Technische Universität Graz

Molecular and Solid State Physics

Calculate the macroscopic properties from the microscopic structure.

Peter Hadley

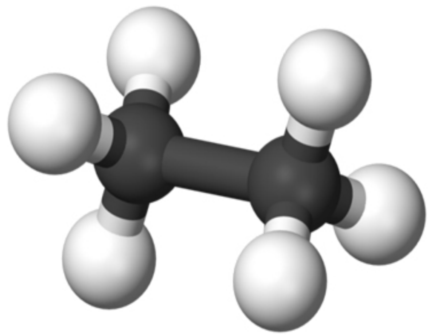
Goals

The microscopic structure determines the macroscopic properties.

At the end of this course you should be able to explain how any property of any molecule or solid can be calculated using quantum mechanics and statistical physics.

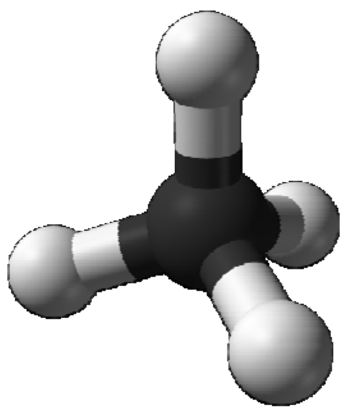
For example: knowing how the atoms are arranged in a crystal, you must be able to say if it is an electrical conductor or not.

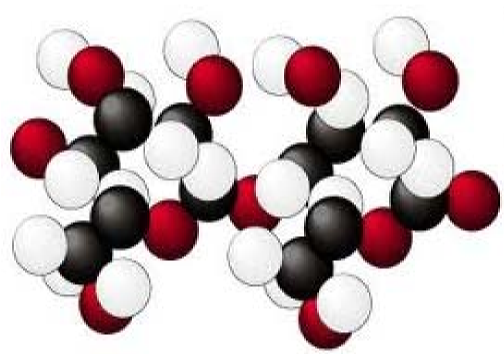
Molecules

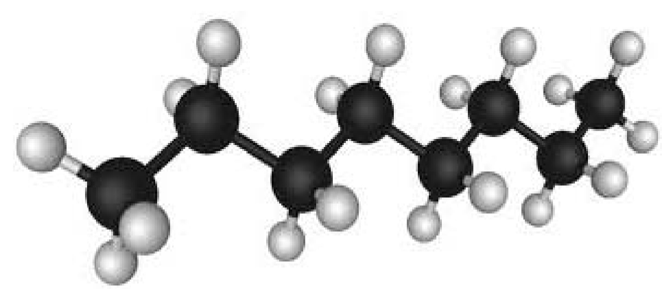


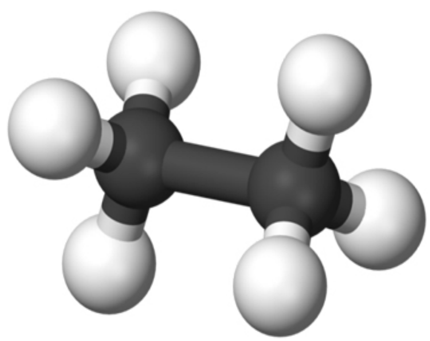
There are billions of useful molecules.

Acids, esthers, alkanes, ...
Biological molecules: DNA, RNA, proteins









Molecules

Every property of a molecule can be calculated using multi-particle quantum mechanics.

$$H_{\text{mp}} = -\sum_i \frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_a \frac{\hbar^2}{2m_a}\nabla_a^2 - \sum_{a,i}\frac{Z_a e^2}{4\pi\epsilon_0|\vec{r}_i - \vec{r}_a|} + \sum_{i<j}\frac{e^2}{4\pi\epsilon_0|\vec{r}_i - \vec{r}_j|} + \sum_{a<b}\frac{Z_a Z_b e^2}{4\pi\epsilon_0|\vec{r}_a - \vec{r}_b|}$$

We will calculate:

