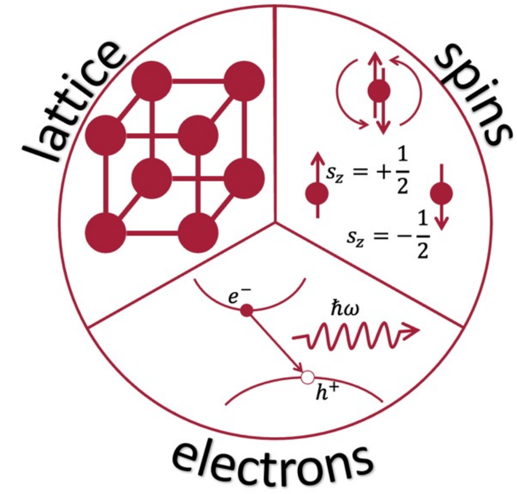
# Advanced topics in condensed matter (ATCOMA)
# (together with "Experimental Techniques")




(Acronym: PHY-VFATCM)

| | |
|---|---|
| Lectures on: | **Wednesdays, 16:15-17:45** |
| Auditorium: | **C9A03 (in person)** |
| First lecture: | October 16th, 2024 |
| Lecturers: | Dr. Ivan Zaluzhnyy |
| | Prof. Dr. Dr. h.c. Frank Schreiber |
| Language: | English |
| Credit: | 3 ECTS |

Synopsis

The series of lectures will present advanced topics in condensed matter physics.
It will be complementary to "BM KoMa" (basic module condensed matter).
The course can be taken in parallel with or subsequent to "BM KoMa".
We will introduce each topic with a brief revision of the basics and explore it in depth.
We will cover theoretical concepts as well as experimental methods.
All blocks from "BM KoMa" will be covered, i.e. Block I (structures and their dynamics), Block II (electrons) and Block III (ordering phenomena and phase transitions, including e.g. magnetism).
The course will be useful for bachelor, master and PhD students.

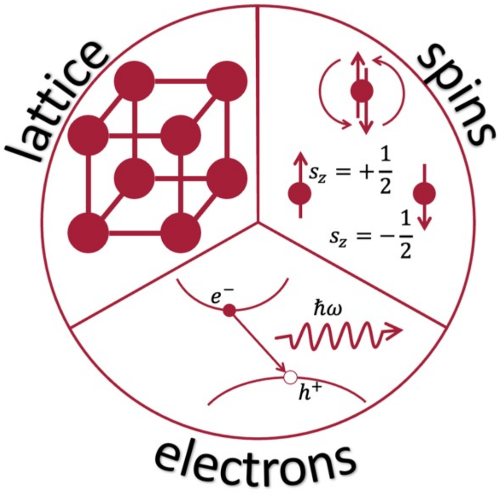
Selected keywords

- Crystal structures and scattering of X-rays and neutrons
- Lattice dynamics and inelastic scattering of neutrons from phonons
- Determination of electron band structure using photoelectron spectroscopy
- Linear response theory and optical properties
- Ordering phenomena
- Phase transitions

Link at group homepage

www.soft-matter.uni-tuebingen.de/vorlesung_ws24_advkoma.html
login & password

# ATCOMA road map for today




Who are we ? (lecturers)
Who are you ? (audience)
Why study condensed matter ?
Length, time, and energy scales
Some relevant numbers
Table of contents / Block I / II / III
Examples
Interaction of waves with matter

# Why study condensed matter ?

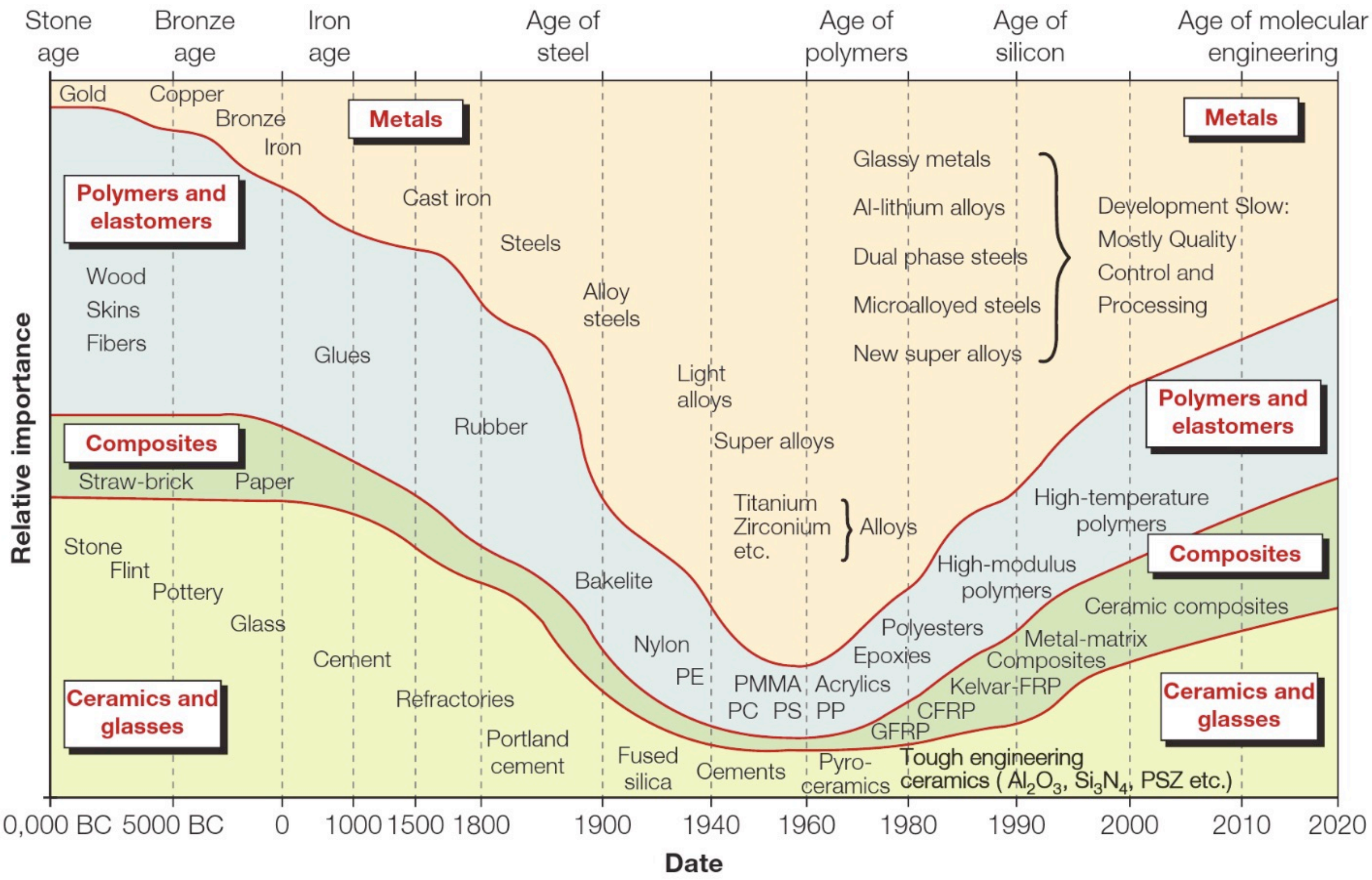
inspired by Steven H. Simon, The Oxford Solid State Basics

1) because it is the world around us
... why are metals shiny and why do they feel cold ?
... why is glass transparent ?
... why is rubber soft and stretchy ?

2) because it is useful
... applications; all sorts of materials; construction; magnetic; electronic; optoelectronic (solar cells, LEDs) ...

