

Theoretical Materials Science

Matthias Scheffler & Christian Carbogno: Lecture

Christian C. & Henrik Kowalski et al.: exercises

Fritz-Haber-Institut der Max-Planck-Gesellschaft

Reading: • these notes (not complete...)

• script (grown and updated since ~30 years) ~ 2 days after lecture

• books

they work together

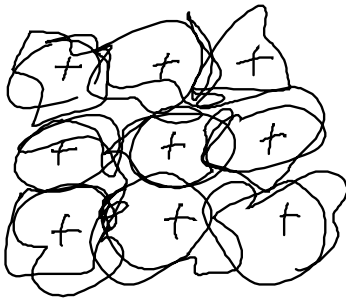
0. Foreword

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

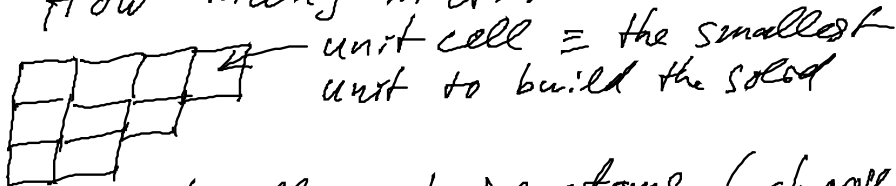
$\sim 10^{23}$ electrons

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?



- 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-performance
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- T_c 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 materials science.