Psi-k/CECAM/CCP9 Biennial Graduate School in Electronic-Structure Methods

Oxford

10th-16th July 2011

Sponsors: CECAM, Psi-k, CCP9 (UK), ESF

Nicola Marzari (Oxford University)
Walter Temmerman (Daresbury Laboratory)
Jonathan Yates (Oxford University)

http://mml.materials.ox.ac.uk/Support/GraduateSchool2011

Summary

The Psi-k/CECAM/CCP9 Biennial Graduate School in Electronic-Structure Methods was held in Oxford from Sunday 10th July until Saturday 16th July 2011. This was a combined theory and hands-on school, with morning sessions dedicated to lectures introducing theory and application of electronic structure methods, and afternoon sessions providing hands-on experience with the relevant codes on a high-performance compute cluster provided by the Oxford Supercomputer Centre.

Graduate School was aimed to give 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.

Scientific Content

The first two days were dedicated to density functional theory within the planewave pseudopotential formalism and its implementation in the PWSCF program. Lectures were given by Stefano Baroni and Nicola Marzari, and the hand-on session run by Davide Ceresoli and Nicola Bonini. The topics covered including an introduction to modelling in Materials science, and background to density functional theory, practical aspects of DFT simulations, time-dependant DFT and electronic excitation, density functional perturbation theory and the simulation of Raman and Infrared spectroscopies.

A poster session was held on the Tuesday evening to allow the student to present their research to their fellow students and the course tutors. This proved a well attended and much appreciated event.

The following day was dedicated to linear scaling methods and with both the morning lectures and afternoon practicals run by the developers of the ONETEP code; Peter Haynes, Arash Mostofi and Chris Skylaris. The days covered the concepts of near-sightedness, the range of linear scaling approaches (eg divide and conquer), linear scaling in the ONETEP program including non-orthogonal generalised wannier functions and the

psinc basis. Finally an overview of applications in biology and materials science was provided.

Thursday moved to the linear muffin tin approach (MLTO) taught by Martin Leuders, Leon Petit, Dzidka Szotek and Walter Temmerman. Here the LNTO approach was developed stating with the Atomic Sphere Approximation (ASA) and covering ideas such as linearisation and downfolding. Move advanced topics were then introduced such as relativistic effect, full potential implementations and moving beyond the local density approximation.

The final day of the school was dedicated to Quantum Monte Carlo with morning lectures by Richard Needs and an afternoon practical session on the Casino code run by Neil Drummond. Topics covered included diffusion and variation Monte Carlo, practical concerns including optimisation of Jastrow factors and non-local pseudopotentials, and applications such as calculation of Van der Waals interactions.

Results and Outcomes

The School proved very popular and was significantly over-subscribed. We were able to find places for 38 students representing 13 different countries. The feedback was overwhelmingly positive, and many constructive suggestions were provided: typically students wanted us to add a particular topic - GW and Wannier functions were popular suggestions.

One a broader scale we believe that the Graduate School has addressed the following issues:

(1) 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 graduate school has provide exactly this level of training.

(2) Bridged the gap between education provided by university lectures and the much higher level of science in real research and at international workshops and conferences.

(3) The combined training and research program has given young researchers the opportunity to develop in the European Psi-k network at a very early stage of their career.

APPENDIX 1

Program

Monday 11th July
09:00-10:00 *Density-functional Theory* Stefano Baroni
10:00-11:00 *Density-functional Theory* Stefano Baroni
11:30-12:30 *Density-functional Practice* Nicola Marzari
14:00-17:30 *Quantum Espresso Hands-on 1* Davide Ceresoli, Nicola Bonini

Tuesday 12th July
09:00-10:00 *Density-functional Perturbation Theory* Stefano Baroni
10:00-11:00 *Time-dependent DFT* Stefano Baroni
11:30-12:30 *Density-functional Perturbation Theory* Nicola Bonini
14:00-17:30 *Quantum Espresso Hands-on 2* Nicola Bonini, Davide Ceresoli