3) because it is deep and reductionism does not work
... new and collective effects / emergent phenomena
(phase transitions 1st vs 2nd order; magnetism; superconductivity;...)
... see Phil Anderson's argument on "more is different"
(inability to reduce everything to the fundamental laws governing the behavior of elementary particles and then deduce from there the behavior of complex condensed matter
... this does not even work with the basic (but very fundamental !) appearance of different symmetries in crystals

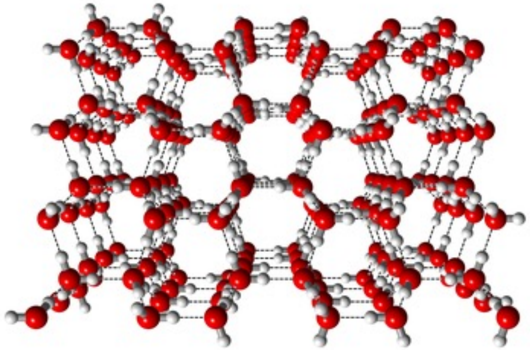
# Condensed matter (co)determines history
## "Without materials, there is nothing"



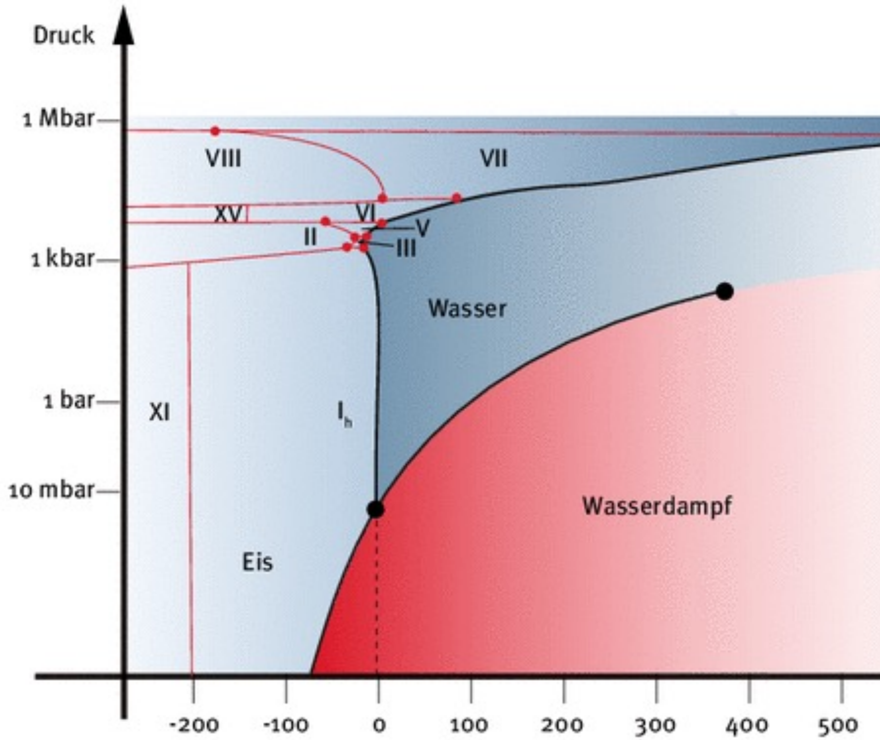

Michael F. Ashby (a slightly subjective compilation)

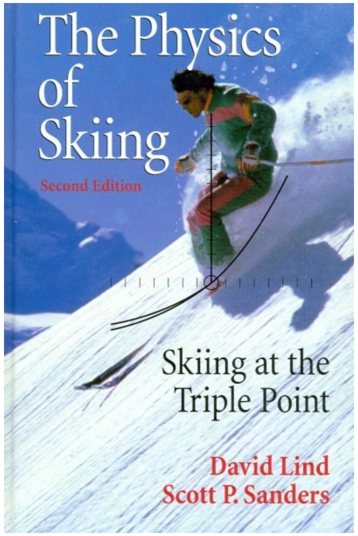
# Phase diagrams and the melting of ice

17 different crystalline forms of ice known as f(T,p): Differences in ordering and density



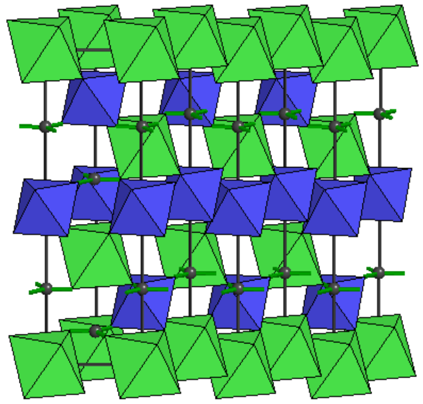
- H2O is material with the most known anomalies (Density etc.)
- High melting and evaporation (than other light molecules)
- High heat capacity (important for climate)
- all 3 states found on Earth

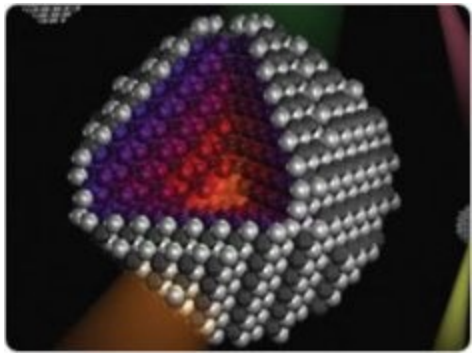



https://www.weltderphysik.de/thema/hinter-den-dingen/eis-ist-nicht-gleich-eis/

# Crystals: From „Nano“ to „Mega“



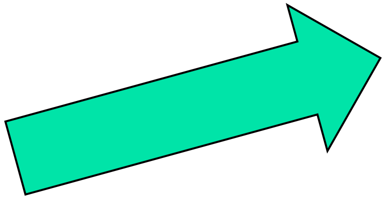


**Gold-Nano-Crystaly (some nm)**

Structure determination as a challenge

Watari et al., Nature Materials 2011

Schreiber, Nature Materials 2011



**Gypsum-Crystals (up to 12 m)**

$CaSO_4 \cdot 2H_2O$

Naica-Mine, Mexico

Ultraslow growth rates of giant gypsum crystals

A. E. S. Van Driessche et al., PNAS (2011)

http://www.ubergizmo.com/2009/05/non-blinking-nanocrystals/

http://giantcrystals.strahlen.org/america/naica.htm

# Length scales

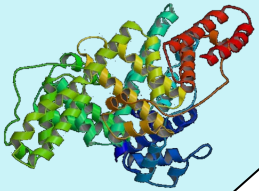
Note on the $10^{-10}$ m scale
- so important that it has its own name (Ångstrom)
- condensed matter, molecules etc. consists of atoms ~ 1 Å
- this makes X-rays ($\lambda$ ~ 1 Å) special in anything related to condensed matter

galaxy ~ $10^{21}$ m

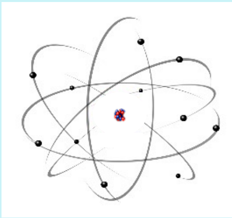
earth ~ $10^{7}$ m

human ~ $10^{0}$ m

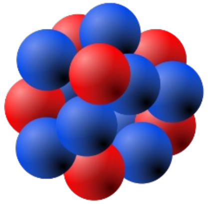
protein ~ $10^{-8}$ m



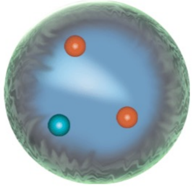
atom ~ $10^{-10}$ m



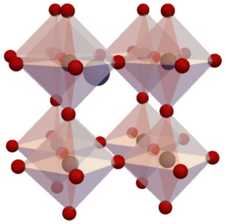
nucleus ~ $10^{-15}$ m



quarks < $10^{-18}$ m

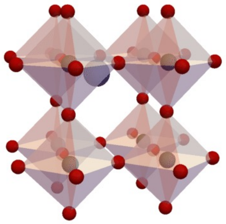


Note on intermediate length scales
- manipulation and emergent effects (engineering; condensed matter; nanoscience; biophysics etc)
- these are associated with time scales



