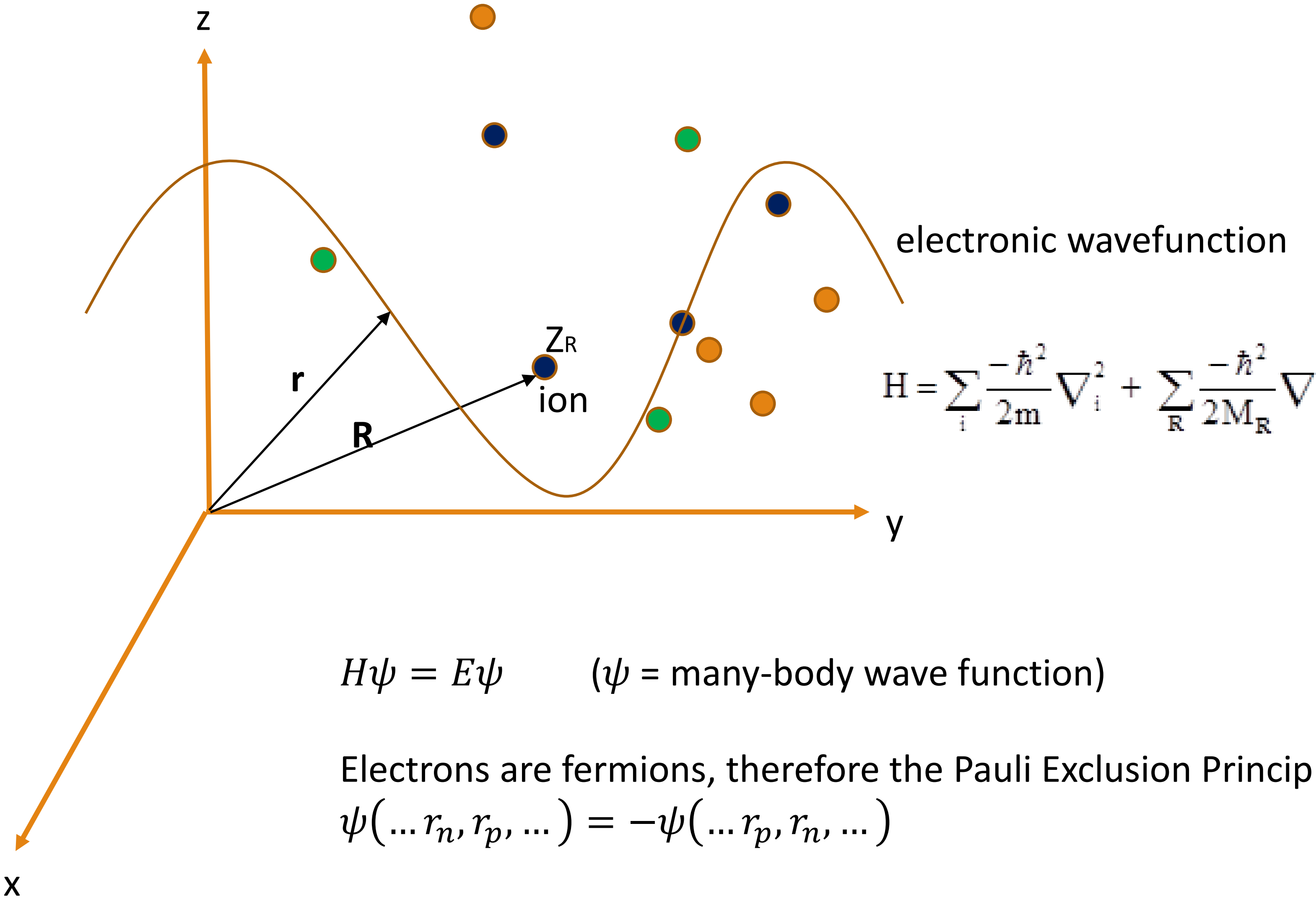
- Various probes, e.g. light (UV, IR), x-rays, electric fields and magnetic fields, temperature and pressure, neutrons, electrons, positrons to create a variety of excitations and collective excitations, such as spinons (spin waves), phonons (lattice waves), magnons (magnetic waves), polarons (electron-hole excitations), etc.





Much complexity in Solid State Physics
- Largest discipline in physics

Unifying theory is Quantum Mechanics



Responsible for binding

$$H = \sum_i \frac{-\hbar^2}{2m}\nabla_i^2 + \sum_R \frac{-\hbar^2}{2M_R}\nabla_R^2 + \frac{1}{2}\sum_{i \neq j}\frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + \frac{1}{2}\sum_{R \neq R'}\frac{Z_R Z_R e^2}{|\mathbf{R} - \mathbf{R}'|} - \sum_{iR}\frac{Z_R e^2}{|\mathbf{r}_i - \mathbf{R}|}$$

$H\psi = E\psi$ (ψ = many-body wave function)

We need to know the structure and the chemical composition

Electrons are fermions, therefore the Pauli Exclusion Principle applies

$$\psi(\ldots r_n, r_p, \ldots) = -\psi(\ldots r_p, r_n, \ldots)$$

ie : wavefunction is anti-symmetric in the exchange of electron coordinates

The energy is central

Why is graphite the more stable form of solid carbon?