Wednesday 13th July
09:00-09:40 *Introduction to Linear Scaling* Peter Haynes
09:40-10:20 *The Onetep code* Chris Skylaris
10:50-11:30 *Applications of Linear Scaling* Arash Mostofi
11:30-12:30 *Materials Modelling in Oxford* Jonathan Yates
14:00-17:30 *Onetep Hands-on* P. Haynes, A. Mostofi, C. Skylaris

Thursday 14th July
09:00-10:00 *LMTO* Martin Leuders
10:00-11:00 *Wannier functions and Model Hamiltonians* Jonathan Yates
11:30-12:30 *LMTO 2* Leon Petit
14:00-17:30 *LMTO* Hands-on D. Szotek, M. Lueders, L. Petit

Friday 15th July
09:00-10:00 *Quantum Monte Carlo* Richard Needs
10:00-11:00 *QMC 2* Richard Needs
11:30-12:30 *The Casino Code* Richard Needs
14:00-17:30 *Casino Hands-on* Neil Drummond, Priyanka Seth

APPENDIX 2

Organisers and lecturers

Stefano Baroni	SISSA Italy
Nicola Bonini	University of Oxford UK
Davide Ceresoli	University of Oxford UK
Neil Drummond	University of Lancaster UK
Peter Haynes	Imperial College London UK
Martin Leuders	Daresbury Laboratory UK
Nicola Marzari	University of Oxford UK
Arash Mostofi	Imperial College London UK
Richard Needs	University of Cambridge UK
Leon Petit	Daresbury Laboratory UK
Chris Skylaris	University of Southampton UK
Dzidka Szotek	Daresbury Laboratory UK
Walter Temmerman	Daresbury Laboratory UK
Jonathan Yates	University of Oxford UK

Participants

Philippe Aeberhard	University of Oxford UK
Merid Legesse Belayneh	University College Cork Ireland
Raffaello Bianco	Universita Degli Studi di Trieste Italy
Frederic Blanc	University of Cambridge UK
Pietro Bonfa	Universita degli Studi di Pavia Italy
Peter Bryrne	University of Durham UK
Pascal Bugnion	University of Cambridge UK
Thomas Cathart	Trinity College Dublin Ireland
Shin Liang Chin	University of Cambridge UK
Nguyen Huu Chuong	Universite Libre de Bruxelles Belgium
Riza Dervisoglu	University of Cambridge UK
Marco di Gennaro	Universite de Liege Belgium
Domenico di Sante	University of L'Aquila Italy
Hongbiao Dong	University of Leicester UK
Maofeng Dou	Royal Institute of Technology Sweeden
Cyrus Dreyer	University of California USA
Marina Rucsandra Filip	University of Bucharest Romania
Sinead Griffin	ETH Zurich Switzerland
Thomas Hollins	University of Durham UK
Kiptiemo Kiprono Korir	Politecnico di Torino Italy
Greg Lever	University of Cambridge UK
Jun Liu	University of Leicester UK
Elisa Londero	Chalmers University of Technology Sweden
Yasheng Maimaiti	University College Cork Ireland
Sanghamitra Mukhopadhyay	University of Oxford UK
Andrea Neroni	CNR-IMRM Italy
Xueyong Pang Ruhr	University Bochum Germany
Giovanni Pizzi	Scuola Normale Italy
Samuel Ponce	Universite Catholique de Louvain Belgium
Sankari Sampath	ICAMS Germany
Alvaro Ruiz Serrano	University of Southampton UK
Priyanka Seth	University of Cambridge UK

Daniel Sethio	University of Groningen Netherlands
Kim Han Seul	Korea Advanced Institute of Science and Technology Korea
John Sharp	University of Liverpool UK
Sathyanarayana Sowmya	University of Vienna Austria
Natalie Tillack	University of Oxford UK
Vincent van Hinsberg	University of Oxford UK