

## Lecture announcement

### Quantum Mechanics in Materials Science

The course will provide an overview of the fundamentals and the application of Quantum Mechanics in Materials Science. After the course the students will be able to read and understand textbooks and the research literature in the field. The course will treat the principles of electronic structure calculations in Materials Science and also provide some insight in the numerical implementation of electronic structure methods. The relations between electronic structure properties and the crystal structure and other properties of materials will be pointed out.

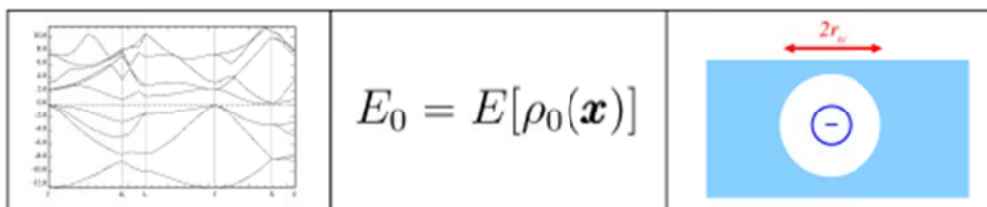
The lectures will be complemented by classes on analytic problems. The course is intended for M. Sc. Students. Successful completion with written exam will correspond to 4 credit points.

#### Keywords:

- Schrödinger equation, many-body problem, Hartree, Hartree-Fock
- band structure, symmetry groups, density of states
- density-functional theory, basis-sets, pseudo potentials
- simplified models of the electronic structure

#### Literature:

- N.W. Ashcroft and N.D. Mermin, Solid States Physics
- D. G. Pettifor, Bonding and Structure of Molecules and Solids



Semester	Summer Semester 2015
Modul	3a
Hold by	Prof. Ralf Drautz
Time	Monday 8.30-10.00 am & Thursday 8.30-10.00 am
Room	ICAMS seminar room IC 02/718
First Lecture	Monday 18.04.2016 and Thursday 21.04.2016
Contact	Prof. Ralf Drautz, IC 02/521, <a href="mailto:ralf.drautz@rub.de">ralf.drautz@rub.de</a> , Phone +49 234 32 29308