$p = -\frac{\partial E}{\partial V}$ basis for pressure induced phase transitions

$F = -\frac{\partial E}{\partial R}$ basis for calculation of equilibrium structures, molecular dynamics

Elastic constants, phonon frequencies, electrical conductivity, etc, etc etc

Calculate charge density from wavefunction, basis for understanding bonding

Single particle energy spectrum basis for understanding electronic properties of solids (e.g. metals, semiconductors, magnetism, etc., etc.)

- Impossible to solve the Schrödinger equation analytically
- Solve numerically, still very difficult without meaningful approximations
- atom = nucleus + electrons

  = (nucleus + core electrons) + valence electrons

  = "ion core" + valence electrons

  Assumed to be chemically inert → "frozen core" approximation

- Ions are massive, more than 2000× greater than the mass of the electron, hence we may treat ions classically (except H, He), and treat electrons quantum mechanically
- Electrons are assumed to be in the ground state at all times – as the ions move in a gas, liquid or solid, we assume that the electrons follow the motion of the ions adiabatically. This is known as the Born – Oppenheimer approximation
- Relativistic effects are important

Density Functional Theory

Energy is a unique functional of the density

Recasts the many electron problem into an effective non-interacting problem

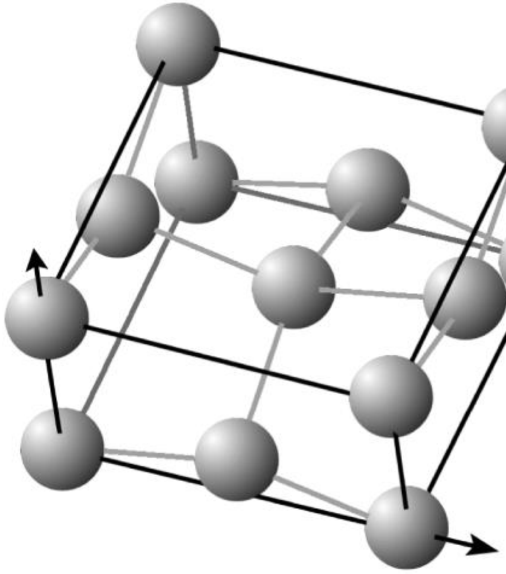
$$< \Psi|H|\Psi > \; = E = T_s + E_C + E_{e-ion} + E_{ion-ion} + E_{xc}$$

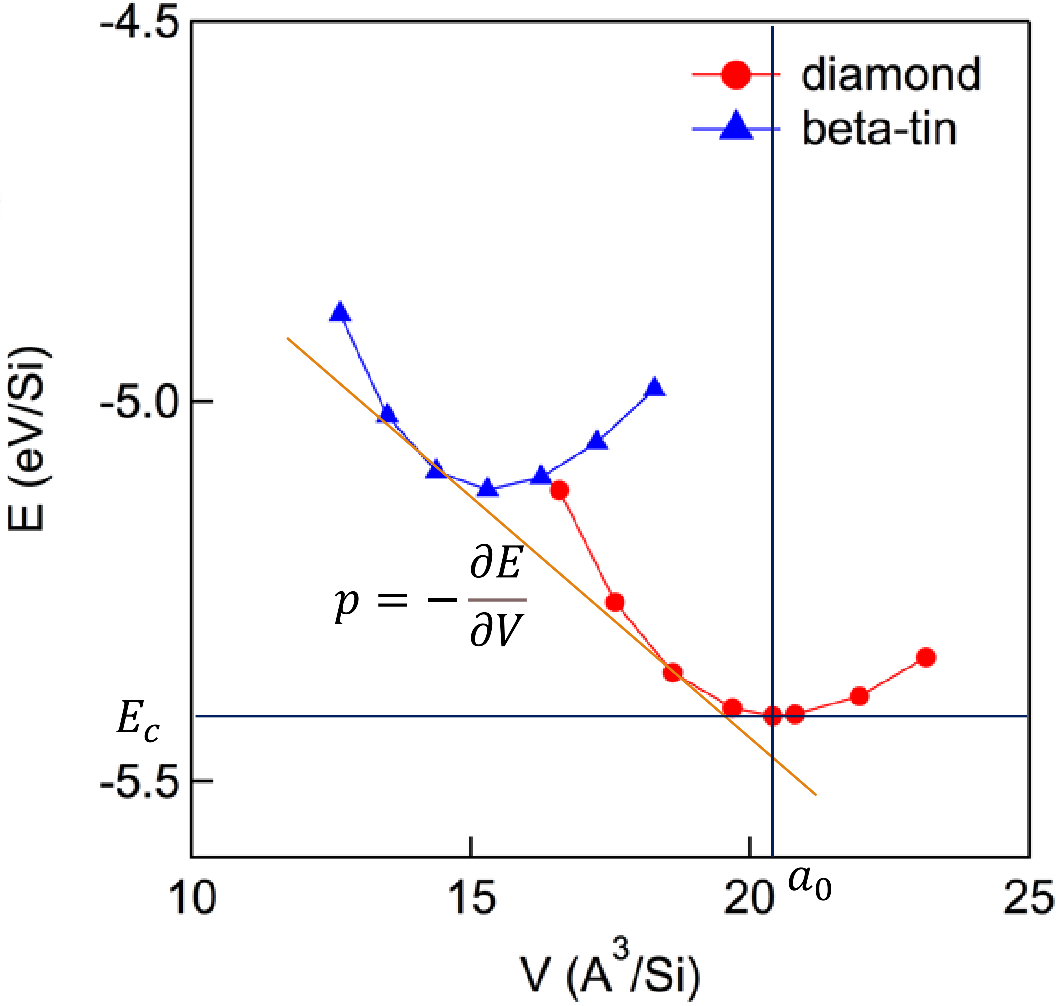
Many body formulation
Hamiltonian exactly known
Wavefunction difficult to compute

