Report of the Daresbury Laboratory CECAM node activities

WM Temmerman

October 2011

REPORT OF THE DARESBURY LABORATORY CECAM NODE ACTIVITIES

5 OCTOBER 2011

WALTER TEMMERMAN

Prologue

This report describes the activities which took place in the second year of CECAM's Daresbury node based at the STFC Daresbury Laboratory.   The report is prepared by Professor Walter Temmerman who was accepted as its Director for a period of four years. The Daresbury Node appointed Dr Leon Petit as Deputy Director.

The governance of the Daresbury node is its Director and Deputy Director assisted by a steering committee comprising

James Annett (University of Bristol)
Mike Ashworth (Advanced Research Computing ,Daresbury)
Paul Durham (Vice-President CECAM Council, Daresbury)
David Emerson (Computational Engineering, Daresbury)
Leon Petit (Deputy Director CECAM Daresbury Node)
Mike Payne (University of Cambridge)
Paul Sherwood (Computational Chemistry, Daresbury)
Zdzislawa Szotek (Band Theory Group, Daresbury)
Walter Temmerman (Director CECAM Daresbury Node)
Stanko Tomic (University of Salford)
Martyn Winn (Computational Biology, Daresbury)

The committee will be joined by Daan Frenkel FRS, University of Cambridge from 1 April 2012.

A budget of €50K provided by the STFC was at the Director's disposal.

During its second year of operation, one highly successful workshop was organized, two tutorials, one other Event and two collaborative meetings between Nodes.

To finish, I would like to thank all members of the CSE Department for their continued enthusiasm and support to make this another successful year of CECAM's Daresbury node.

In particular, I would like to acknowledge Richard Blake, the CSE Director, for providing support and funding, Shirley Miller for providing secretarial services to this Committee and the Administration Team at Daresbury for their exemplary organization of the workshops and so much more.

Walter Temmerman
Daresbury
4 October, 2011

Report -2011

I/ WORKSHOPS

Theoretical and Experimental Magnetism Meeting
16 June - 17 June 2011, STFC Rutherford Appleton laboratory, Oxfordshire
Organisers: Devashi Adroja (ISIS Facility, STFC Rutherford Appleton Laboratory) and
Walter Temmerman (STFC Daresbury Laboratory)

II/ TUTORIALS

CCP5 Summer School in Molecular Simulation 2011
17 July - 26 July 2011, Queen's University of Belfast
Organisers: John Harding (Sheffield University), John Purton (STFC Daresbury Laboratory), Mario G. Del Popolo (Queen's University Belfast)

The CCP5 Summer School in Molecular Simulation was held at Queen's University (Belfast) between the 17th and 26 July 2011

The Summer School is intended to provide newcomers to the science of molecular simulation a comprehensive introduction to the methodology. The power and versatility of computer simulation methods are demonstrated through a series of lectures and coupled practical sessions. Research seminars are presented by a mixture of new and more senior academics on a variety of disciplines.

As usual the event was oversubscribed and the event will be held in 2012 at the University of Cardiff between the 22nd and 31st July. The final report of the meeting is attached.

Psi-k/CECAM/CCP9 Biennial Graduate School in Electronic-Structure Methods
10 July - 15 July 2011, University of Oxford
Organisers: Martin Lueders, Leon Petit, Zdzislawa (Dzidka) Szotek, Walter Temmerman (STFC Daresbury Laboratory), Feliciano Giustino, Nicola Marzari, Jonathan Yates (University of Oxford)

The Psi-k/CECAM/CCP9 Biennial Graduate School in Electronic-Structure Methods was held in Oxford from Sunday 10th Julyuntil 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.

III/ OTHER RESEARCH MEETINGS

Self-Interaction Correction: State of the Art and New Directions
18 September - 21 September 2011, Ramada Hotel, Chester
Organisers: Zdzislawa (Dzidka) Szotek, Martin Lueders and Leon Petit (STFC Daresbury Laboratory)

The paramount goal of this event is to bring together, for the first time, all the groups that have applied and worked on self-interaction correction, in order to discuss and assess the state of the art of all the different flavours of SIC, share the experiences and identify the most important and burning issues, unsolved problems, and perhaps find a common direction for future developments.