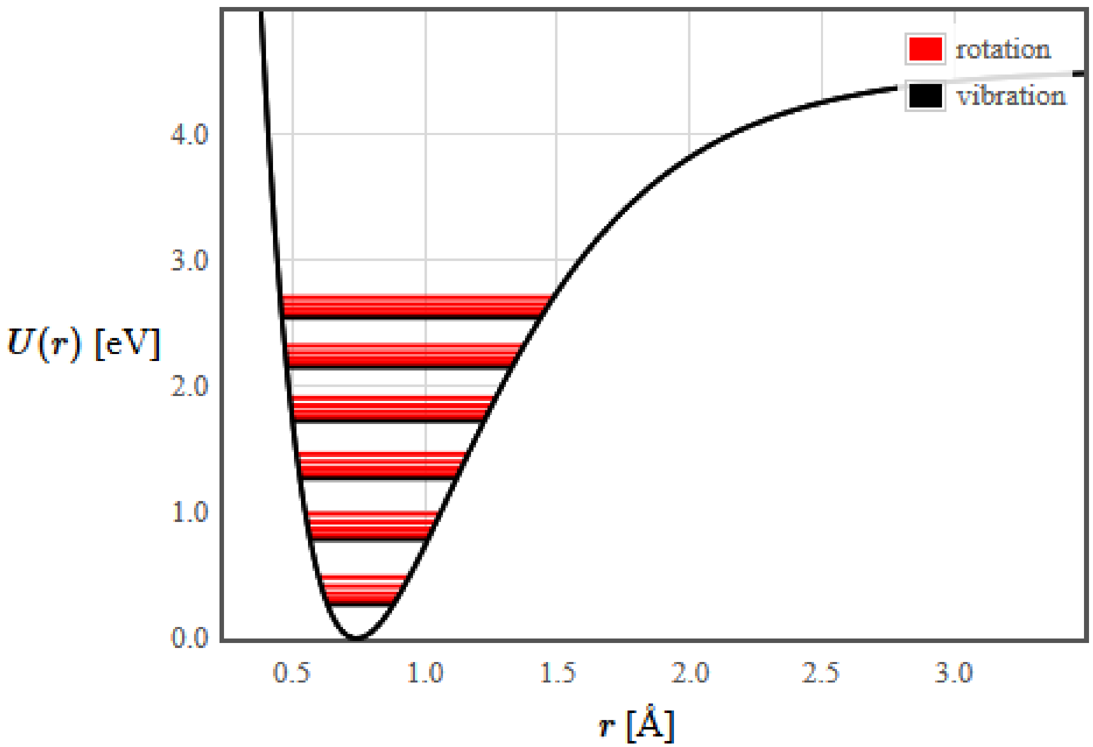
- bond length
- bond strength
- molecular energy levels

http://en.wikipedia.org/wiki/File:Erwin_Schr%C3%B6dinger.jpg

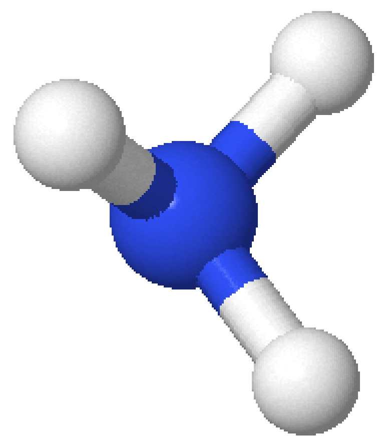
Molecules

$$H_{\rm mp} = -\sum_i \frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_a \frac{\hbar^2}{2m_a}\nabla_a^2 - \sum_{a,i}\frac{Z_a e^2}{4\pi\epsilon_0|\vec{r}_i - \vec{r}_a|} + \sum_{i<j}\frac{e^2}{4\pi\epsilon_0|\vec{r}_i - \vec{r}_j|} + \sum_{a<b}\frac{Z_a Z_b e^2}{4\pi\epsilon_0|\vec{r}_a - \vec{r}_b|}$$

$$E = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$



Bond length: 0.74144 Å.
Dissociation energy: 4.52 eV.



Solids

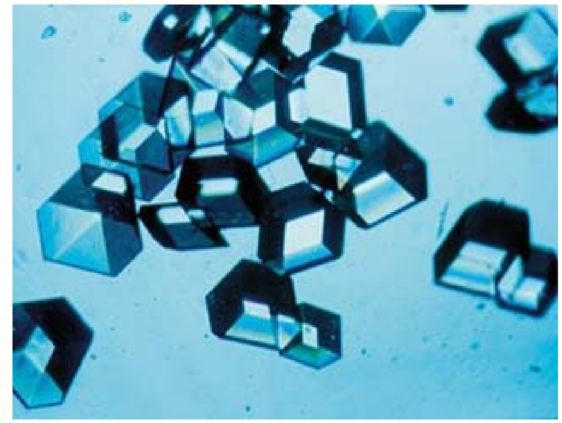
Solids are large molecules

Crystal structures
Determining crystal structures with x-ray diffraction
Photons in solids
Phonons in solids (lattice vibrations)
Thermal properties
Free electron model
Band structure (metals, semiconductors, insulators)
Semiconductors