n(r) →

Single particle formulation
Hamiltonian not exactly known
Wavefunction computable using numerical techniques

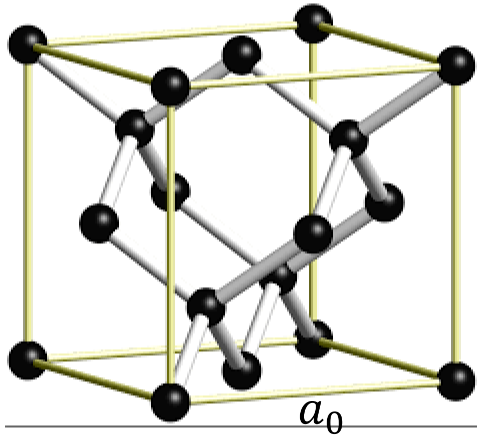
Energies are the same

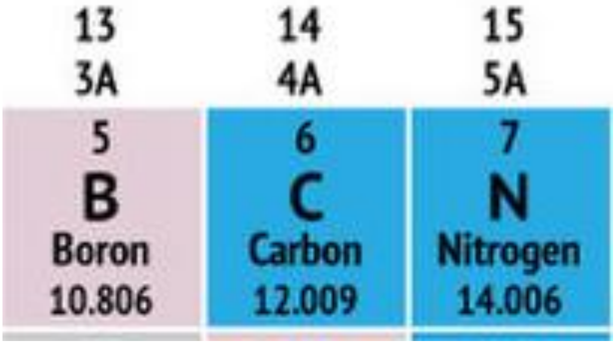




$$p = -\frac{\partial E}{\partial V}$$

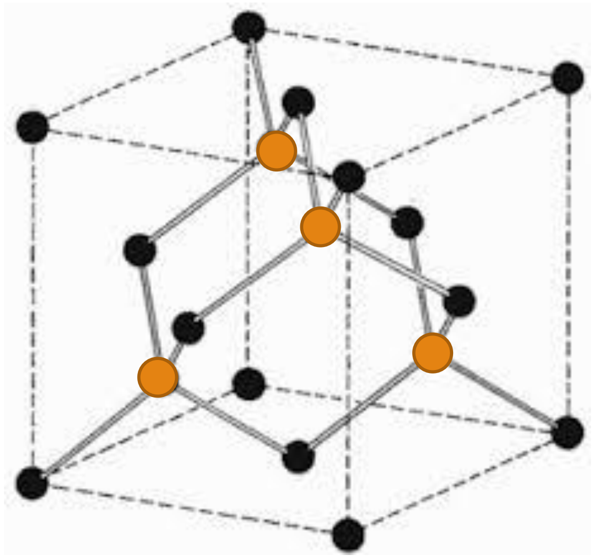
Bulk Modulus $B = \frac{\partial^2 E}{\partial V^2}$