IV/ VISITORS PROGRAMME

Thomas Schultess (ETC Zurich) visited Dzidka Szotek and Walter Temmerman collaborating on the development of full potential self-interaction free LAPW code.

V RESEARCH collaborations

Quixote Collaboration Meeting
22 - 23 March 2011, STFC Daresbury Laboratory
Organiser: Jens Thomas (STFC Daresbury Laboratory)

The Quixote Collaboration Meeting in Daresbury, rather than being a discussion and planning meeting, had a very distinct practical goal, to complete a demonstration by which outputs from quantum chemistry calculations could be parsed and the results stored in an searchable public database. This target was achieved, and since then two data collections have been added to the database, which is available at http://quixote.ch.cam.ac.uk/

Theoretical and Experimental Magnetism Meeting,

16 June - 17 June 2011, STFC Rutherford Appleton laboratory, Oxfordshire
Organisers: Devashi Adroja (ISIS Facility, STFC Rutherford Appleton Laboratory) and
Walter Temmerman (STFC Daresbury Laboratory)

The Theoretical and Experimental Magnetism Meeting (TEMM) was held at Rutherford Appleton Laboratory, UK from June 16-17 2011. This two-day meeting was organised by the CECAM, Hartree Centre, ISIS-facility, SEPnet, Hubbard Theory Consortium and the Magnetism and Neutron scattering Groups of the Institute of Physics. This year, for the first time, TEMM 2011 was scheduled to coincide with the SEPnet Condensed Matter in the City programme, being part of a week focused on Frustrated Magnetism. The meeting was also combined with UK-Korea workshop on strongly correlated systems. The meeting attracted 89 registered participants from eight different countries. There were 29 oral presentations, out of which 15 were given by the international speakers, and 11 poster presentations. This provided a substantial boost to the visibility to CECAM, ISIS, SEPnet and IOP. The participants included academics, senior researchers, post-doctoral fellows and Ph.D. students. This was the ninth highly successful meeting in this series. This meeting has become an important part of the UK as well as European scientific calendar for those in the filed of magnetism. The meeting presented an excellent opportunity to hear and discuss with leading experts from all over the world on topics of current research in magnetism such as exotic superconductivity in Fe-based systems as well as in high temperature superconductors and heavy fermion systems, manganites, multiferroics, orbital ordering, low-dimensional and frustrated magnetism, molecular and nano magnetism and quantum phase transitions. Steve Bennington, group leader of ISIS excitations group, on behalf of the organizing committee, welcomed the participants at the beginning of the meeting.

The meeting commenced with an excellent scientific presentation by Jens Jensen (NBI, Denmark) on the theoretical aspects on the chiral spin-wave excitations of the spin-5/2 trimers in the langasite compound $Ba_3NbFe_3Si_2O_{14}$. He made a direct comparison between experimental and theoretical results and showed how the complex spin waves can observed in this system. He was followed by John Chalker (Oxford) who discussed the effects of impurities in a quantum spin liquid. In his talk he showed how the disorder can act as a distraction, as a probe as well as a source of new physics. He focused the role of disorder in the Kitaev model. The third talk of the session was given by Bella Lake (HZB, Berlin) on a quantum dimer magnet with extended lattice fluctuations in $Sr_3Cr_2O_8$. In the fourth talk Je-Geun Park (SNU, Seoul) explained the origin of unusual ferromagnetism in $SrRuO_3$. The last talk of the first session was given by Peter Baker (ISIS) on µSR measurements of the correlated iridates.

The discussion was focused on multiferroics and quantum magnetism, especially on new material CuO, in the second session after the lunch. In the first talk of the second session José Lorenzana (INFM-CNR, Italy) gave an excellent review on High-Tc multiferroic effect emerging from magnetic degeneracy in CuO. He was followed by Silvia Picozzi (NFN, Italy) who discussed on the modelling and understanding of multiferroics and magnetoelectrics. Christian Ruegg (PSI) who talked on quantum spin ladders with frustration and non-magnetic vacancies and he was followed by Oleg Petrenko (Warwick) who talked on the low-temperature magnetism in $SrRE_2O_4$, a family of geometrically frustrated materials. The final talk of the session was by Philip Lightfoot (St Andrews) who discussed on synthesis and magnetic properties of a new vanadium oxyfluoride exhibiting a unique S=1/2 kagome lattice.

