2 Psi-k Training Graduate Schools

2.1 Report on Bristol Training Graduate School

Psi-k Training Graduate School

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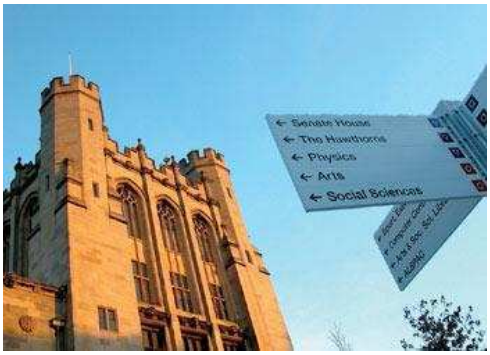
Workshop Details

Time and location: 25-31 March, 2007, Bristol University, U. K.



Description

This Graduate School is an activity of the Psi-k Training Programme in the EU-funded 'Series of Events' Marie Curie Conferences and Training Courses. It was funded by MOLSIMU, the Psi-k Programme of the ESF and the EPSRC's CCP9.

The combined theory-hands-on Graduate School on electronic structure methods took place at Burwalls and the Physics Department in Bristol from Sunday March 25 until Saturday March 31, 2007. There were 20 lectures over 6 days, 10 lectures on theory and 10 lectures on electronic structure methods. The rest was all hands-on experience with relevant codes. The 10 lectures on theory were:

- 3 lectures on Density Functional Theory (DFT) by Hardy Gross
- 3 lectures on many body perturbation theory (MBT) by Rex Godby
- 3 lectures on dynamical mean field theory (DMFT) by Karsten Held
- 1 lecture on the Bethe-Salpether equation (BSE) by Francesco Sottile.

The 10 lectures on methods gave a bird's eye view of 5 electronic structure methods:

- the plane-wave methods (PW) by Xavier Gonze
- the full potential local orbital method (FPLO) by Manuel Richter
- the linear augmented plane waves (LAPW) by Peter Blaha
- the linearized muffin tin orbital method (LMTO) by Ole Andersen
- the Korringa-Kohn-Rostoker (KKR) method by Hubert Ebert.

Each electronic structure method was introduced by two lectures followed by hands on experience with a modern state of the art code.

Scientific Objectives

The Bristol University Graduate School aimed towards giving masters students and beginning PhD students

- an understanding of the theories underlying electronic structure calculations;

- hands-on experience in electronic structure calculation codes;
- a perspective how these methods are used in state of the art research.

The Graduate School was motivated by

- The importance of electronic structure calculations of materials at the nano scale (such as catalysis, fuel cell research, magnetic recording and spin electronics, semiconductor technology, pharmacy etc.), has resulted in a sharp increase in the number of European groups (including industrial groups) starting with electronic structure calculations; these groups, however, do not have the optimal knowledge expertise for adequate training of their PhD students.
- The field of electronic structure calculations has become so broad that single institutions do not have the expertise to provide training of the entire field; only at the European level this expertise exists.
- The gap between education provided by university lectures and the much higher level of science in real research and at international workshops and conferences is steadily increasing. The school aimed at bridging this gap.
- The combined training and research program, will give young researcher the opportunity to develop in the European Psi-k network at a very early stage of their career.

Report

The Graduate School had 37 participants of which 23 were students. The fundamentals of electronic structure calculations for condensed matter were covered by lectures on density functional theory, on many body perturbation theory, dynamical mean field theory and on the Bethe-Salpether equation. A selection of 5 electronic structure methods and codes was made in order to stress such concepts as pseudopotentials and plane waves, multiple scattering, partial waves and screening, downfolding and minimal basis, local orbitals and linear augmented plane waves. Hands-on exercices complemented these lectures on the electronic structure methods.
The lecture notes can be found under
`http://psi-k.dl.ac.uk/data/Psik-training/psi-k_training2007.html`

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Program

Day 1: March 25 2007
Session : 1 Registration and Welcome
16:00 to 20:00 :

Day 2: March 26 2007
Session : 1 DFT I + II (Gross)
09:00 to 10:00 : Presentation
Gound-state density functional theory: An overview.
Basic Theorems
10:10 to 11:10 : Presentation
Gound-state density functional theory: An overview.
Optimized effective potential method (OPM, OEP)
Construction of orbital functionals to tackle van der Waals interactions
Non-collinear OEP
Session : 2 PW I (Gonze)
11:30 to 12:30 : Presentation
Plane waves and pseudopotentials:
I. Formalism

II Iterative techniques

Session : 3 MBT I (Godby)

