UNIVERSITY OF VIENNA

VIENNA, AUSTRIA

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SS11: VO Computational Quantum Mechanics
2 Stunden, 2,5 ECTS credits
Unterrichtssprache: Englisch
Ort: Seminarraum, Sensengasse 8/7, 1. Stk.
Erster Termin: 08.03.2011, 14.00-15.30

Course Description:

Contents: This course focuses on the atomistic modeling of materials-specific properties through the solution of the many-electron Schrödinger equation. The students will be introduced to computational methods used in electronic structure calculations to reduce the complexity of the Schrödinger equation at various levels of sophistication. Specific topics include: numerical solution of the Schrödinger equation, linear algebra and matrix diagonalization, the many-body problem, tight-binding approximation, Hartree-Fock (HF) and density functional theories (DFT), post- HF and DFT methods. The applicability of the computational tools to diverse materials problems will be discussed (also through computational experiments). This course requires some prior experience in quantum mechanics and solid states physics.

Aim: Computational quantum-mechanical modeling of materials. The lecture will give students the theoretical background and the practical experience to model, understand, and predict the properties of real materials.

Schedule:

Date	Time	Subject
01.03.2011	14.00	Presentation
08.04.2011	14.00-15:30	Schrödinger Equation I
15.03.2011	14.00-15.30	Schrödinger equation II
22.03.2011	14.00-15:30	Linear algebra problems
29.03.2011	14.00-15:30	Grid-based methods
04.05.2011	14.00-15:30	The many body problem
05.04.2011	14.00-15:30	The Hartee-Fock method I
12.04.2011	14.00-15:30	The Hartee-Fock method II
12/18.04.2011	–	Easter Holidays
03.05.2011	14.00-15:30	Density Functional Theory I
10.05.2011	14.00-15:30	Density Functional Theory II
17.05.2011	14.00-15:30	Band Structure methods I
24.05.2011	14.00-15.30	Band Structure methods II
31.05.2011	14.00-15.30	Band Structure methods III
07.06.2011	14.00-15:30	Extra (Beyond DFT)
14.06.2011	14.00-15.30	Extra (Beyond DFT, Monte Carlo)