Following tea, the third session was on HTSC and quantum criticality and the talks on HTSC were given by Henrik Ronnow (EPFL, Lusanne) on the mechanism of High-Temperature Superconductivity with a pinch of Iron, followed by Martin Greven (Stanford University) who talked on Two Ising-like collective magnetic excitations in a single-layer cuprate superconductor and Stephen Hayden (Bristol) talked on the magnetic excitations in the normal and superconducting states of $YBa_2Cu_3O_{+x}$ studied by polarized neutron spectroscopy. Ernst Bauer (TU Vienna) gave an excellent talk on reentrant quantum criticality in Yb_2Pd_2Sn and Edward Yelland (St Andrews) talked on high-field superconductivity at an electronic topological transition in ferromagnetic URhGe. The first day was concluded with a late evening poster session and drinks with many discussions on complex magnetism and a delightful conference dinner.

The discussion on exotic superconductivity and quantum magnetism was continued on the second day. The first session was on Fe-based superconductors. The first talk of the session was on theoretical aspects. The fist talk was given by Qimiao Si (Rice University) on the new iron chalcogenide $(K,Tl)Fe_xSe_2$: pairing strength and symmetries, and some   general lessons about iron pnictides. He was followed by Ray Osborn (Argonne) who discussed on the phase competition and superconductivity. The third talk of the session was given by Russell Ewings (ISIS) who talked on antiferromagnetic spin fluctuations in LiFeAs observed by neutron scattering. The fourth and final talk of the session was given by Alan Tennant (HZB, Berlin) on thermal transport and magnetic quasiparticles.

The second session, after tea, of the meeting was focused on computational magnetism. Arthur Ernst (Halle) gave a talk on first-principles design of magnetic oxides, who was followed by Jan Minar (Munich) who talked on correlation effects-from simple metals to complex systems. Julie Staunton (Warwick) talked on magnetism in transition metal and rare earth materials described by ab-initio electronic structure theory. The final talk of the session was given by Zsolt Gercsi (Imperial College) who gave an experimental talk on designed metamagnetism in Mn-based orthorhombic alloy*s*.

The third session, after lunch, was on transition metal magnetism in low dimensions. The first talk was given by Byoung-Chul Min (KIST, Seoul, Korea) on MgO-based magnetic tunnel junctions for spin-transfer torque devices and the second talk by Changyoung Kim (Yonsei Univ, Korea) on electronic structures and magnetic phases of 4d transition metal oxides. Tatiana Guidi (ISIS) gave an experimental talk on direct access to the spin correlations within zero dimensional spin systems and Pascal Manuel (ISIS) discussed on frustrated magnetism in the $RBaCo_4O_7$ antiferromagnet. The meeting closed with an excellent presentation by Nikitas Gidopoulos (ISIS) on the distinct phase transition at the surface of an antiferromagnet.

Overall, the meeting was a great success, very useful and enjoyable opportunity for experimentalists to have discussions with theoreticians on various aspects of current research in magnetism. Finally, on behalf of the organizing committee we would like to express our gratitude to all speakers who had taken great care for giving excellent and stimulating presentations. We would like to CECAM, Hartree Centre, SEPnet, ISIS, UK-GPF and the IOP magnetism and neutron scattering groups for providing funding.

CCP5 Summer School in Molecular Simulation 2011

17 July - 26 July 2011, Queen's University of Belfast
Organisers: John Harding (Sheffield University), John Purton (STFC Daresbury Laboratory),
Mario G. Del Popolo (Queen's University Belfast)

Report on the Methods in Molecular Simulation Summer School 2011

Organizers

The Methods in Molecular Simulation Summer School 2011 was held at Queen's University
Belfast from 17 - 26 July, at the Atomistic Simulation Centre and the School of Mathematics
and Physics. The School was organised by the CCP5 Summer School Working Group,
which
consisted of J. Harding (Chairman), J. Purton (Secretary), P. Camp, Jamshed Anwar, M. Del
Popolo and D. Willock. The local organisation was handled by M. Del Popolo, from the
Atomistic Simulation Centre at Queen's University.

