

## 0.1 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)

Web Page:

<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.

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. A poster session was held on the Tuesday evening which proved a well attended and much appreciated event. The following day was dedicated to linear scaling methods and was run by the developers of the ONETEP code; Peter Haynes, Arash Mostofi and Chris Skylaris. Thursday moved to LMTO taught by Martin Leuders, Leon Petit, Dzigka Szotek and Walter Temmerman. That evening the conference dinner was held at The Queen's College with pre-dinner drinks in the Provost's Garden courtesy of the current Provost, Paul Madden, and the dinner itself in the impressive 18th century Dining Hall. 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.

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.

The school has run biennially for a number of years. From this year's experience we feel there is a clear need for this level of graduate training and we hope that there is support for such a school in 2013.

## 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* W. Temmerman, 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

## Participants

### 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*

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

<b>Allocated funding</b>			
CECAM	€9,000.00		
ESF	€2,500.00		
Psik	€2,500.00		
CCP9	£6,000.00		
<b>Income</b>			
CECAM	80% of €9000		£6,108.41
ESF	80% of €2500		£1,729.80
Psik	80% of €2500		£1,710.13
CCP9	80% of £6000		£4,800.00
Fees	30x£100		£3,000.00
		<b>Total</b>	<b>£17,348.34</b>
<b>Outgoing</b>			
Accommodation and Meals			£16,453.96
Hire of Computer Suite			£1,462.50
Poster Session			£75.00
Morning refreshments			£375.00
Speakers travel expenses			£914.11
Photocopying and Stationary			£340.51
Bank Charges			£112.33
		<b>Total</b>	<b>£19,733.41</b>
		<b>Outstanding</b>	<b>£2,385.07</b>
Amounts requested to balance account			
ESF	20% of €2500 = €500		£432.45
CCP9	20% of £6000 = £1200		£1,200.00
Psik	20% of €2500 = €500		£432.45
CECAM	€370		£320.17
Notes:			
1- The charge for each participant to attend the School was £100			
2- Accommodation and meals covers 6 nights bed and breakfast for all participants at the Queen's College, plus evening meal on the first night and the conference dinner			
3- The accounting is carried out in GBP.			
Jonathan Yates, Oxford, 1st Sept 2011			