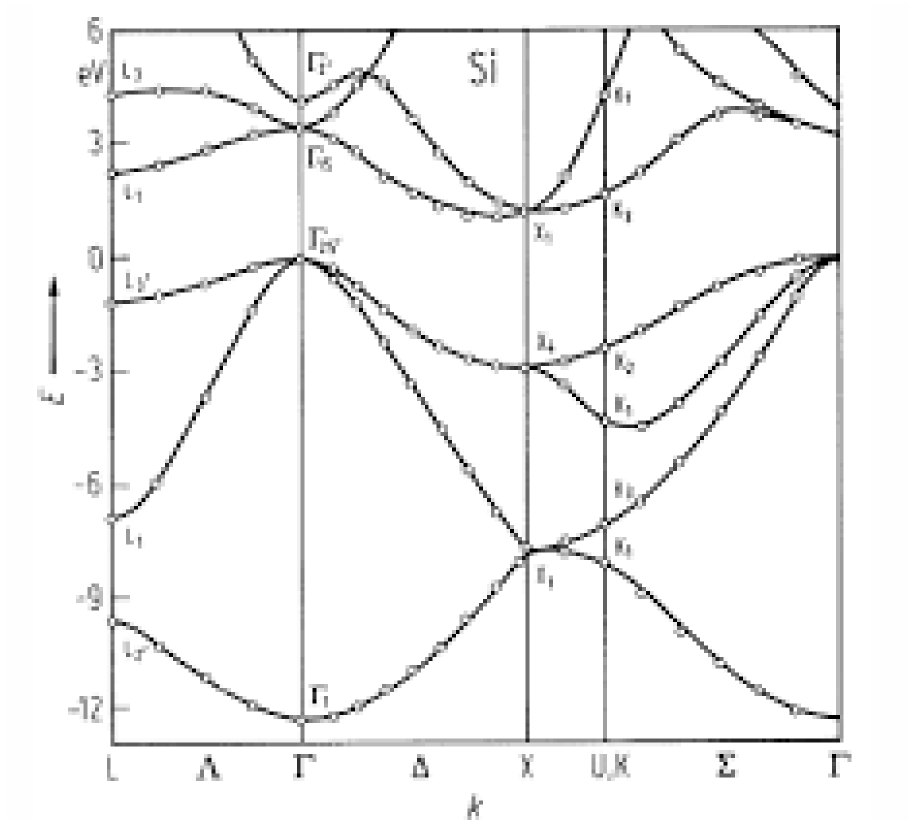
13 3A	14 4A	15 5A
5 B Boron 10.806	6 C Carbon 12.009	7 N Nitrogen 14.006