Location and Facilities

The School was held on the University campus, more precisely at the Elmwood Learning
and Teaching Centre (ELTC) and at the Peter Froggatt Centre (PFC). The computer
exercises also took place in the ELTC, which had sufficient places for 70 students working
independently.

The computing equipment consisted of desktop personal computers running Microsoft
Windows, augmented by Virtual Box software, which provided a Linux environment for
running the programs of the basic course. An additional multiprocessor platform was
available for the advanced courses.

3. Participation

We received 97 applications to attend the School and these were screened by the
organisers with the intention of giving priority to students in the first year of postgraduate
study and whose research required a significant amount of molecular simulation. Students of
the disciplines of chemistry, physics, biology, mathematics and computational science were
considered acceptable. 67 students attended. Those attending originated from 17 countries:
29 were from the host nation (UK) and 34 were from elsewhere in Europe. 4 students were
from outside Europe. A full list of participants and their nationalities is presented in Appendix
i.

4. Support

A registration fee of £200 was charged to the students, which covered the bulk of the
costs.Queen's University of Belfast provided the use of the lecture theatres and the
computing equipment at nominal cost. The organisers express their sincere appreciation of
the support received from the supporting organisations.

5. Accommodation

The residential students and lecturers were accommodated in the halls of residence of in
Queen's Elms Village, within 15 minutes walking distance of ELTC and PFC. Plenary

Lecturers were located in local hotels, near the university. Breakfast, lunch and evening meals were provided for all the School participants.

6. Programme

The programme of the School consisted of two parts. The basic course in molecular simulation methodology covered the first 5 ½ days. This was followed by an advanced course lasting 2 ½ days, for which there were three options for the students (see below).

The Basic Course

The basic course was designed to introduce students to the fundamentals of molecular simulation. It covered the basic elements of statistical mechanics, the methodologies and applications of Monte Carlo and molecular dynamics simulation, potential energy functions and optimization methods. More advanced aspects of statistical mechanics, the treatment of long ranged (electrostatic) forces, hyperdynamics and the calculation of free energies by simulation methods were also included. All students were required to attend the basic course and were presented with prepared course notes beforehand. The course content was reviewed after the summer school of 2010 and the student responses were taken into account, as far as was practical, in 2011.

The lectures given in the basic course and the speakers presenting them were as follows (numbers in brackets indicate the number of lectures devoted to the subject):

- (1) Potentials. J Harding
- (1) An overview of molecular simulation. S. Parker
- (2) Statistical mechanics. M. Del Popolo.
- (4) Molecular dynamics. D. Willock
- (4) Monte Carlo. P. Camp.
- (1) Long range forces. J. Harding
- (1) Long timescales methods. J. Harding
- (2) Free energy methods. J. Anwar
- (1) Parallel programming. K. Refson

Three (1 hour) lectures were given in the morning of each day, with a coffee break between lectures 2 and 3. The timetable for the School is presented in Appendix ii.

Computing Workshops

Following the lectures in the morning, the afternoons were devoted to computational workshops. In these the students were required to complete exercises based on the topics covered in the basic course. The exercises thus expanded on the material presented in the basic course while giving the students opportunity to study the underlying computational methodology and allowing them to experience problems and solutions in actual computational work. One afternoon was devoted to a `mini-project' in which students were required to conduct realistic research on the diffusion of methane in a zeolite cage (Willock). The bulk of the material was supplied by the organisers, with additional material from Prof. M.P. Allen at the University of Warwick and Dr. W. Smith at Daresbury laboratory. As in previous years, the exercises were accessed via a web browser, allowing the students to read instructions online, and then download the necessary software from a website at Queen's University, or from a backup at the CCP5 website at Daresbury Laboratory. The work was performed entirely on the PCs running a linux operating system via the Virtual Box software with essential C- and Fortran compilers. The gfortran Fortran compiler was the

compiler of choice. Also available were CCP5's DL_POLY program and assorted graphics tools such as RasMol, VMD and JMol.