Crystal = periodic arrangement of atoms

Gallium crystals

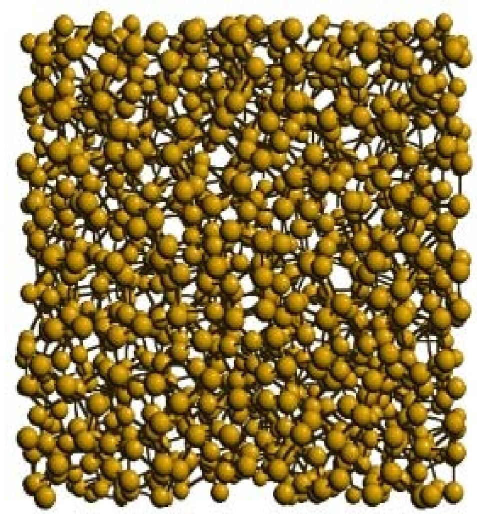
quartz



Insulin crystals

amorphous metal

glass

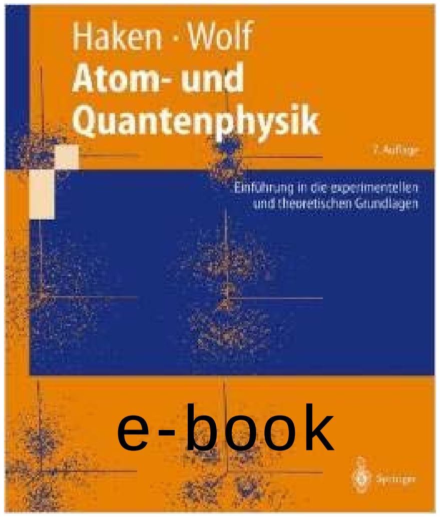


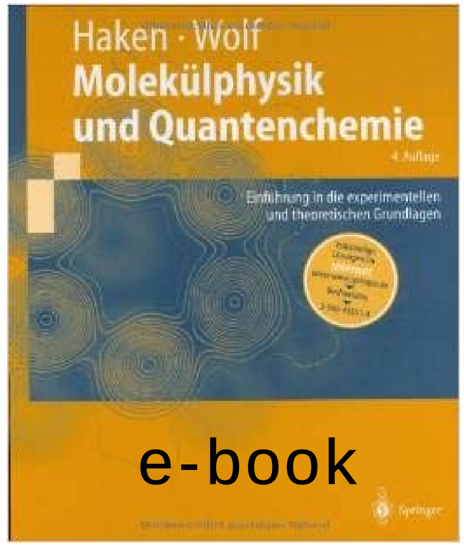
amorphous silicon

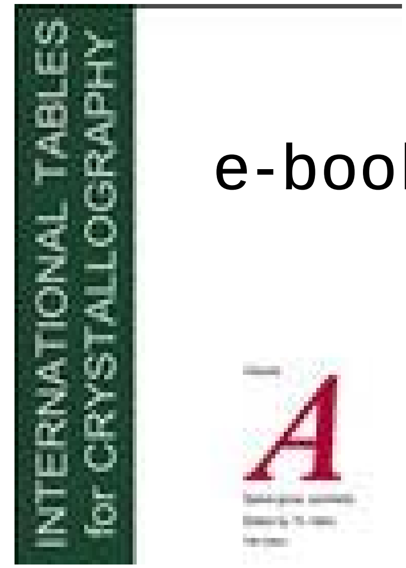
http://www.wikipedia.org

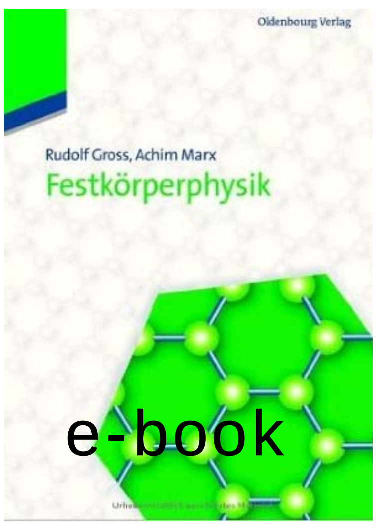
http://www.pmc.umontreal.ca/~mousseau/site_an/uploads/Main/si1000.jpg