Diamond structure
2 identical atoms per cell

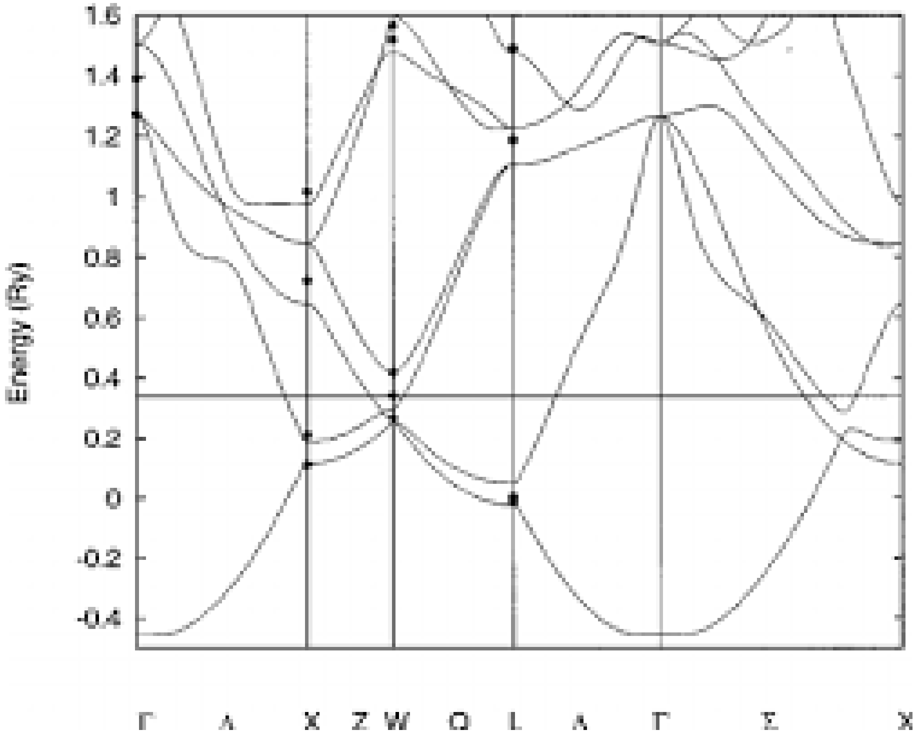


Bulk modulus of diamond 445 GPa
Bulk modulus of cubic BN 367 GPa

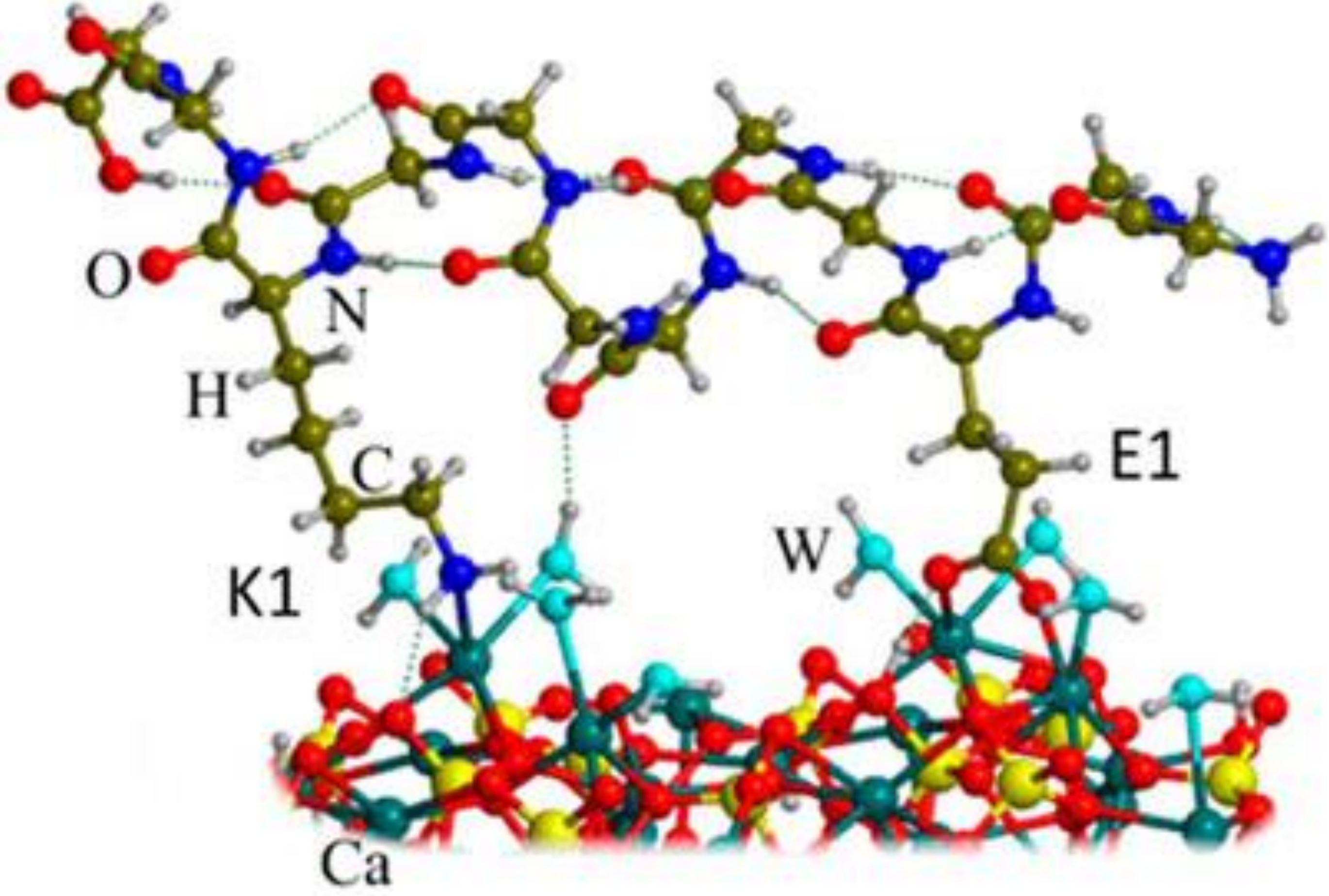
Zincblend structure
2 different atoms per cell

