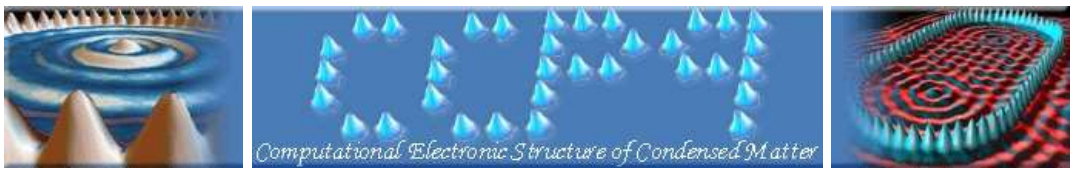
4 News from UK's CCP9 Programme



UK's Collaborative Computational Project 9 (CCP9) on "Computational Studies of the Electronic Structure of Solids"

4.1 Report on the CCP9 Conference

http://www.ccp9.ac.uk/ccp9workshops_2008_cambridge_sept.shtml

Robinson College, Cambridge, 4-5 September 2008

Short report

The Conference was held at the Robinson College in Cambridge on 4th and 5th September 2008 and was attended by 58 participants both from the U. K. and abroad. The scope of the Conference covered all ab-initio and materials specific calculations of the electronic properties of condensed matter systems such as metals, semiconductors, magnets, superconductors, biological systems, minerals, surfaces, etc. Topical areas incorporated in the Conference were magnoelectronics, catalysis, nanotechnology, high temperature superconductors, novel wide band gap semiconductors, etc. Techniques covered by the Conference included QMC, DFT, GW, TDDFT, DMFT, SIC-LSDA, LSDA+U. In general, all the applications dealing with the solution of the Schrödinger/Dirac equation in condensed matter systems were represented.

The Conference was structured around five excellent plenary talks, 9 invited talks, and 21 poster presentations, covering a broad range of ab initio computational topics. The first, very impressive, plenary presentation was by Hardy Gross (FU Berlin, Germany) who talked about density functional theory for superconductors, treating both electrons and ions on equal footing, and demonstrated it on a number of impressive applications. Vladimir Anisimov (Ekaterinberg, Russia) gave a very complete presentation on a practical implementation of the DFT+DMFT method and its application to real d and f electron materials, where electron correlations fall

in the range of moderate to strong and metallic to insulating limits. Gustavo Scuseria (Rice University, USA) presented a nice overview and outlook for the screened hybrid functionals and their applications to solid-state physics and chemistry. Nicola Marzari (MIT, USA) discussed the key challenges for the for the density functional theory in catalysis and electrochemistry. Finally, and David Ceperley (University of Illinois, USA) talked about a new method, called Coupled-Electron Ion Monte Carlo, that allow for simulations in much lower temperatures than with other methods. He discussed an application of the method to the dense Hydrogen.

The first invited talk was by Neil Drummond (University of Cambridge, UK) who talked about an application of Quantum Monte Carlo to the two-dimensional homogeneous electron gas". Leon Petit (University of Aarhus, Denmark) discussed large scale simulations of materials properties through grid applications, based on the study of the whole series of rare earth monopnictides and monochalcogenides using the SIC-LSD method. Marcus Neumann (AVMATSIM) gave a presentation on effective prediction of crystal structures for pharmaceutical industry, combining DFT and tailor-made force fields. Dario Alfe (UCL, UK) talked about the application of Quantum Monte Carlo free energy calculations to melting of iron at Earth's core conditions. Robert Laskowski (TU Wien, Austria) discussed h-BN nanomesh on transition metal surfaces. Jonathan Yates (University of Cambridge, UK) gave a talk with an intriguing title of "Atomic espionage: J-resolved NMR spectroscopy". Hubert Ebert (LMU Muenchen, Germany) presented the first KKR implementation of the LSDA+DMFT method for the application to spectroscopies. Massimiliano Stengel (Santa Barbara, USA) discussed dielectric, piezoelectric and magnetoelectric properties based on first-principles calculations at constant electric displacement. The final invited presentation was by Keith Refson on "Plane-wave Optimised Effective Potential Studies of Transition Metal Oxides".

On both days of the Conference there were poster presentations after lunch and they attracted all the participants, generating a very lively atmosphere of scientific discussions and exchange of opinions. Despite the very unfortunate heavy rain, the conference was very successful and informative to all involved. Considering that at the time of the conference there was a number of similar events happening both in the U. K. and elsewhere, this CCP9 Conference could be considered as very successful.