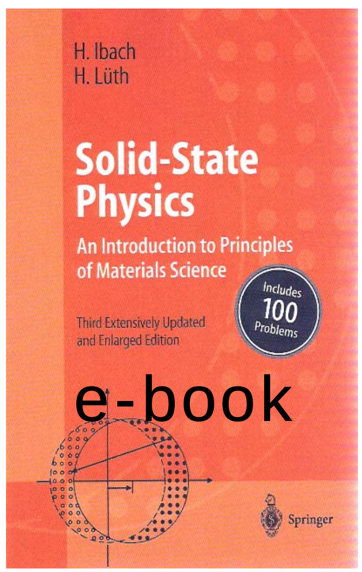
Books

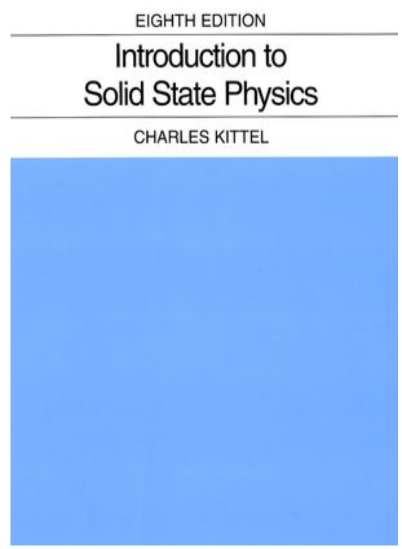

Haken · Wolf
Atom- und Quantenphysik
7. Auflage
Einführung in die experimentellen und theoretischen Grundlagen
Springer
e-book

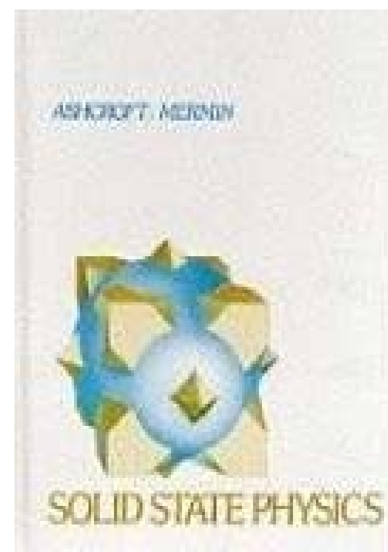

Haken · Wolf
Molekülphysik und Quantenchemie
4. Auflage
Einführung in die experimentellen und theoretischen Grundlagen
Springer
e-book


INTERNATIONAL TABLES for CRYSTALLOGRAPHY
A
e-book


Oldenbourg Verlag
Rudolf Gross, Achim Marx
Festkörperphysik
e-book


H. Ibach
H. Lüth
Solid-State Physics
An Introduction to Principles of Materials Science
Includes 100 Problems
Third Extensively Updated and Enlarged Edition
Springer
e-book


EIGHTH EDITION
Introduction to Solid State Physics
CHARLES KITTEL


ASHCROFT MERMIN
SOLID STATE PHYSICS

http://www.if.tugraz.at/ss1.html

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Menu | Sections | **PHY.F20 Molecular and Solid State Physics**

Course outline

- **Introduction** ▶ EN 6:45
- **Review of atomic physics**
  - The solutions to the Schrödinger equation for the hydrogen atom ▶ DE 5:13
    - Plots of the atomic orbitals
  - Helium
  - Many-electron wavefunctions
  - Slater determinants W
  - Singlet and triplet states
  - Exchange W
  - The intractability of the Schrödinger equation
  - Many-electron atoms
- **Molecules**
  - Molecular orbital theory W
    - Solving the total molecular Hamiltonian W
      - The Born-Oppenheimer approximation W
      - Many-electron wavefunctions
      - Bond potentials
      - Vibrational states
      - Rotational states
    - Solving the molecular orbital Hamiltonian

Student Projects

Do something that will help other students

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Google Custom

Menu | Sections | **PHY.F20 Molecular and Solid State Physics**

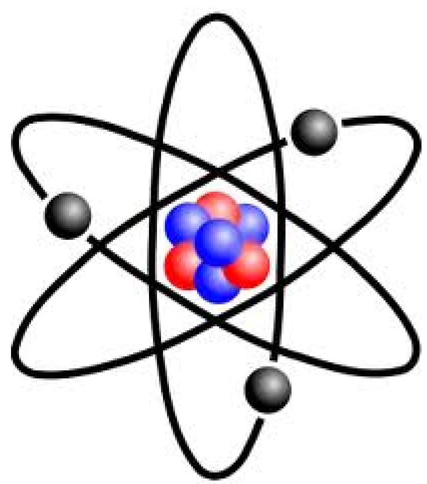
Student projects

- Over the years there have been many contributions to the course from students and now we need to correct errors and remove unclear contributions before too much more is added. If you find something that is wrong or unclear and can improve it, that would be a suitable project.