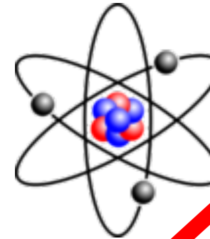
# Time scales

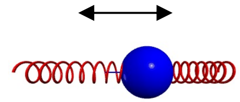
πάντα ῥεῖ
(everything flows)



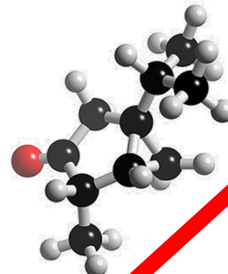
# Time scales

πάντα ῥεῖ
(everything flows)





Attosecond
($10^{-18}$ s)



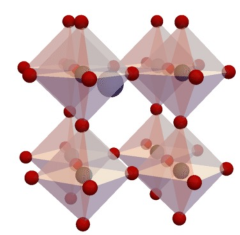
Femtosecond ($10^{-15}$ s)

Picosecond ($10^{-12}$ s)

Nanosecond ($10^{-9}$ s)

Microsecond ($10^{-6}$ s)

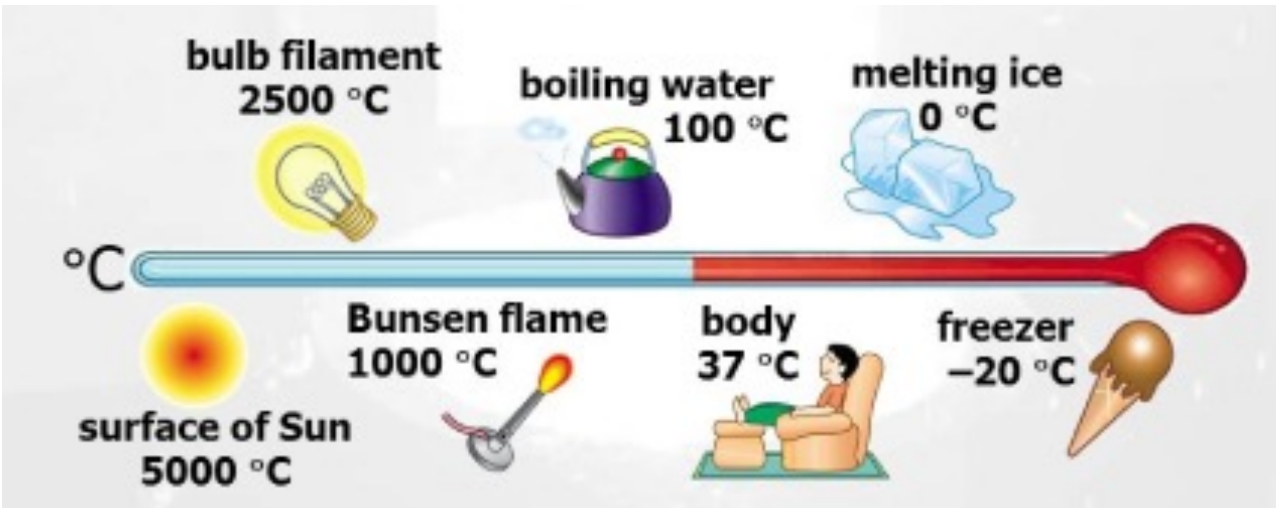
Millisecond ($10^{-3}$ s)

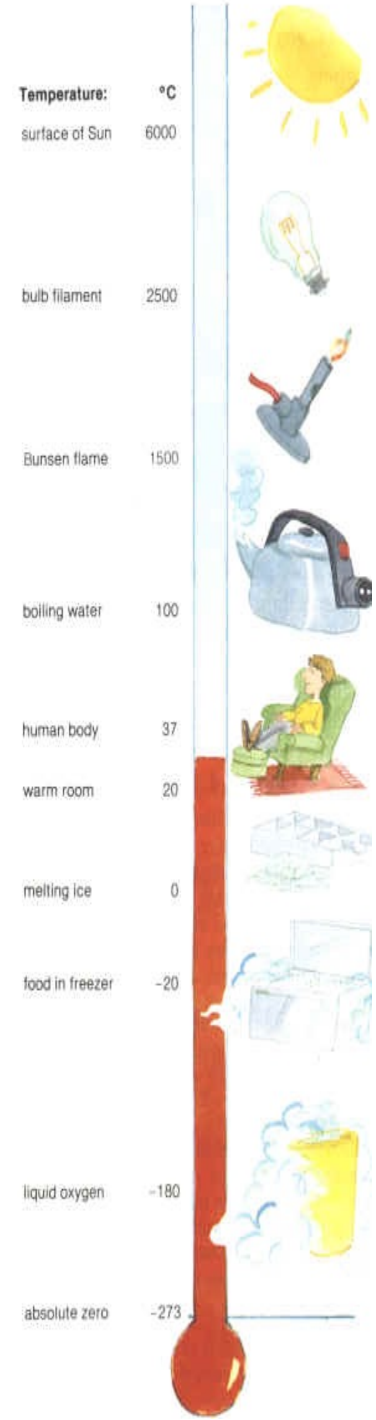


Second

# Temperature scales

Generally, for our lives, $T \sim 300$K is most relevant!
This makes $k_B T(300\text{ K}) = 25$ meV an important reference energy!




http://ramadan.50megs.com/IGC_Temperature.htm

# Some relevant numbers

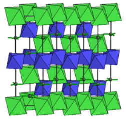
- Length scales … Angstroems, i.e. 0.1 nm
- … relevant for inter-atomic distances

- Energy for Angstroem wavelength ... 12 keV (X-rays) ... or 80 meV (neutrons)
- … relevant for scattering experiments

- Wavelength for 2 eV energy ... 600 nm
- … relevant for band structure and gap, e.g. for photovoltaics

- Thermal energy near room temperature $k_B T$ (300 K) = 25 meV
- … relevant for thermal excitations of lattice vibrations, electrons etc
- … incidentally (and favorably) near that of 1 Å –neutrons, i.e. ... 80 meV

# Road map of ATCOMA loosely connected to BM KoMa



Sub-themes:

… how to probe the properties of condensed matter?

Block I Structure and dynamics
… … how to probe structures
… … how to probe dynamics
… … some deeper insight into dynamics
(non-linearities etc)

Block II Electronic and optical properties
… … how to measure the bandstructure ?
… … fundamentals of response functions
and Kramers-Kronig relationship

Block III Magnetism and other ordering phenomena
… … localized vs itinerant magnetism
… … phase transitions

# Block I … preview

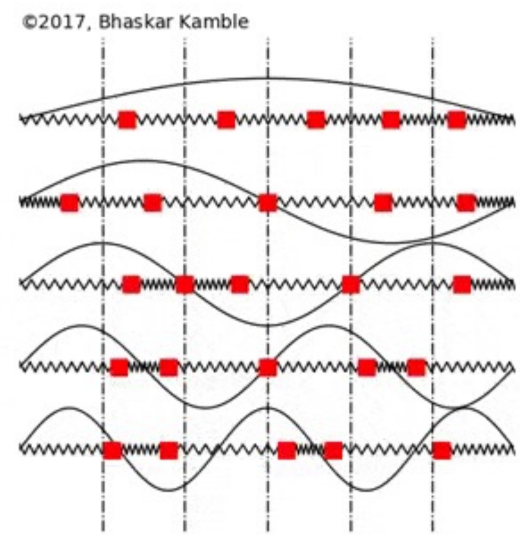
# Structures g(r) and their Dynamics G(r,t)