14:30 to 15:30 : Presentation

Many-body theory for electronic structure

Introduction to many-body perturbation theory

The GW approximation (non-SC and SC)

Session : 4 KKR I (Ebert)

15:30 to 16:30 : Presentation

The Munich SPRKKR program package

Introduction

Green's functions

Scattering theory

Angular momentum representation

Calculating the scattering path operator

Session : 5 MBT II (Godby)

17:00 to 18:00 : Presentation

Many-body theory for electronic structure

Implementation of GW

Spectral properties

Day 3: March 27 2007

Session : 1 PW II (Gonze)

09:00 to 10:00 : Presentation

Plane waves and pseudopotentials:

III Applications

IV The ABINIT software

Session : 2 PW: Hands-on

10:30 to 12:30 : ABINIT tutorial session

Session : 3 KKR II (Ebert)

14:30 to 15:30 : Presentation

The Munich SPRKKR program package

The impurity problem

Substitutional disordered alloys

Relativistic formalism

Combination of the KKR with the DMFT

Applications

Session : 4 KKR: Hands-on

16:00 to 18:00 : KKR tutorial session

Day 4: March 28 2007

Session : 1 FPLO I + II (Richter)

09:00 to 10:00 : Presentation

FPLO: Full-potential Loal-orbital approach to electronic structure of solids and molecules

Introduction: why yet another DFT solver?

Linear combinbation of local orbitals (LCLO) equations and core-valence transformation

Optimum local basis: strategies

10:10 to 11:10 : Presentation

FPLO: Full-potential Loal-orbital approach to electronic structure of solids and molecules

Performance and application

Summary and licence

Session : 2 FPLO: Hands-on

11:30 to 12:30 : FPLO tutorial session

Session : 3 FPLO: Hands-on

14:30 to 15:30 : FPLO tutorial session

Day 5: March 29 2007

Session : 1 LMTO I + II (Andersen)

09:00 to 10:00 : Presentation

Muffin tin orbitals

Introduction

The idea

Crystals

Muffin tin orbitals: EMTOs, NMTOs

10:10 to 11:10 : Presentation

Localized minimal basis sets by downfolding and N-ization

Wannier functions and tight binding Hamiltonians

Metal insulator transition in V_2O_3

Superconductivity in hole and eletron doped graphite

Session : 2 LMTO: Hands-on

11:30 to 12:30 : LMTO tutorial session

Session : 3 LMTO: Hands-on

14:30 to 15:30 : LMTO tutorial session

Session : 4 DFT III (Gross)

15:30 to 16:30 : Presentation

Extensions of density functional theory.

Finite temperatures

Superconductivity

Time dependent DFT

Time dependent DFT and Quantum Transport

Session : 5 DMFT I (Held)

17:00 to 18:00 : Presentation
Dynamical mean field theory
DMFT - an introduction
LDA + DMFT
Beyond DMFT

Day 6: March 30 2007
Session : 1 LAPW I + II (Blaha)
09:00 to 10:00 : Presentation
The FP-LAPW and APW +lo methods
APW Augmented plane wave method
Linearization
Full-potential
Core-semicore and valence states
Problems of the LAPW method
Extending the basis: local orbitals
The LAPW+lo method
10:10 to 11:10 : Presentation
The FP-LAPW and APW +lo methods
The Wien2k software package
General remarks on Wien2k
w2web GUI (graphical user interface)
Program structure
Properties with Wien2k
Advantages/disadvantages
Session : 2 LAPW: Hands-on
11:30 to 12:30 : LAPW tutorial session
Session : 3 LAPW: Hands-on
14:30 to 15:30 : LAPW tutorial session
Session : 4 DMFT II (Held)
15:30 to 16:30 : Presentation
LDA + Dynamical mean field theory
(Physical) Hamiltonian point of view
Spectral density functional point of view
Colossal magnetoresistance in $La_{1-x}Ca_xMnO_3$
Kinks in $SrVO_3$ and everywhere
Session : 5 DMFT III (Held)
17:00 to 18:00 : Presentation
Beyond DMFT
Cluster extensions
Diagrammatic extensions
Dynamical vertex approximation DΓA

Results: Hubbard model

Day 7: March 31 2007

Session : 1 MBT III (Godby)

09:00 to 10:00 : Presentation

Many-body theory for electronic structure

GW total energy

Vertex correctbions beyond GW

Session : 2 BSE (Sottile)

10:00 to 11:00 : Presentation

The Bethe-Salpeter equation

Spectra in linear response approach

The Bethe-Salpeter equation

Results

Session : 3 Wrapping Up

11:30 to 12:30 : Discussion