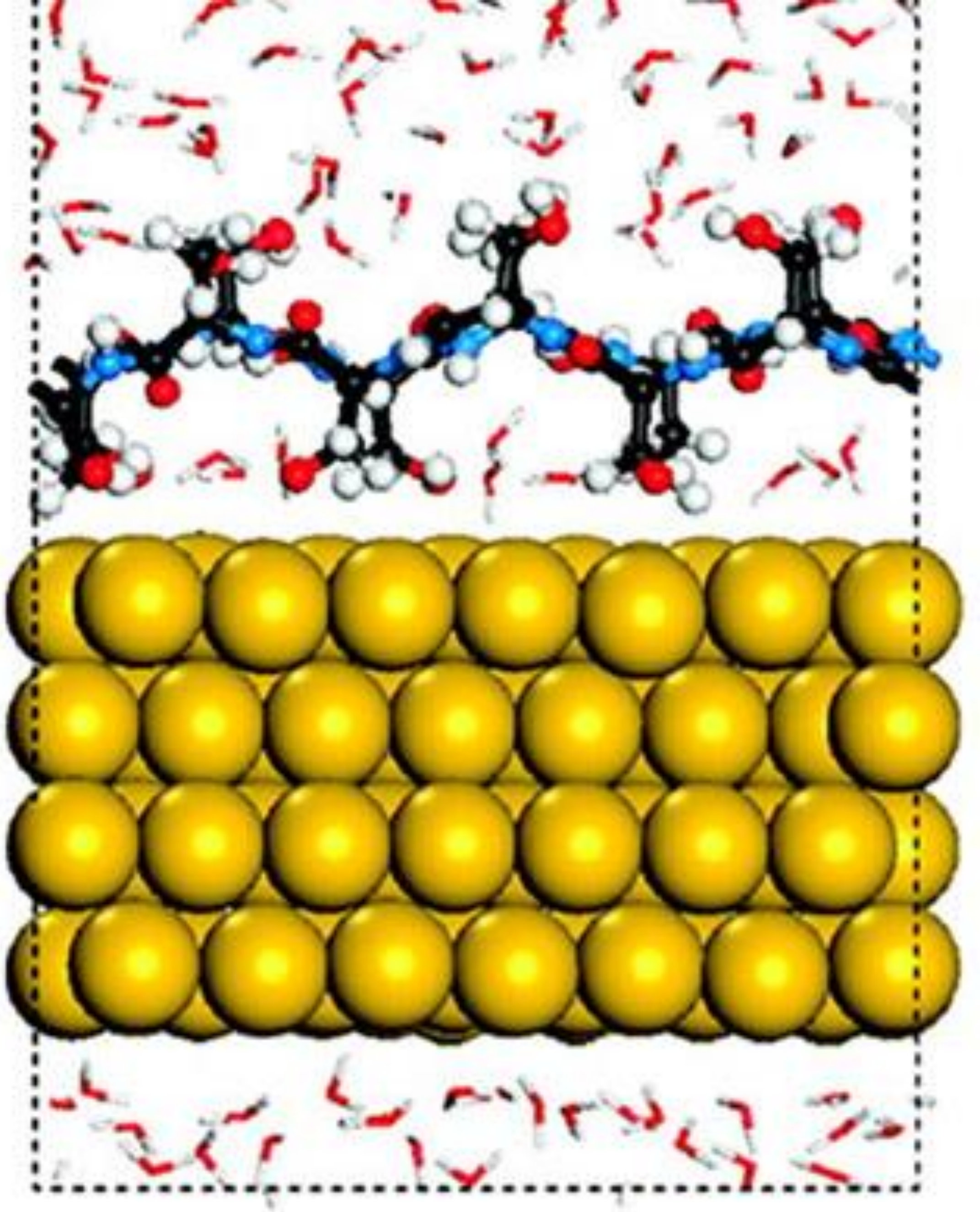


Electronic bandstructure for Si



Electronic bandstructure for Al


O
N
H
C
K1
W
E1
Ca



Success of DFT

Energies of many electron systems; difference in energies; bond lengths; magnetic systems; phase transitions under pressure; finite temperature molecular dynamics; phase transitions under temperature; defect states; interfaces; nanosystems, 2D systems, transport phenomena, etc., etc.

Experimental, Theory, Computational studies of solids

- QM is sufficiently accurate that it is now used as a predictive tool in studies of solids; limited only by access to sufficiently large computing resources
- Molecular mechanics (classical methods) have limited universality; can study large systems

10 most cited papers in Physical Review over 110 years

#	Title	Author(s)
1.	*Self-Consistent Equations Including Exchange and Correlation Effects* *(1965)*	W. Kohn, L. J. Sham
2.	*Inhomogeneous Electron Gas* *(1964)*	P. Honenberg, W. Kohn
3.	*Self-Interaction Correction to Density-Functional Approximations for Many-Electron Systems* *(1981)*	J.P. Perdew, Alex Zunger
4.	*Ground State of the Electron Gas by a Stochastic Method* *(1980)*	D. M. Ceperley, B.J. Alder
5.	*Theory of Superconductivity* *(1957)*	J. Bardeen, L.N. Cooper, J.R. Schrieffer
6.	*Model of Leptons* *(1967)*	S. Weinberg
7.	*Linear Methods in Band Theory* *(1975)*	O. K. Andersen
8.	*Effects of Configuration Interaction on Intensities and Phase Shifts* *(1961)*	U. Fano
8.	*Disordered Electronic Systems* *(1985)*	P.A. Lee, T.V. Ramakrishnan
9.	*The Electronic Properties of Two-Dimensional Systems* *(1982)*	T. Ando, A.B. Fowler, F. Stern
10.	*Special Points for Brilloun-Zone Integrations* *(1976)*	H.J. Monkhorst, James D. Pack

The African School of Electronic Structure Methods and Applications (ASESMA)

Began in 2008

Richard Martin, Sandro Scandolo (ICT), Nithaya Chetty

Jim Gubernatis (IUPAP)

Biennial School Series in QM studies of real materials over 2 weeks

Rotates through different African countries

ASESMA

About 40 PhD students and young academics drawn from sub-Saharan Africa for each School

Involves developers of Quantum Espresso

Lecturers and mentors from around the world
  - Lots of goodwill and excitement

Administered by ICTP

Access CHPC in Cape Town

Work continues well after School is over
  - Networking
  - Communications
  - Collaborations
  - Exchange

Fosters a collaborative network for research and higher education within Africa.