- Often in atomic and molecular physics it is necessary to evaluate matrix elements of the form, $\langle \phi_m | H | \phi_n \rangle$. Where ϕ_n are the atomic orbitals. To evaluate the integral, we need to know the atomic orbitals and the Laplacians of the atomic orbitals, $\nabla^2 \phi_n$. A student made a list of the first few atomic orbitals which can be found at the bottom of the page on atomic orbitals. This list could be expanded.
- There are some examples of using the atomic orbitals to calculate matrix elements such as the 1s orbital and the 2p orbital. Code in various languages such as Fortran, c, Java, JavaScript, Matlab, and Mathematica would be useful to have.
- Check the integration and the numerical calculations on the pages for these atomic orbitals 1s, 2s, $2p_z$.
- Plot the bond potential for a hydrogen molecular ion H_2^+. See the discussion of the Hydrogen molecular ion H_2^+.
- Calculate the molecular orbitals of ethylene, and butadiene similar to the calculation for benzene. Since these molecules are chain of carbon atoms, refer to the discussion of molecular chains. Separate projects would be the numerical calculation of H_{11}, H_{12}, and S_{12} for ethylene, butadiene, or benzene.
- Upload a video to YouTube (<10 minutes) that explains some topic in the course outline.
- Upload a video to YouTube that explains how to use a piece of laboratory equipment in the physics building related to this course.
    - x-ray diffractometer

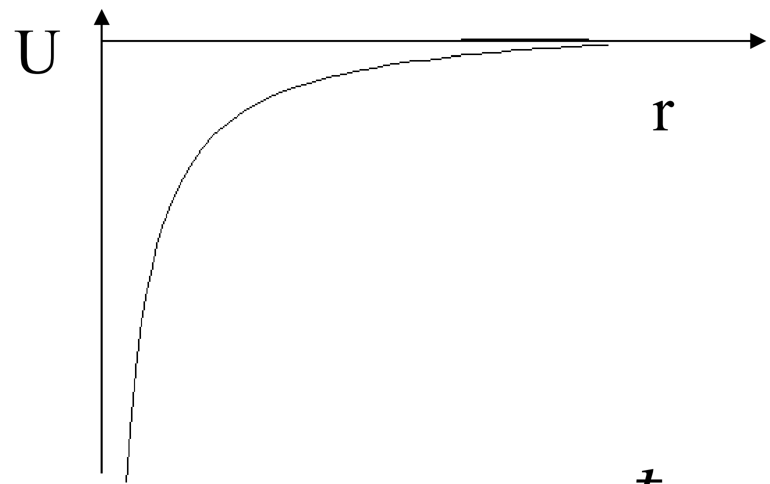
Review of atomic physics

Estimating the size of an atom
The hydrogen atom
The helium atom
Many electron atoms



Estimate the size of a hydrogen atom

Potential energy $U(r) = -\frac{e^2}{4\pi\varepsilon_0 r}$



Uncertainty relation $\Delta x \Delta p_x \geq \frac{\hbar}{2}$

For an atom: $\Delta x \sim r_0$

$$\Delta p_x \geq \frac{\hbar}{2r_0}$$

Estimate the size of a hydrogen atom

$$\Delta p_x \geq \frac{\hbar}{2r_0}$$

$$\Delta p_x = \sqrt{\langle p_x^2 \rangle - \langle p_x \rangle^2} \qquad \langle p_x \rangle = 0$$