Plenary Lectures
The plenary lectures are an integral feature of the School and are intended to demonstrate to students what science may be accomplished by molecular simulation methods. This year the plenary lectures were:

• **Julia Yeomans**, University of Oxford, *Swimming and scattering at low Reynolds numbers.*
• **Rebecca Wade**, Heidelberg Institute for Theoretical Studies*, Modeling protein interactions and dynamics: From single protein to multi-protein systems.*
• **Dominik Marx**, Ruhr Universitat Bochum*, Magnetostructural Dynamics of [2Fe-2S] Protiens from Spin-Projected Two-Determinant Ab Initio Molecular Dyanmics.*
• **David Coker**, University College Dublin*, Quantum Dynamics in Condensed Phases*
• **David Quigley**, University of Warwick*, Busting the myth of classical nucleation theory, molecular simulations of crystal growth.*
• **Paola Carbone**, The University of Manchester*, Combining atomistic and coarsecoarse grained models to simulate soft matter*
A plenary session was also dedicated to short (15 min.) talks given by the students. The four talks selected this year were:
• **Aaron Finney**, University of Warwick, UK. *Applying Belonoshko's Z Method to Molecular Solids*
• **Sarah Khanniche**, University of Savoie, France. *Molecular Modelling of Chemical Sensor Based on Silica Surfaces*
• **Cloé Lanthony**, LAAS-CNRS, France. *Basic Mechanisms of Al/CuO Bilayer Films Formation: a Theoretical Study*
• **Fredrick Robin Devadoss Victor Paul Raj**, University of Konstanz, Germany. *Analysis and Visual Summarization of Molecular Dynamics*
The contributions of the students were complemented by a **Poster Session**, which featured a wide range of research activity.

In recognition of the high standard of presentations made by the students in both the talks and posters, the organizers made a small award to Mrs. Cloé Lanthony, for best short seminar, and Mrs. Weina Du, for best poster.

Advanced Courses

The School offered a choice of three advanced courses:
• **Biomolecular simulation** (Xavier Daura, University of Barcelona)
• **Mesoscale simulation** (Ian Halliday, Sheffield Hallam University; Michael Seaton, Daresbury Laboratory)
• **First principles simulation** (Keith Refson, Rutherford Appleton Laboratory)

Each of these courses was comprised of 4 one-hour lectures and associated practical sessions on the computer. As with the basic course, students were presented with prepared course notes beforehand.

The Biomolecular Simulation course was run by Dr. Xavier Daura of the University of Barcelona. The course described the nature of biomolecular structures, the force fields Amber, Gromos and Charmm and the methods and programs used to simulate biomolecular systems and analyse the results.

Dr. Ian Halliday from Sheffield Hallam University and Dr. Michael Seaton from Daresbury Laboratory, gave the advanced course on Mesoscale Simulation. The course described the current techniques applied in this area: Lattice Gas Automata, Lattice Boltzmann and Dissipative Particle Dynamics.

The advanced course on First-principles simulation was given by Dr. K. Refson (Rutherford Appleton Laboratory).The course introduced simulation from first-principles quantum mechanics, covering the electron-ion Hamiltonian, the Schroedinger equation and the impossibility of a direct solution. Various necessary topics from the quantum theory of the solid state were introduced and the major approximate methods of the Hartree, Hartree-Fock and density-functional theory described including the LDA and GGA approximations to the XC functional discussed. Basis sets and SCF solves were described and the computer representation as used in several major codes discussed. The second half of the course concentrated on practical aspects of FP simulation, with a strong emphasis on convergence issues. The aim was to equip the students with sufficient practical knowledge to perform correctly converged calculations. This was reinforced in the practical sessions which gave the students hands-on experience of running *ab initio* lattice dynamics and molecular dynamics calculations.

7. Performance Assessment

To assess the quality of the School, each student was asked to complete a questionnaire inviting their response to various specific and general aspects of the School. The analysis of the survey was conducted by Prof. J. Harding and is attached to the present document.

8. The Future
The Summer School in 2012 is planned for Cardiff University. CCP5 will provide some funding and additional funding will be requested from CECAM.