Conference Programme

Wednesday 3rd September

18.00 - 19.30	REGISTRATION OPEN

Thursday 4th September

08.30 - 09.00	REGISTRATION AND COFFEE
09.00 - 10.00	Hardy Gross (plenary) "Ab-Initio Theory of Superconductivity"
10.00 - 10.25	Neil Drummond "Quantum Monte Carlo Studies of the Two-Dimensional Homogeneous Electron Gas"

10.30 - 10.55 Leon Petit
"Large scale calculations of materials properties through grid applications"

11.00 - 11.30 COFFEE

11.30 - 11.55 Marcus Neumann
"From dispersion corrected DFT to tailor-made force fields - accurate lattice energy calculations for crystal structure prediction"

12.00 - 12.25 Dario Alfe
"Melting of iron at Earth's core conditions from quantum Monte Carlo free energy calculation"

12.30 - 15.30 LUNCH AND POSTER SESSION

15.30 - 16.30 Vladimir Anisimov (plenary)
"Density Functional and Dynamical Mean-Field Theory (DFT+DMFT) method and its applications to correlation effects in electronic structure of real materials"

16.30 - 16.55 Robert Laskowski
"h-BN nanomesh on transition metal surfaces"

17.00 - 17.25 Jonathan Yates
"Atomic espionage: J-resolved NMR spectroscopy"

17.30 MEETING CLOSES FOR THE DAY

Friday 5th September

09.00 - 10.00 Gustavo Scuseria (plenary)
"Screened hybrid functionals for solid-state physics and chemistry"

10.00 - 10.25 Hubert Ebert
"A self-consistent relativistic implementation of the LSDA+DMFT-scheme and its application in spectroscopy"

10.30 - 10.55 Massimiliano Stengel
"Dielectric, piezoelectric and magnetoelectric properties via first-principles calculations at constant electric displacement"

11.00 - 11.30 COFFEE

11.30 - 12.30 Nicola Marzari (plenary)
"DFT challenges in catalysis and electrochemistry"

12.30 - 15.00 LUNCH AND POSTER SESSION

15.00 - 16.00 David Ceperley (plenary)
"Simulation of dense hydrogen using Coupled-Electron Ion Monte Carlo"

16.00 - 16.25 Keith Refson
"Plane-wave Optimised Effective Potential Studies of Transition-Metal Oxides"

16.30 MEETING CLOSES - COFFEE AVAILABLE

List of Posters

Chris Adriaanse (University of Cambridge, U. K.)
"Computation of the free energy change in some steps in the reduction of O_2 in aqueous solution".

Simon Binnie (University College London, U. K.)
"Benchmarking DFT Surface Energies with Quantum Monte Carlo"

Gareth Conduit (University of Cambridge, U. K.)
"DMC calculations in valley degenerate semiconductors"

Calvin Davidson (Sussex University, U. K.)
"A Density Functional Theory Study of the Adsorption of Tetracene on Reconstructed Oxygen Terminated Copper (110) Surfaces"

Giulia C De Fusco (Imperial College London, U. K.)
"Ab Initio Study of the Electronic Structure and Magnetic Properties of the High-Temperature $V(TCNE)_2$ Organic-Based Magnet"

Nicholas Hine (Imperial College London, U. K.)
"Supercell Size Scaling of Formation Energies of Charged Defects"

Leandro Liborio (Imperial College London, U. K.)
"Magneli Phases: An ab initio Approach"

Giuseppe Mallia (Imperial College London, U. K.)
"Doping Titania with transition metal to make a dilute ferromagnetic semiconductor: insights from hybrid density functional simulations"

Andrew Morris (University of Cambridge, U. K.)
"Defects in Semiconductors using Random Structure Searching"

Arash Mostofi (Imperial College London, U. K.)
"Linear-Scaling DFT+U"

Duncan Riley (University of Salford, U. K.)
"Hydrogen Storage in Metal-Organic Frameworks"

Mark Robinson (University of Cambridge, U. K.)
"Ab initio Study of Peptide Stacking in an Amyloid Fibril"

Jon Swaim (Imperial College London, U. K.)
"The Electronic Structure of CrO_2 Revisited: A Hybrid-Exchange Density Functional Theory Study"

Z (Dzidka) Szotek (STFC Daresbury Laboratory, U. K.)
"Application of Local Self-Interaction Correction (SIC) to Transition Metal Oxides"

Walter Temmerman (STFC Daresbury Laboratory, U. K.)
"Finite Temperature Magnetism of Heavy Rare Earths: SIC-DLM Study"

Fabien Tran (Vienna University of Technology, Austria)
"PBE+U Calculations of the Jahn-Teller Effect in PrO_2"

Claudia Utfeld (University of Bristol, U. K.)