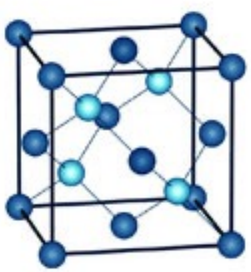
**From single atoms to solids**

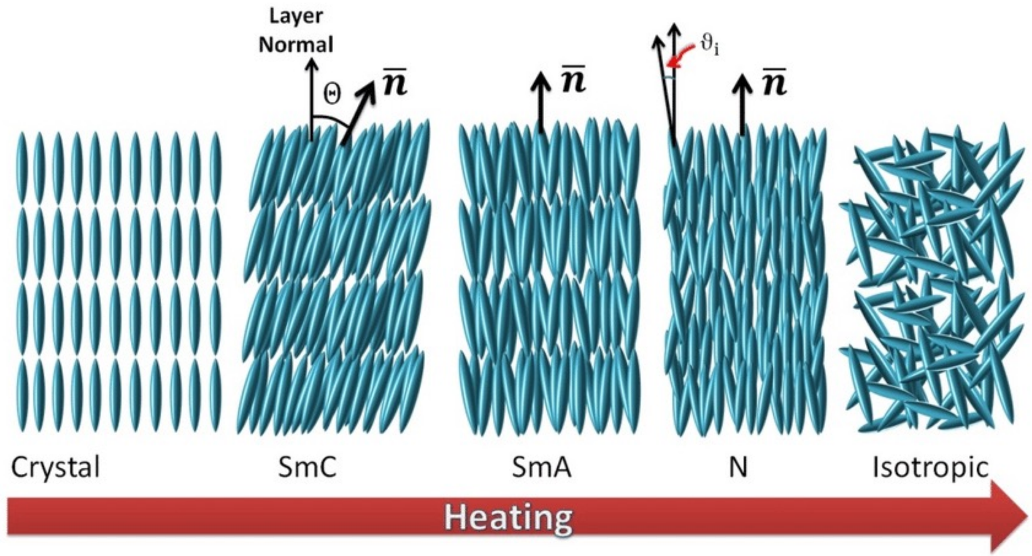
- S(q) ~ FT[g(r)]
- Definition and description of crystal structures
- Determination of crystal structures
- Quasi-crystals, liquid crystals and other forms of condensed matter

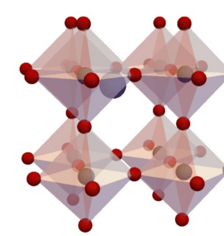
**Condensed matter with dynamics**

- S(q,ω) ~ FT[G(r,t)]
- Lattice vibrations (phonons)
- Diffusion





- Wikipedia
- Nanomaterials 2017
- Pradip, PRL 2016

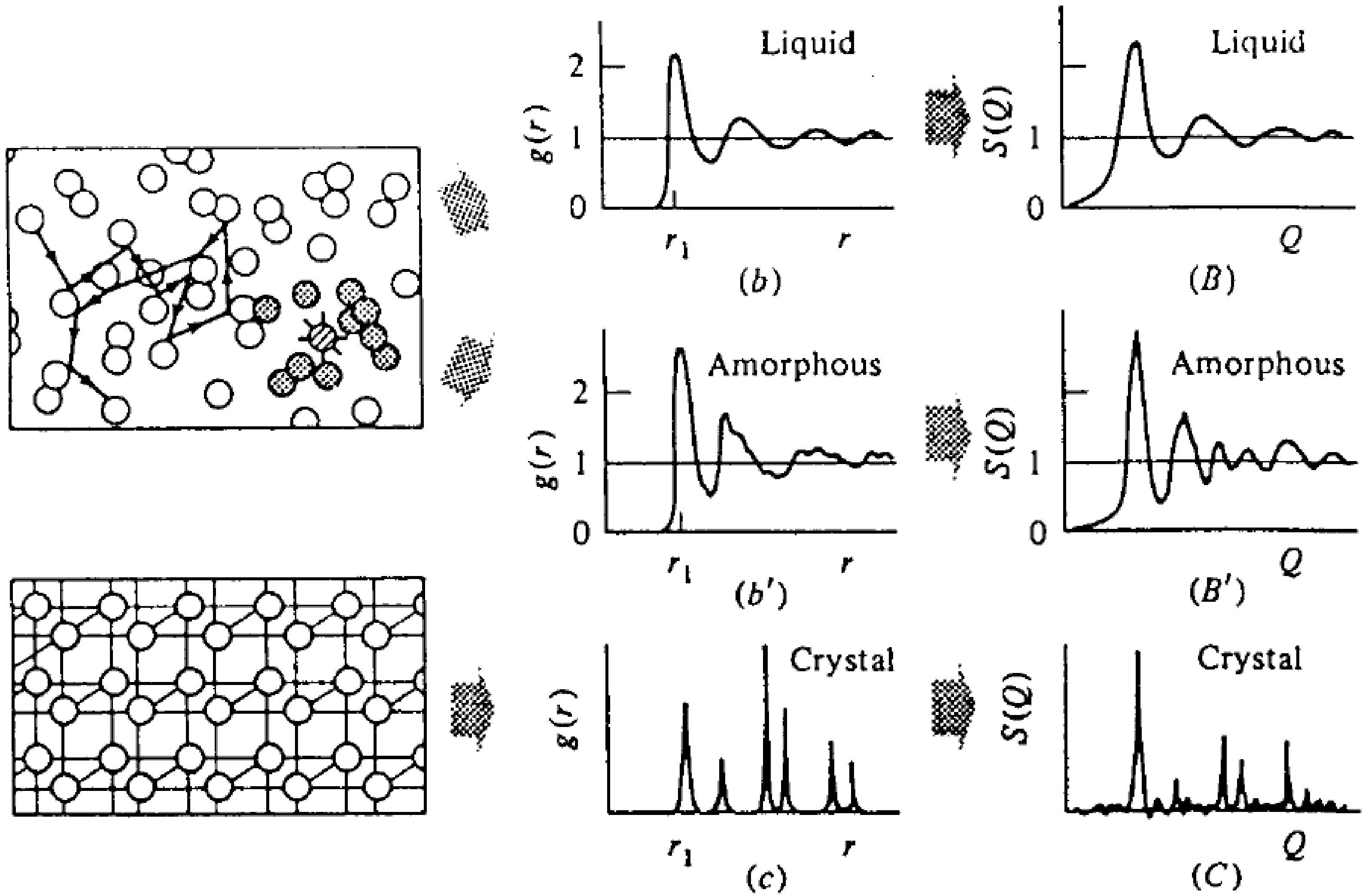
# Structures g(r) and their Dynamics G(r,t)

**From single atoms to solids**

- S(q) ~ FT[g(r)]

