

Psi-k/CECAM/CCP9 graduate school in electronic-structure methods

Organizers: Martin Lueders, Leon Petit

The Psi-k/CECAM/CCP9 Biennial Graduate Schools is aimed towards giving beginning PhD students, a) an understanding of the theories underlying electronic structure calculations, b) hands-on experience in electronic structure calculation codes, and c) a perspective how these methods are used in state of the art research.

The 2016 incarnation of the school was held in 5 – 9 September at Daresbury Laboratory. There were 25 participants. An in-depth introduction to Density Functional and band structure theory, was followed by tutorials on four different electronic structure methodologies.

ABINIT : a plane-wave pseudopotential method
ELK : an all-electron method
SIESTA : a local orbital order-N method
YAMBO : a method based on GW

Each method was introduced by two lectures followed by hands on experience. This allows the students to become aware and comfortable with a range of different methods and provides a guide on how to choose the appropriate code for a particular problem.

Programme

Monday 05

10:00-12:00 Registration
12:20-13:30 Lunch
13:30-15:00 Density Functional Theory and Beyond
15:00-15:30 Coffee
15:30-17:00 Band structure methods

Tuesday 06

9:00 -12:30 ABINIT tutorial
12:30-14:00 lunch
14:00-17:30 ABINIT hands on

Wednesday 07

9:00 -12:30 ELK tutorial
12:30-14:00 lunch
14:00-17:30 ELK hands on

Thursday 08

9:00 -12:30 SIESTA tutorial
12:30-14:00 lunch
14:00-17:30 SIESTA hands on

Friday 09

9:00 -12:30 YAMBO tutorial
12:30-14:00 lunch
14:00-17:30 YAMBO hands on

List of speakers

Emilio Artacho, CIC nanoGUNE, San-Sebastian, Spain
Kay Dewhurst, Max Planck Institute of Microstructure Physics, Halle, Germany
Hardy Gross, Max Planck Institute of Microstructure Physics, Halle, Germany
Myrta Gruening, Queen's University Belfast, UK
Fabiano Corsetti, Imperial College London, UK
Matteo Giantomassi, Catholic University of Louvain, Belgium