Appendix i) Attendance List

Sandeep Kumar	Singh	University of Antwerp	Belgium
Trond	Ingebrigtsen	Roskilde University	Denmark
Lasse	Bøhling	Roskilde University	Denmark
Artur	Tamm	University of Tartu	Estonia
Sarah	Khanniche	University of Savoie	France
Aurelie	Ortiz	Université Pierre et Marie Curie	France
Cloé	Lanthony	LAAS-CNRS	France
Alvarado	Orozco	French Institute of Petroleum	France
Baptiste	Farbos	Universite de Bordeaux 1	France
Gaëlle	Filippini	LTIM, Blaise Pascal University	France
Amir	Niazi	AICES Graduate School, RWTH Aachen	Germany
Fredrick Robin Devadoss	Victor Paul Raj	University of Konstanz	Germany
Olga	Ivchenko	University of Heidelberg	Germany
Paul	Gorman	University College Dublin	Ireland
Nicodemo	Di Pasquale	Politecnico di Torino	Italy
Irene	Bessi	Università di Firenze	Italy
Veranika	Zobnina	University of Roma Tre	Italy
Ismael	Rattalino	IIT Italian Institute of Technology	Italy
Emiliano	Poli	University of Bologna	Italy
Simona	Mariani	University of Modena and Reggio Emilia	Italy
Wagner	Homsi Brandeburgo	University of Amsterdam	Netherlands
Weina	Du	University of Amsterdam	Netherlands
Emmet	McBride	Queen's University Belfast	Northern Ireland
Terence	Sheppard	Queens University Belfast	Northern Ireland
Alexey	Zatula	University of Oslo	Norway
Andres	Henao Aristizabal	Technical University of Catalonia	Spain
Ramiro	Perezzan	Universidad Complutense de Madrid (UCM)	Spain
Miguel Angel	Gonzalez	Universidad Complutense de Madrid	Spain
Francisco José	Martínez Ruiz	University of Huelva	Spain
Bing	Sun	Uppsala University	Swden
Tanveer	Hussain	Uppsala University	Sweden
Joakim	Jämbeck	Stockholm University	Sweden
Jonas	Fagerberg	Uppsala University	Sweden
Matti	Hellström	Uppsala University	Sweden
Ferruccio	Palazzesi	ETH Zurich	Switzerland
Federico	Giberti	Swiss Federal Institute of Technology (ETH)	Switzerland
Sertan	Kurnali	Zonguldak Karaelmas University	Turkey
Tugba	Isik	Zonguldak Karaelmas University	Turkey
Mark Andrew	Lewis	University of Liverpool	UK
Stepan	Ruzicka	University of Warwick	UK
Annalaura	Del Regno	University of Manchester	UK
Daniel	Holden	University of Liverpool	UK
Olga	Lobanova	Imperial College London	UK
Aaron	Finney	University of Warwick	UK
Sally	Bridgwater	University of Warwick	UK
Amaal	Albackri	Lancaster University	UK
Yawen	Zhang	Imperial College London	UK

Zhuo	Zhang	Heriot-Watt University	UK
Mykhailo	Melnykov	University of Leicester	UK
Hendrik	Frentrup	Imperial College London	UK
Thomas	Pope	Lancaster University	UK
Christopher	Cave-Ayland	University of Southampton	UK
Konstantinos	Papachristos	University of Leeds	UK
Sophia Rebecca	Wheeler	University of Southampton	UK
Anthony	Nash	University of Warwick	UK
Sang Young	Noh	University of Warwick	UK
Thomas	Fenech	University of Bristol	UK
Stefano Artin	Serapian	Imperial College London	UK
Somwang	Sae-tang	University of Bradford	UK
Andreas	Stegmueller	University of Cambridge	UK
Alessio	Atzori	University of Manchester	UK
Hugh Patrick George	Thompson	University of Cambridge	UK
Edward Oliver	Pyzer-Knapp	University of Cambridge	UK
Mark	Siddorn	University of Exeter	UK
Jahangir	Malik	University College London	UK
Jesse	Kern	University of Kansas	USA
Kyle	Hart	Pennsylvania State University	USA
Maria Monica	Castellanos Mantilla	Pennsylvania State University	USA

Appendix ii) The CourseTimetable

Methods in Molecular Simulation 2011

Click on a Lecture or Workshop for details. For information on using the workshop computers click here.