**Distinction by dynamics ?**

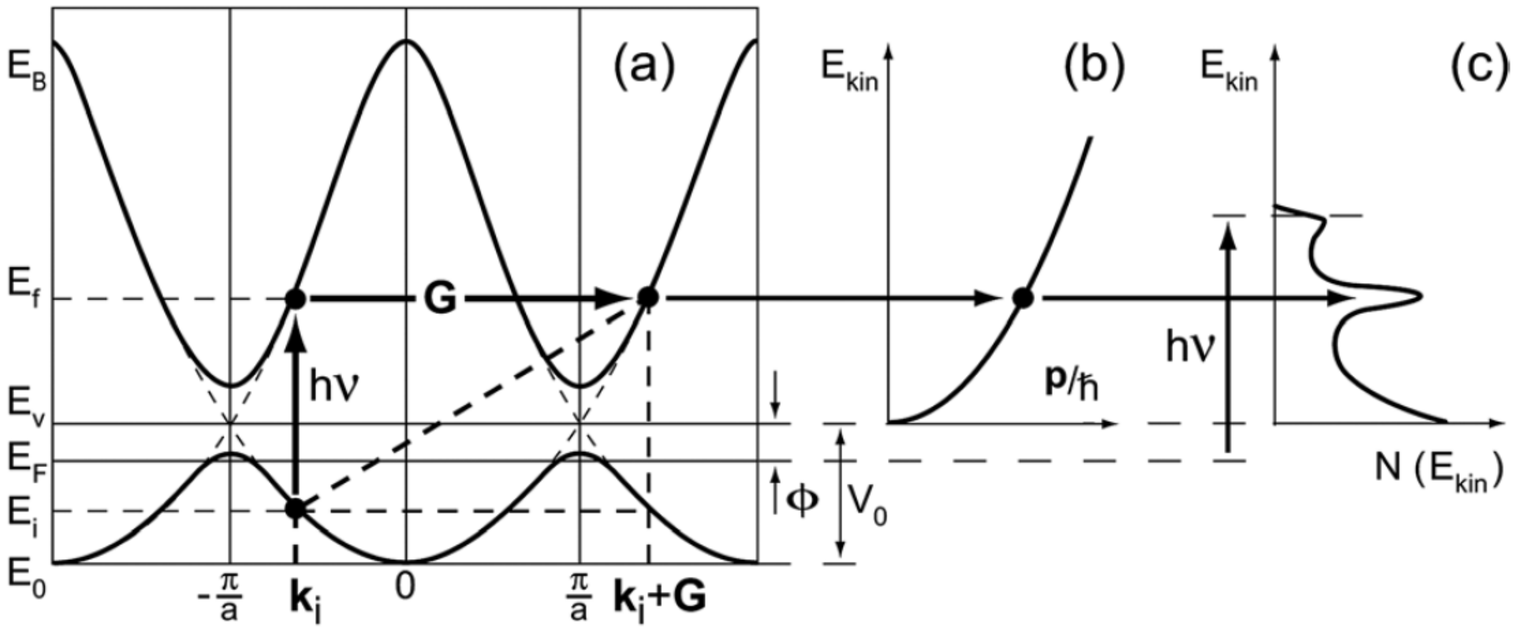
- S(q,ω) ~ FT[G(r,t)]



# Block II … preview

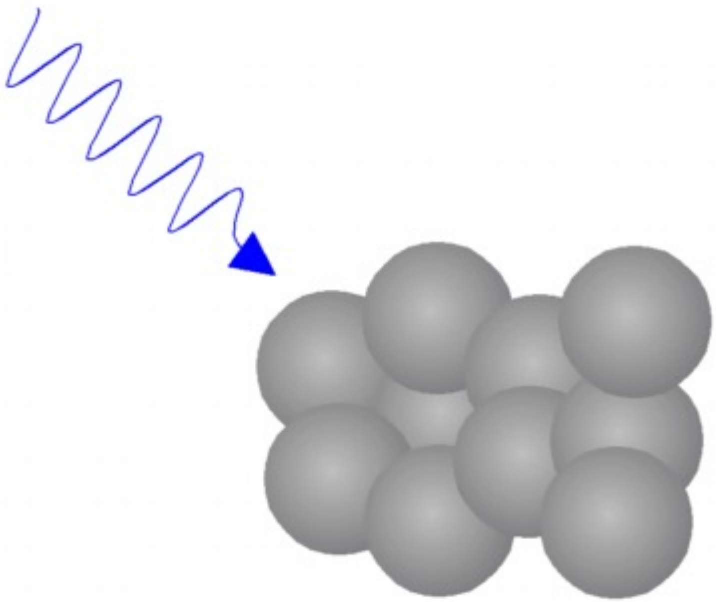
# Electronic Structure using AR-UPS

**Electronic bandstructure E(k) and photo-excitation in a periodic potential**




Observe energy and momentum conservation
to resolve bandstructure E(k)

