Theoretical Materials Science

Matthias Scheffler & Christian Carbogno: lecture
Christian C. & Henrik Kowalski et al.: exercises

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they work together

Reading:
- these notes (not complete ...)
- script (grown and updated since ~30 years) ~ 2 days after lecture
- books

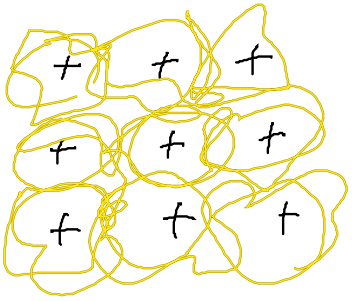
0. Foreword

Solid State physics; Condensed Matter Physics, Materials Science & Engineering

A very broad, multilayered field; probably the most active & important for wealth & health.

1) quantum-mechanical many-body problem
2) dynamics & Statistical Mechanics

A solid



$\sim 10^{23}$ nuclei per cm^3

$\sim 10^{23}$ electrons

200,000 materials are known to exist

but their properties are largely unknown
↳ hardness, elastic constants, electrical conductivity, thermal conductivity, e.t.c.

How many materials do we not know?

unit cell ≡ the smallest unit to build the solid

- a unit cell contains atoms (choose from ~100 atoms in Periodic table)
- many atoms per cell (1, 2, ... 100, ...)
- also inorganic & organic materials
- organic/inorganic hybrids
- heterostructures 
- nanostructures

⇒ amount of possible materials is practically infinite

2 "science & engineering initiative"

a) National nanotechnology initiative
B. Clinton (2000)

b) Material genome initiative ...
B. Obama (2011)

Very active field many new developments

Still many open questions
- basic theory
- new methods
- algorithm
- new computer codes

} high-permance computers ~ 100 mio CPU-core hours every day

Since 1978 we can predict solid state properties ab initio (from first principles)
↑ starting from the many-body Schrödinger eq.

only now approximations check
⇒ new, hitherto unknown materials can be calculated

several phenomena are not yet fully understood:
phase transitions, disorder/amorphous, crystal growth & crystal-structure prediction, f-electrons, high-Tc superconductivity, electrical conductivity, electronic excitations, thermal conductivity.

The main challenges for theory

1) Explain exp. observations
Reduce the explanation to the Key physical

properties.

2) predict properties of yet unknown system, or at harsh conditions

e.g.: Fe at the center of earth core

- predict new materials (cleaner & cheaper): fuel for heating or mobility batteries ...

⇒ enormous socio-economic relevance since 1980: 38 Nobel Prizes related to material science.