"$Co_xFe_{1-x}S_2$: How close to half-metallicity?"

Rebecca Varns (University of Kent, U. K.)
"A First Principles Study of Group 13 Simple Metal Clusters: Superatom or Cluster?"

Rebecca Varns (University of Kent, U. K.)
"A First Principles Study of the Electronic Structure and Chemical Bonding of Neutral and Charged Boron Clusters"

Rudolf Zeller (Institut fuer Festkoerperforschung, Juelich, Germany)
"A Reformulation of the KKR Green-Function Method for Large-Scale Density-Functional Calculations"

Nicholas Zonias (University of Southampton, U. K.)
"Large-Scale DFT Calculations on Silicon Nanocrystals"

List of Participants

Title	First Name	Surname	Affiliation
Mr	Chris	Adriaanse	University of Cambridge
Prof	Dario	Alfe	University College London
Prof	Vladimir	Anisimov	Institute for Metal Physics
Prof	James	Annett	University of Bristol
Mr	Albert	Bartok-Partay	University of Cambridge
Mr	Simon	Binnie	University College London
Prof	David	Ceperley	University of Illinois
Mr	Gareth	Conduit	University of Cambridge
Dr	Gabor	Csanyi	University of Cambridge
Mr	Calvin	Davidson	Sussex University
Ms	Giulia C	De Fusco	Imperial College London
Dr	Neil	Drummond	University of Cambridge
Prof	Paul	Durham	STFC Daresbury Laboratory
Prof	Hubert	Ebert	Ludwig-Maximilians-University of Munich
Dr	Asier	Eiguren	Donostia International Physics Center
Prof	Matthew	Foulkes	Imperial College London
Prof	Michael	Gillan	University College London
Prof	Hardy	Gross	FU Berlin
Mr	Nic	Harrison	STFC Daresbury Laboratory
Dr	Philip	Hasnip	University of York
Prof	Volker	Heine	University of Cambridge
Mr	Tilina	Herath	University of Warwick
Dr	Nicholas	Hine	Imperial College London
Mr	Damian	Jones	STFC Daresbury Laboratory
Dr	Thomas	Kuehne	ETH Zurich
Dr	Robert	Laskowski	TU Wein
Dr	Leandro	Liborio	Imperial College London
Dr	Giuseppe	Mallia	Imperial College London

Prof	Nicola	Marzari	Massachusetts Institute of Technology
Dr	Victor	Milman	Accelrys Inc.
Dr	Carla	Molteni	King's College London
Mr	Andrew	Morris	University of Cambridge
Prof	Ian	Morrison	University of Salford
Dr	Arash	Mostofi	Imperial College London
Dr	Andres	Mujica Fernaud	Universidad de La Laguna
Prof	Richard	Needs	University of Cambridge
Dr	Marcus	Neumann	Avant-Garde Materials Simulation
Prof	Mike	Payne	University of Cambridge
Dr	Alexander	Perlov	Accelrys Inc.
Dr	Leon	Petit	University of Aarhus
Dr	Chris	Pickard	"SUPA, University of St Andrews"
Dr	Keith	Refson	STFC Daresbury Laboratory
Dr	Duncan	Riley	University of Salford
Mr	Mark	Robinson	University of Cambridge
Prof	Gustavo E.	Scuseria	Rice University
Dr	Chris-Kriton	Skylaris	University of Southampton
Dr	Michiel	Sprik	University of Cambridge
Dr	Massimiliano	Stengel	University of California
Prof	Paul	Strange	University of Kent
Mr	Jon	Swaim	Imperial College London
Prof	Z (Dzidka)	Szotek	STFC Daresbury Laboratory
Prof	Walter	Temmerman	STFC Daresbury Laboratory
Dr	Fabien	Tran	Vienna University of Technology
Ms	Claudia	Utfeld	University of Bristol
Ms	Rebecca	Varns	University of Kent
Dr	Jonathan	Yates	University of Cambridge
Dr	Rudolf	Zeller	Institut fuer Festkoerperforschung
Mr	Nicholas	Zonias	University of Southampton

Conference Organizers:

Prof James F. Annett (Bristol University)
Prof Mike C. Payne (Cambridge University)
Prof Walter M. Temmerman (STFC Daresbury Laboratory)

Local Organizers:

Damian Jones (STFC Daresbury Laboratory)
Shirley Miller (STFC Daresbury Laboratory)