# Electronic Structure using AR-UPS



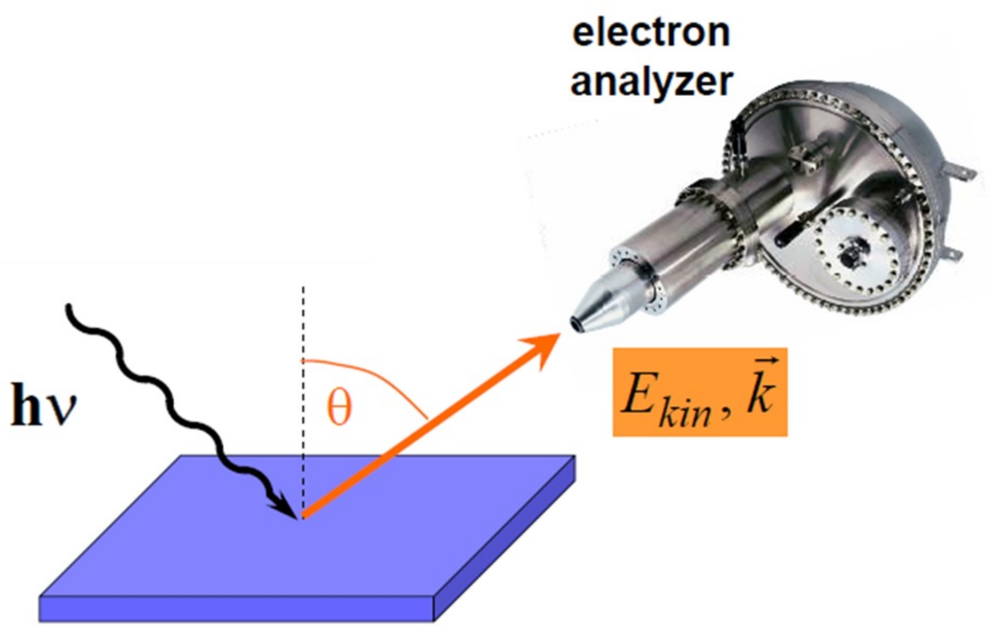
$$M + h\nu \rightarrow M^{+} + e^{-}$$

- X-ray photoelectron spectroscopy (XPS)
  *hv = 50 … 5000 eV*

- **Ultraviolet photoelectron spectroscopy (UPS)**
  *hv = 10 … 50 eV*

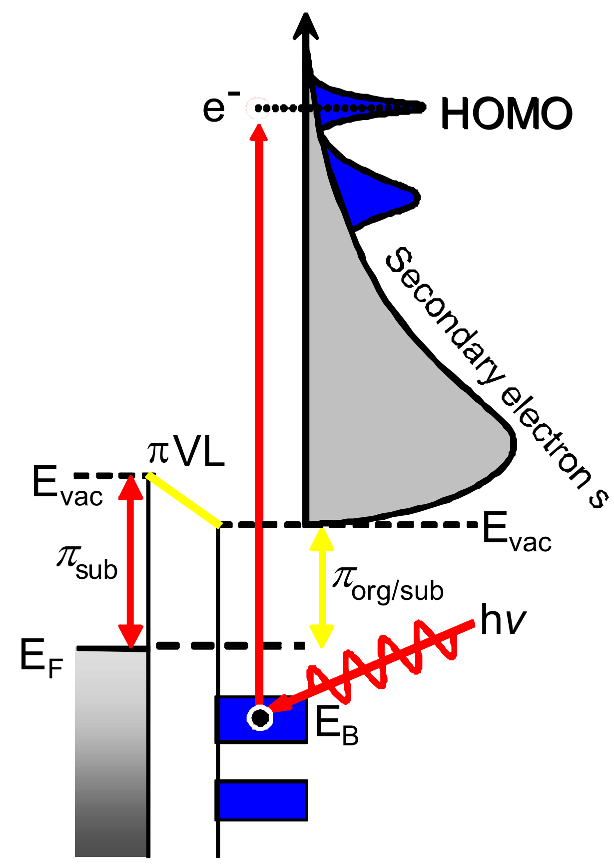
# Electronic Structure using AR-UPS

**Angle-resolved photoelectron spectroscopy (ARPES)**



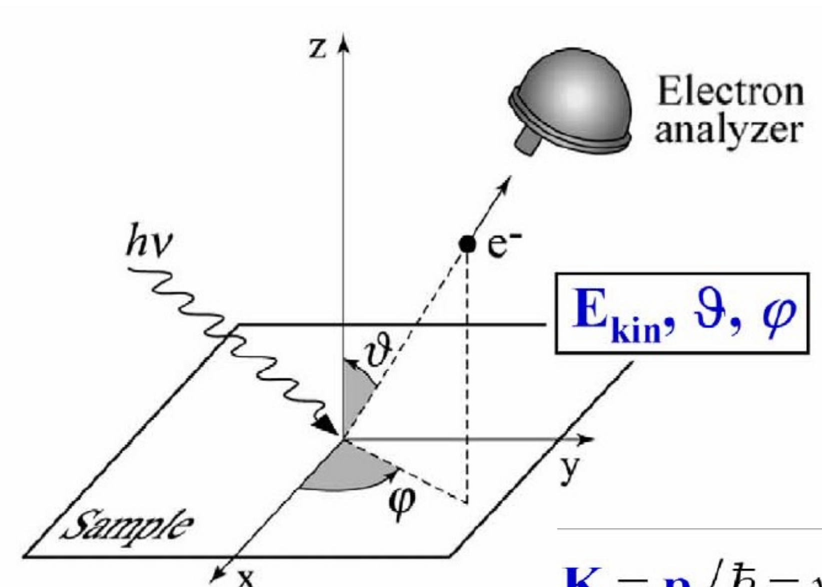

Energy conservation

$$E_{kin} = h\nu - \phi - |E_B|$$



# Electronic Structure using AR-UPS

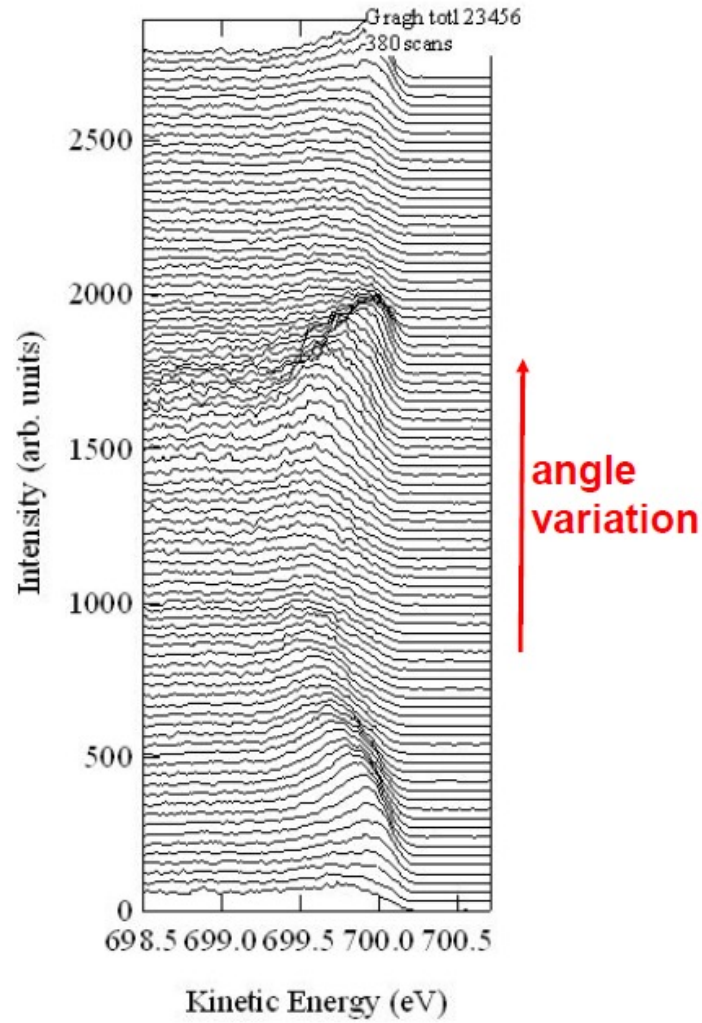
## Angle-resolved photoelectron spectroscopy (ARPES)




$$\mathbf{K} = \mathbf{p} / \hbar = \sqrt{2mE_{kin}} / \hbar$$

Momentum conservation

$$\hbar \mathbf{k}_{||} = \hbar \mathbf{K}_{||} = \sqrt{2mE_{kin}} \cdot \sin\vartheta$$




**example:**
**soft x-ray ARPES on $Sr_2Ru_{1-x}Ti_xO_4$**

# Block III … preview

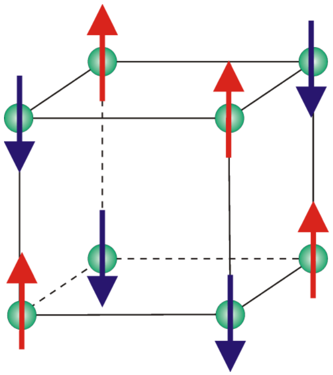
# Magnetic Structures and their Dynamics

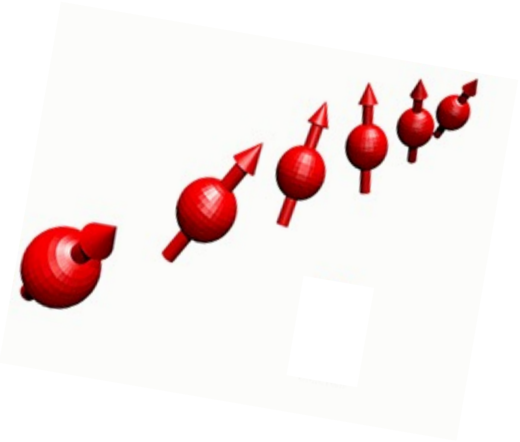
**From single atoms to solids**

- Exchange interactions
- Criteria for stabilizing magnetic order
- Magnetic structures

**Condensed matter with dynamics**

- Spinwaves (magnons)
- Detection of magnetic excitations

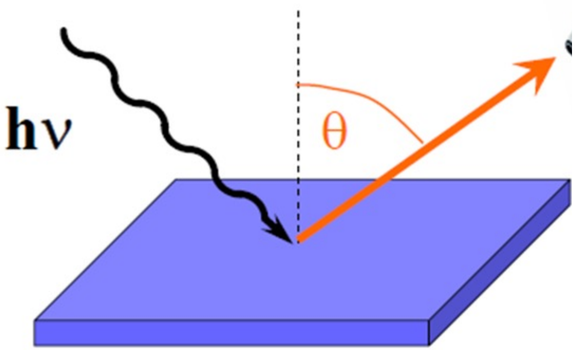




- Wikipedia
- Nanomaterials 2017
- Pradip, PRL 2016

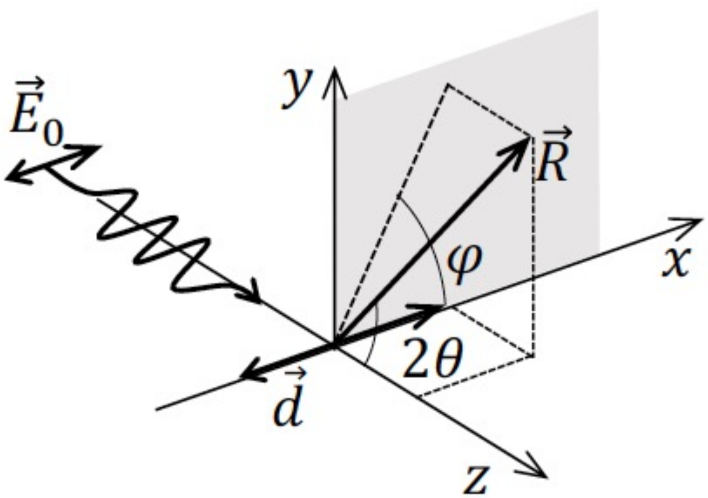
# How to address these questions quantitatively ?

