MSS
MATERIALS SCIENCE AND SIMULATION

ICAMS
INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

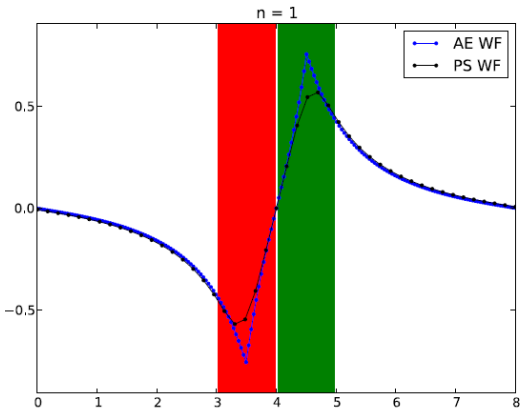
Lecture announcement

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 2015
Modul	6-MS2
Hold by	Prof. Dr. J. Neugebauer, Dr. Georg Madsen
Time	Tuesday 16.00-18.00 & Friday 10.00-12.00
Room	ICAMS CIP-pool
First Lecture	17.04.2015
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