

5 Psi-k Training

5.1 Psi-k Training Graduate School

Bristol University, U. K.

25-31 March 2007

Scientific Summary

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. - The other two activities are Hands-on Tutorials and Summer Schools. - The Bristol University Graduate School is aimed towards giving masters and beginning PhD students (1) an understanding of the theories underlying electronic structure calculations; (2) hands-on experience in electronic structure calculation codes; (3) a perspective how these methods are used in state of the art research.

The Graduate School is 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 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.

Abstract

The Psi-k Graduate School aims to provide an understanding of electronic structure calculations, hands-on experience in running a variety of codes and their usefulness in state of the art research.

Meeting Programme

The combined theory-hands-on Graduate School on electronic structure methods will take place at Burwalls and the Physics Department in Bristol from Sunday March 25 until Saturday March 31, 2007. There will be 20 lectures over 6 days, 10 lectures on theory and 10 lectures on electronic structure methods. The rest is all hands-on experience with relevant codes. Of the 10 lectures on theory there would be 5 on Density Functional Theory (DFT), 3 on many body theory (MBT) and 2 on dynamical mean field theory (DMFT). Of the 10 lectures on methods we will give a bird's eye view of 5 methods: plane-wave methods (PW), the full potential local orbital method (FPLO), linear augmented plane waves (LAPW), the linearized muffin tin orbital method (LMTO) and the Korringa-Kohn-Rostocker (KKR) method, each introduced by two lectures followed by hands on experience with a modern state of the art code.

Speakers/Participants

Lecturers:

Density Functional Theory (including fundamentals of Time Dependent Density Functional Theory); 3 hours (**Hardy Gross**)

Many Body Perturbation Theory; 3 hours (**Rex Godby**)

Bethe-Salpeter Equation and Time Dependent Density Functional Theory; 1 hour (**Francesco Sottile**)

Dynamical Mean Field Theory; 3 hours (**Misha Katsnelson**)

PW 2 hours (**Xavier Gonze**)

FPLO 2 hours (**Manuel Richter**)

LAPW 2 hours (**Peter Blaha**)

LMTO 2 hours (**Ole Andersen**)

KKR 2 hours (**Hubert Ebert**)

Tutors: **James Annett, Dzidka Szotek, Martin Lüders, Peter Hogg and Walter Temmerman.**

Participants:

The school will accommodate about 25-30 enthusiastic students at the start of their Ph.D., or at Master's level. For participants from EU countries most living costs will be paid, although a small workshop fee will be charged. Some participants may be eligible for the fee to be reimbursed after completion of the workshop.

Applications for participation and further details can be obtained by email to *tracie.anderson@bristol.ac.uk*.