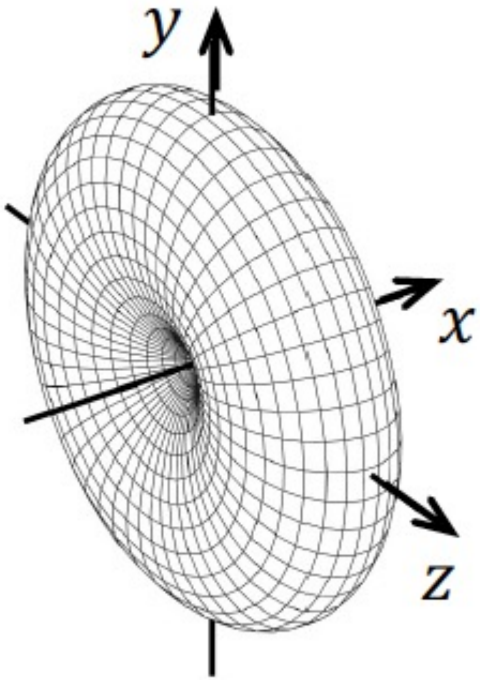
- Scattering of waves from condensed matter
- … elastic scattering … no energy exchange with solid … diffraction
- … inelastic scattering … energy exchange with solid … spectroscopy
- … absorption … and possibly emission of (other) particle … spectroscopy



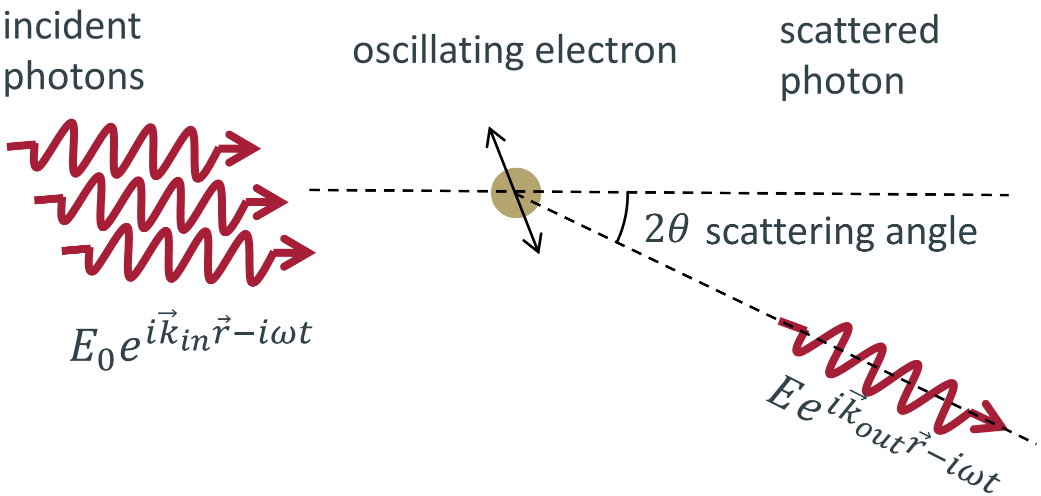

- Need to know cross sections relevant for interaction
- This is what we do today (1st lecture) for elastic scattering

# Scattering of X-rays from electrons (classical picture)



# Scattering of X-rays from electrons (classical picture)




Amplitude of electron's oscillations

$$d = -\frac{eE_0}{m\omega^2} e^{-i\omega t}$$

Electric field radiated by the electron

$$E \propto -\frac{e^2}{mc^2} E_0 e^{-i\omega t}$$

Scattering vector

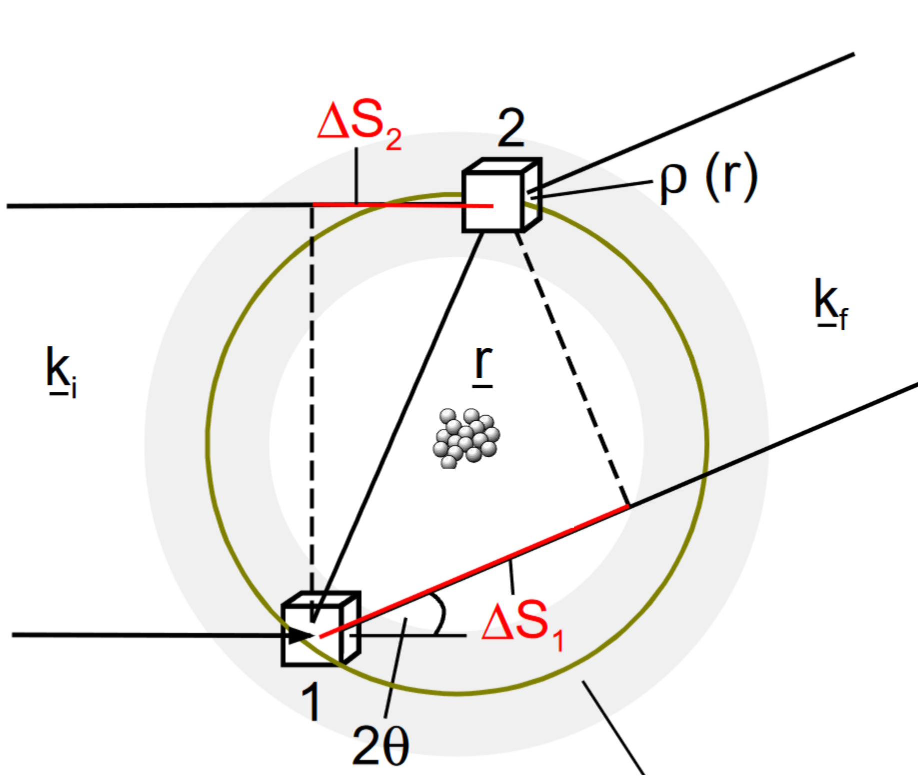
$$\vec{q} = \vec{k}_{out} - \vec{k}_{in}$$