Beijing Supercomputing Centre

IUPAP
International Union of Pure and Applied Physics

Board on International Scientific Organizations
U.S. Liaison Committee for IUPAP
National Academy of Sciences

ICTP
The Abdus Salam
International Centre for Theoretical Physics

NITheP
National Institute for Theoretical Physics

APS physics

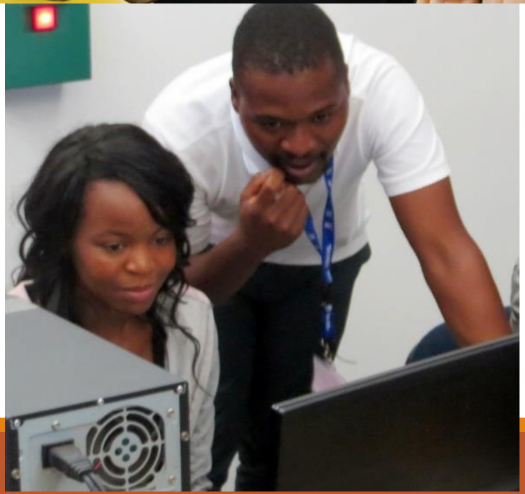
The Thomas Young Centre
TYC

NSF

MARVEL
NATIONAL CENTRE OF COMPETENCE IN RESEARCH

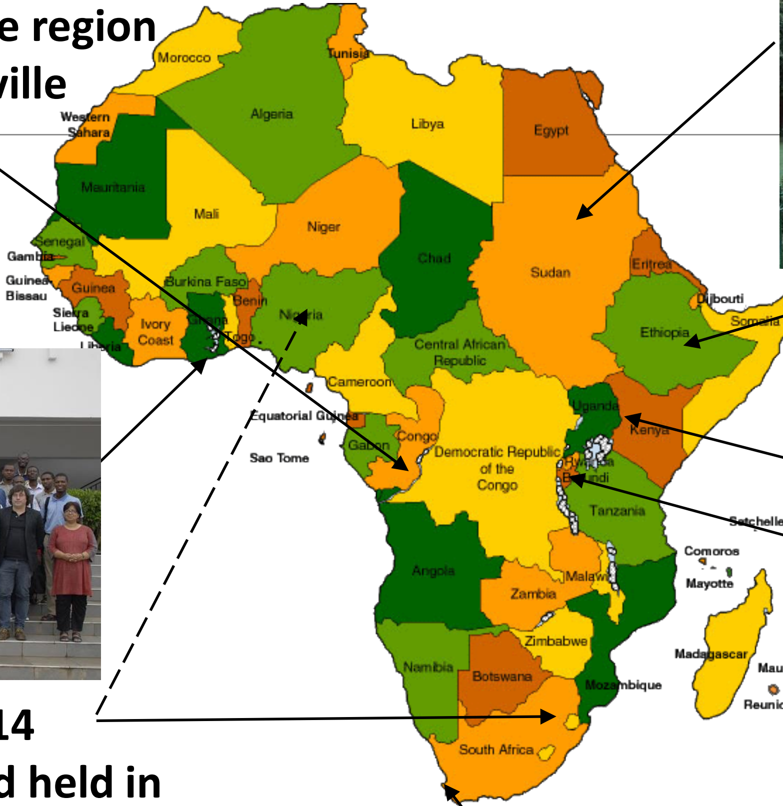
Materials Research Lab Santa Barbara

ASESMA is People and connections



ASESMA Schools

“Mini-ASESMAs”
in Frencophone region
Congo, Brazzaville



Sudan – 2015 Support “KWAMS” school

Ethiopia - 2018

Ghana - 2016

Kenya - 2012

Rwanda – 2021/23

Virtual School in 2021
In-person School in June 2023

Nigeria – 2014
Canceled and held in
Johannesburg - 2015

Capetown – 2010

Active Research Groups

Cameroon - Yaounde

Congo, Brazzaville – Brazzaville

Ethiopia – Addis Ababa

Ghana – Accra, Kumasi

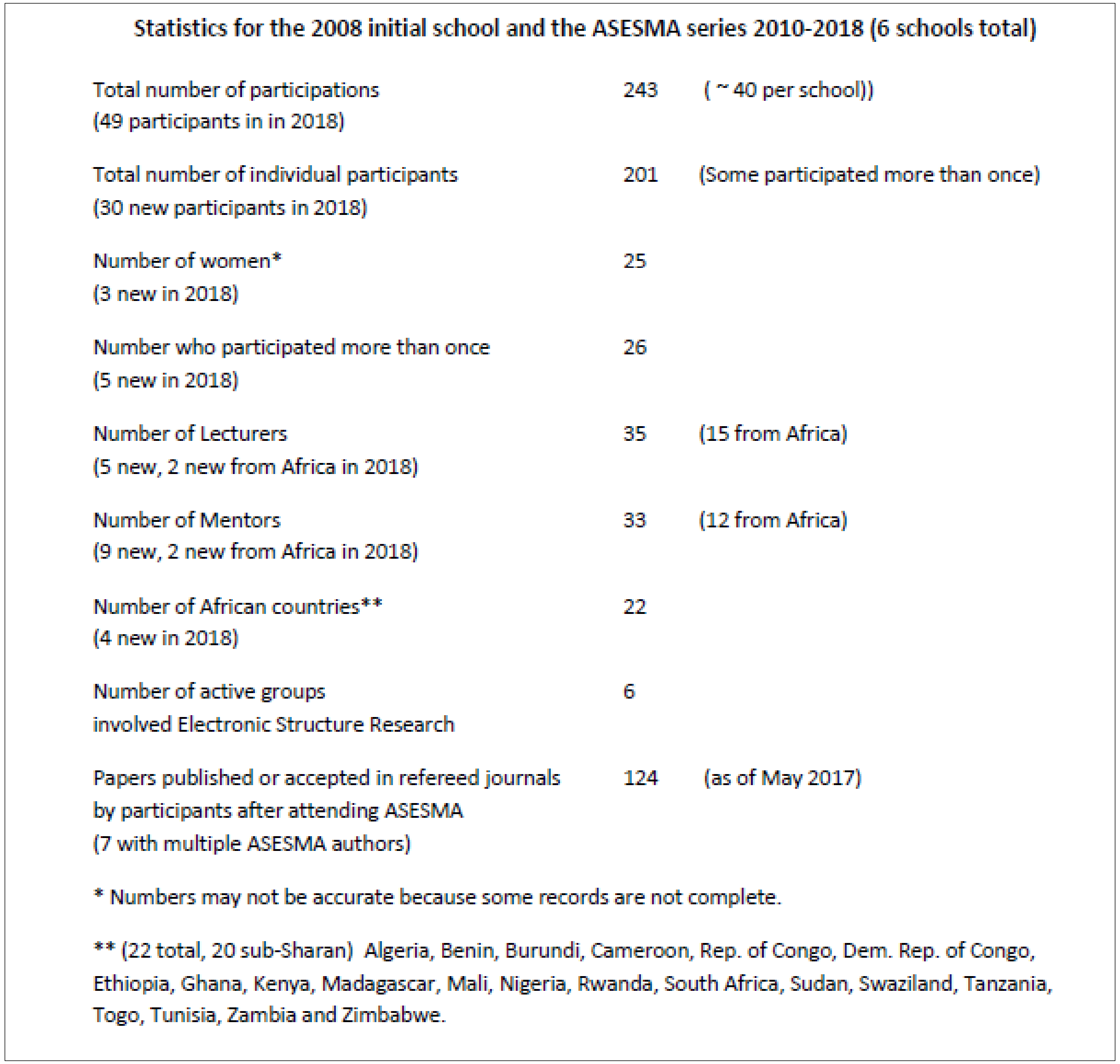
Kenya – Nairobi, Eldoret, Kakamega

Nigeria – Ibadan, AUST

Rwanda – Kigali (New Institute)

South Africa – Many

Others growing



Statistics for the 2008 initial school and the ASESMA series 2010-2018 (6 schools total)

Total number of participations (49 participants in in 2018)	243	(~ 40 per school))
Total number of individual participants (30 new participants in 2018)	201	(Some participated more than once)
Number of women* (3 new in 2018)	25	
Number who participated more than once (5 new in 2018)	26	
Number of Lecturers (5 new, 2 new from Africa in 2018)	35	(15 from Africa)
Number of Mentors (9 new, 2 new from Africa in 2018)	33	(12 from Africa)
Number of African countries** (4 new in 2018)	22	
Number of active groups involved Electronic Structure Research	6	
Papers published or accepted in refereed journals by participants after attending ASESMA (7 with multiple ASESMA authors)	124	(as of May 2017)

* Numbers may not be accurate because some records are not complete.

** (22 total, 20 sub-Sharan) Algeria, Benin, Burundi, Cameroon, Rep. of Congo, Dem. Rep. of Congo, Ethiopia, Ghana, Kenya, Madagascar, Mali, Nigeria, Rwanda, South Africa, Sudan, Swaziland, Tanzania, Togo, Tunisia, Zambia and Zimbabwe.