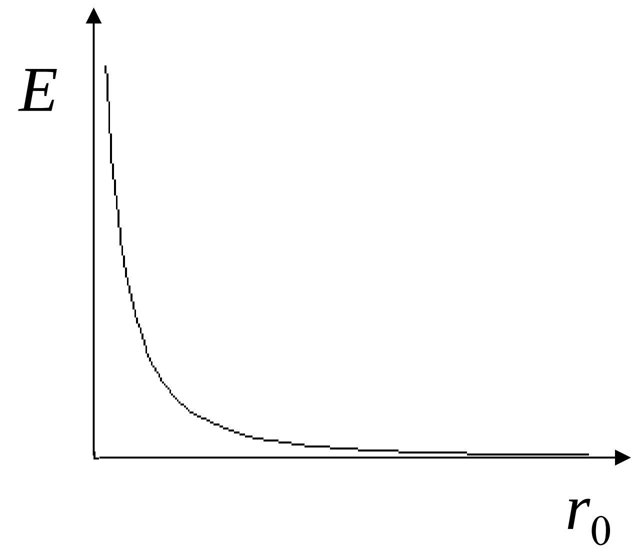
$$(\Delta p_x)^2 = \langle p_x^2 \rangle \geq \left(\frac{\hbar}{2r_0} \right)^2$$

$$E_{kin} = \frac{mv^2}{2} = \frac{p^2}{2m}$$

Kinetic energy in x-direction = $\langle E_{kin} \rangle = \dfrac{\langle p_x^2 \rangle}{2m} \geq \dfrac{\hbar^2}{8mr_0^2}$

Confinement energy

Kinetic energy in *x*-direction = $\langle E_{kin} \rangle = \frac{\langle p_x^2 \rangle}{2m} \geq \frac{\hbar^2}{8mr_0^2}$



Confinement energy:

$$\frac{\langle p_x^2 \rangle}{2m} + \frac{\langle p_y^2 \rangle}{2m} + \frac{\langle p_z^2 \rangle}{2m} \geq \frac{3\hbar^2}{8mr_0^2}$$

Estimate the size of a hydrogen atom

Total energy = Kinetic + Potential

$$E_{tot} = \frac{3\hbar^2}{8mr^2} - \frac{e^2}{4\pi\varepsilon_0 r}$$

$$\frac{dE_{tot}}{dr} = \frac{-3\hbar^2}{4mr^3} + \frac{e^2}{4\pi\varepsilon_0 r^2}$$

$$r_0 = \frac{3\hbar^2 \pi\varepsilon_0}{me^2} = 4.0\times10^{-11}\ \text{m}$$

$$a_0 = 5.3\times10^{-11}\ \text{m}$$

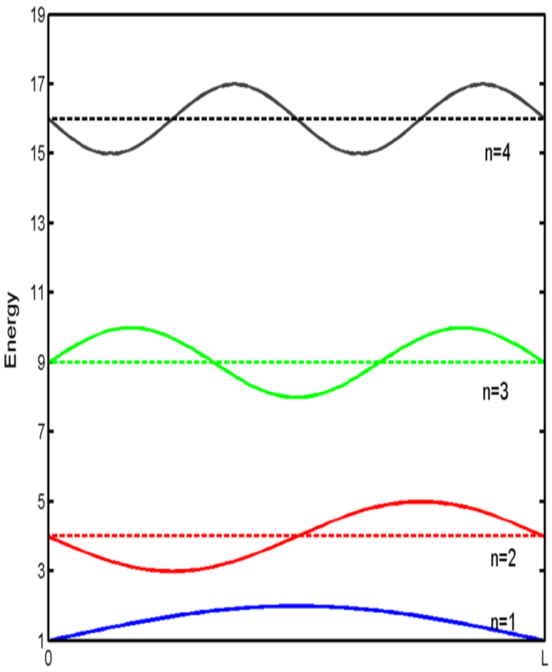
Confinement energy

$$\frac{-\hbar^2}{2m}\nabla^2\Psi - \frac{e^2}{4\pi\varepsilon_0 r}\Psi = E\Psi$$

The kinetic energy term increases as the wavelength gets smaller

$$E_{kin} = \tfrac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \frac{h^2}{2m\lambda^2}$$

$$p = mv \quad p = \hbar k \quad k = \frac{2\pi}{\lambda}$$



PHY.F30UF

Molekül- und Festkörperphysik 1UE

Di 11:45 – 12:30 (TUGraz) - T. Kamencek, P. Hadley

Di. 12:00 – 12:45 (TUGraz) - R. Resel

Di 12:00 – 12:45 (KFUGraz) - L. Egger, M. Schwendt

problems / register: TUGraz TechCenter	- one credit per problem
written exams: 5. May, 23 June	- each 50 credits
optional student projects (until Aug.2020)	- up to 20 credits

from written exams: at least 50 credits

sufficient: 70 … 88 credits

satisfactory: 89 … 106 credits

good: 107 … 124 credits

very good: > 125 credits