$$|\vec{q}| = \frac{4\pi}{\lambda} \sin\theta$$

# Scattering of X-rays from electrons (classical picture)

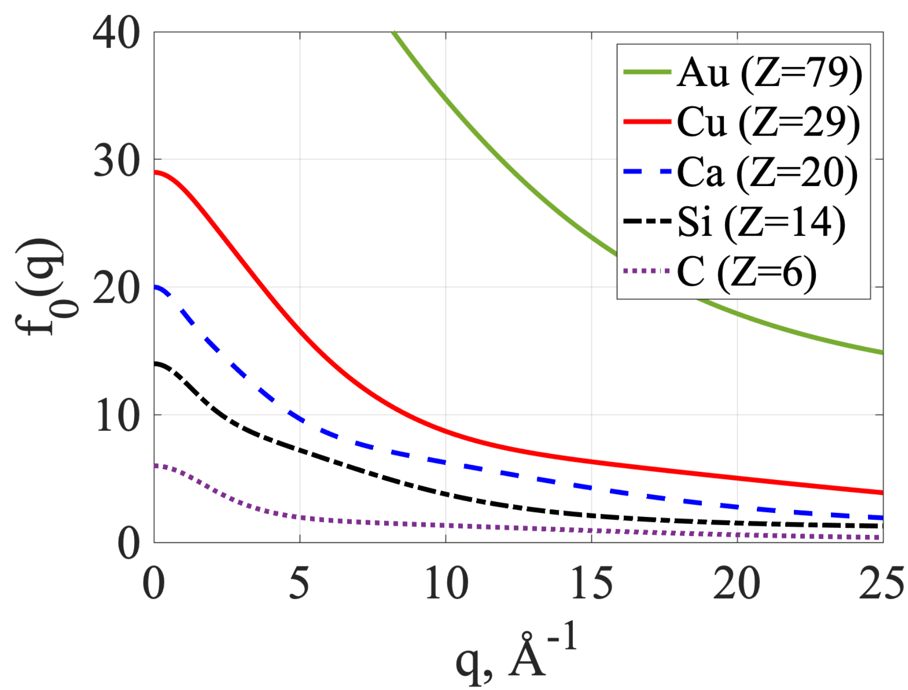
Calculation on blackboard

# Scattering of X-rays from atoms

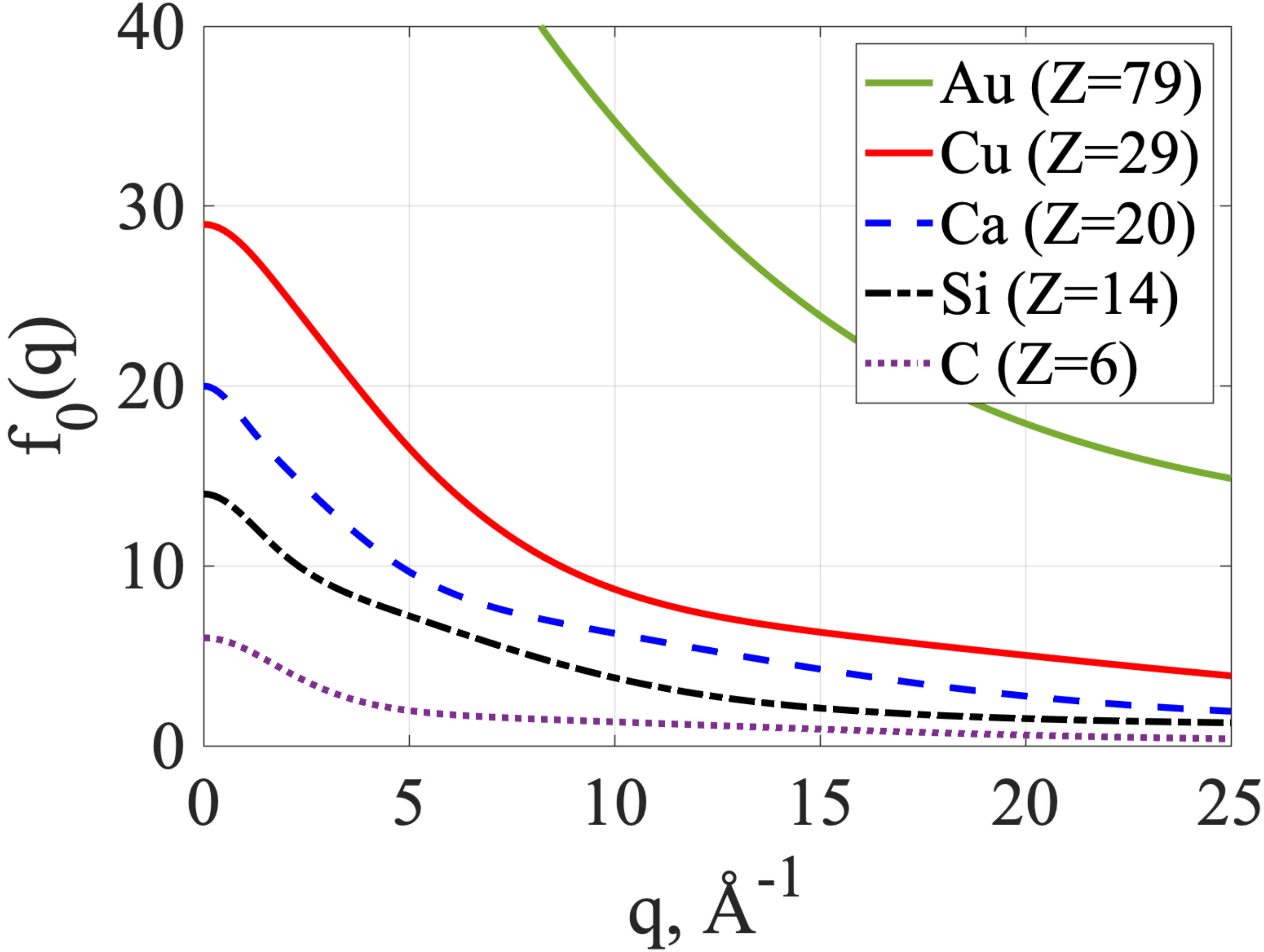



$$A = r_e \int \rho(\underline{r})\, e^{i\underline{q}\cdot\underline{r}}\, d\underline{r}$$

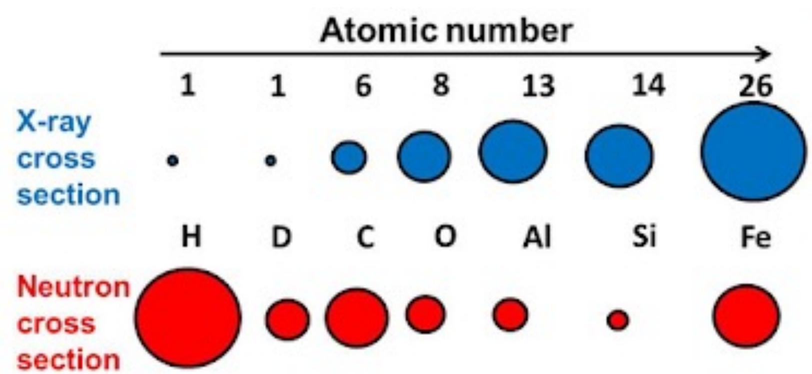
$$\boxed{f(\underline{q}) = \int \rho(\underline{r})\, e^{i\underline{q}\cdot\underline{r}}\, d\underline{r}}$$

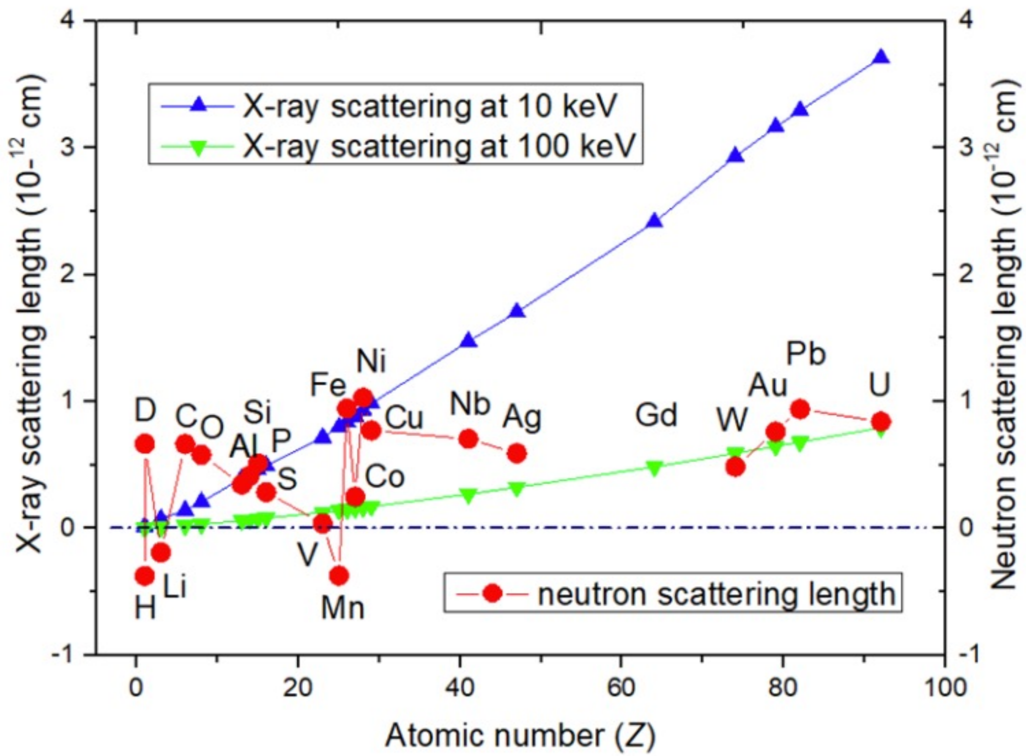


# Scattering of X-rays from atoms



# Scattering of X-rays vs scattering of neutrons




http://worldsciencereport.blogspot.com/

*Ren, Y., Zuo, X.,*
*Small Methods 2018, 2, 1800064*