# Theoretical Materials Science

(Condensed Matter Theory I & II)

## Wahl pflichtfach

Tue & Wed 10 - 12
& excess Wed 14 - 16

combine with
Quantenmechanik gekühlter Atome (Udo Schanz)
Mo 12 - 14

or
Comp. aspects of Stat. phys. (Luca Ghiringhelli)
Mo 10 - 12

## Who are we ?

Matthias Scheffler
Alex Tkatchenko
Patrick Rinke
Volker Blum

} Fritz-Haber-Institut of MPG

http://th.FHI-Berlin.MPG.de

Literature: see 1. exercise sheet

Script: 1) this handwritten material (available directly after the lecture)

2) A typed manuscript available "soon" after the lecture we try 1-2 days

## Chapter 0 A general intro

1) $10^{23}$ electrons & $10^{23}$ nuclei

⇒ basic theory: electrons — electron theory (many-body)

⇒ interaction between atom

⇒ reaction to outside perturbation

⇒ properties

2) properties ⇒ function

3) predict improved functional material (photovoltaic, new catalyst (energy from sun, wind ...) ⇒ "fuel"

⇒ urgent need; to tackle with energy challenge.

≡ fundamental research

Many-body theory

⟹ novel phenomena

do this is only getting possible now

a) new concepts and methods

b) high-performance computers

Future (next 5+x years)

Building a library of hitherto unknown materials

so far experiment trial & error

soon calculate > 10000 potential material

⟹ new level of understanding, trends & mechanism

The field is huge & important

one indicator for → Nobel prizes: since 1980 33 Nobel prizes to materials science

units

SI ← will use this in the beginning

then "atomic units"

$\frac{e^2}{4\pi\varepsilon_0} = 2$

$\hbar = 1$

$m_e = 0.5$

} Rydberg atomic units

natural unit of energy = 1 Ryd = 13,606 eV
= binding energy of electron in H.

length unit: 1 bohr = 0.529 Å
0.0529 nm

nano = $10^{-9}$

# Chapter 1 Introduction

## 1.1 The many body hamiltonian

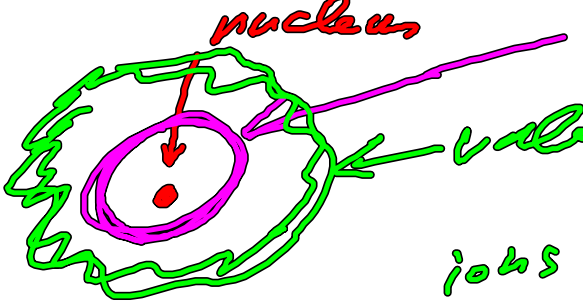
$$H\psi = E\psi$$

$\Updownarrow$

materials build from nuclei & electrons

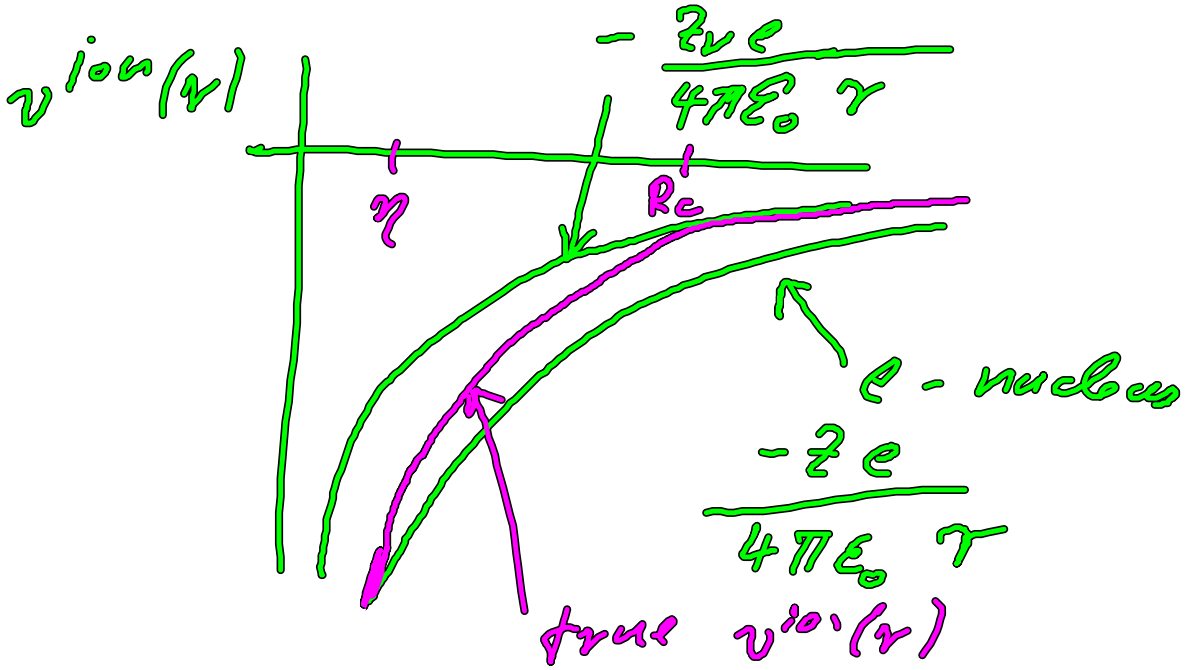
or

ions + all valence electrons




ions $\equiv$ core + valence elect

$\equiv$ fixed object



frozen core approximation
not necessary
but good for talking.

| atom | number of electronic configuration | Z | $Z_V$ | $R_c$ [bohr] | $v_{ion}(r)$ [Ryd] |
|---|---|---|---|---|---|
| H | $1s^1$ | 1 | 1 | 0 | $-\frac{2}{r}$ |
| He | $1s^2$ | 2 | 2 | 0 | $-\frac{4}{r}$ |
| C | $[1s^2]2s^2 2p^2$ | 6 | 4 | 0.7 | $r \geq -\frac{8}{r}$ <br> $\eta < r < R_c$ <br> $r < \eta = -\frac{12}{r}$ |
| Si | $[1s^2 2s^2 2p^6]$ <br> $3s^2 3p^2$ | 14 | 4 | 1.7 | ... |

if interatomic distance $< 2R_c$
then frozen-core approach cannot be used.