

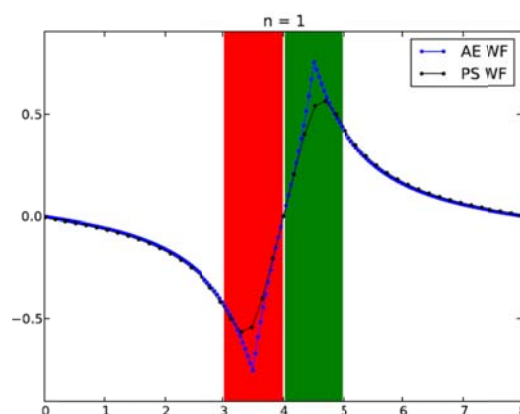
## Lecture announcement

### Application and Implementation of Electronic Structure Methods

Students will be enabled to choose the most appropriate electronic structure computational method for a given researchproject, to formulate and describe the foundation of density functional theory (DFT), to describe the most common approximations employed in DFT, and to contribute to the implementation of a DFT code.

#### Subject aims

- Numerical implementation and solution of a single particle Schrödinger equation (electron in a pseudo potential)
- Basis sets, representation of operators in a basis
- Results and analysis of electronic structure calculations
- Numerical convergence
- The Plane-Wave Pseudo-Potential Method (self-consistent numerical implementation)
- The Tight Binding Method
- Bond-order potentials
- Special topics and applications (structural stability, magnetism)



Semester	Summer Semester 2016
Modul	6-MS2
Hold by	Prof. Dr. J. Neugebauer, Prof. Dr. Drautz
Time	Block Seminar
Room	ICAMS CIP-pool
First Lecture	22.06.2016
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