	17 July	18 July	19 July	20 July	21 July	22 July	23 July	24 July	25 July	26 July
09.00		Overview of Molecular Simulation	Statistical Mechanics 2	Monte Carlo 2	Monte Carlo 3	Molecular Dynamics 4	Long Ranged Forces	**Free Time**	Advanced Seminar 3 FPS BIO MESO	Advanced Seminar 4 FPS BIO MESO
10.00		Potentials	Monte Carlo 1	Molecular Dynamics 2	Molecular Dynamics 3	Monte Carlo 4	Parallel Programming		Practical Session FPS BIO MESO	Practical Session FPS BIO MESO
11.00		*Refreshments*							*Refreshments*	
11.30		Statistical Mechanics 1	Molecular Dynamics 1	Optim--ization Methods	Free Energy Methods 1	Free Energy Methods 2	Long Timescale Methods		Practical Session FPS BIO MESO	Practical Session FPS BIO MESO
12.30		*Lunch*								
14.00	**Arrival**	Practical Workshop 1	Practical Workshop 3	Practical Workshop 5	Practical Workshop 7	Practical Workshop 9	**Free Time**	Advanced Seminar 1 FPS BIO MESO	Practical Session FPS BIO MESO	Practical Session FPS BIO MESO
15.30		*Refreshments*							*Refreshments*	
16.00		Practical Workshop 2	Practical Workshop 4	Practical Workshop 6	Practical Workshop 8	Practical Workshop 10		Advanced Seminar 2 FPS BIO MESO	Practical Session FPS BIO MESO	**Departure**
17.00		Research Seminar R. Wade	Research Seminar J. Yeomans	Student Research Seminars -> Posters	Research Seminar D. Marx	Research Seminar P. Carbone		Research Seminar D. Coker	Research Seminar D. Quigley	

Main lecturers	Advanced Topics	Research Seminars
John Harding (Sheffield)	**Keith Refson (STFC-RAL)**	**R. Wade (HITS)**
Philip Camp (Edinburgh)	**Xavier Daura (A.U. Barcelona)**	**J. Yeomans (Oxford)**
David Willock (Cardiff)	**Ian Halliday (Sheffield Hallam)**	**P. Carbone (Manchester)**
Jamshed Anwar (Bradford)	Local Organiser/Lecturer	**D. Coker (UCD)**
Keith Refson (STFC-RAL)	**Mario del Popolo (Queens University Belfast)**	**D. Quigley (Warwick)**
		D. Marx (Bochum)

John Purton *Last modified 8th April 2011*

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APPENDIX C

<u>Psi-k/CECAM/CCP9 Biennial Graduate School in Electronic-Structure Methods</u>
10 July - 15 July 2011, University of Oxford
Organisers: Martin Lueders, Leon Petit, Zdzislawa (Dzidka) Szotek, Walter Temmerman
(STFC Daresbury Laboratory), Feliciano Giustino, Nicola Marzari, Jonathan Yates
(University of Oxford)

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

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 Lueders, Leon Petit,
Dzidka 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 Lueders
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

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 Lueders 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
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Participants

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Riza Dervisoglu University of Cambridge UK
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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

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

APPENDIX D

Self-Interaction Correction: State of the Art and New Directions
18 September - 21 September 2011, Ramada Hotel, Chester
Organisers: Zdzislawa (Dzidka) Szotek, Martin Lueders and Leon Petit (STFC Daresbury Laboratory)

This CECAM/Psi-k event on "Self-Interaction Correction: state of the art and new directions" is taking place on the thirtieth anniversary of John Perdew and Alex Zunger's seminal paper on correcting self-interaction error inherent in local density approximation to density functional theory [Phys. Rev. B23, 5048 (1981)]. This paper has initiated a variety of new implementations, generalizations, and extensions of the proposed self-interaction correction (SIC) approach. It has also led to a plethora of applications in different fields of physics and chemistry. Over the years, it has become apparent that different "varieties" of SIC have been developed nearly independently of each other, in particular in the field of quantum chemistry and solid state physics, with the experiences/advances gained in one field barely noticed in the other areas.

The paramount goal of this event is to bring together, for the first time, all the groups that have applied and worked on self-interaction correction, in order to discuss and assess the state of the art of all the different flavours of SIC, share the experiences and identify the most important and burning issues, unsolved problems, and perhaps find a common direction for future developments.

We welcome you wholeheartedly to Chester and hope this event will be very successful and beneficial for all the participants.

The Organisers

Programme of SIC Workshop

Chester, 19-21 September, 2011

Sunday 18 September 2011

17:00 - 20:00 Arrival and Registration

Monday 19 September 2011

08:45   Walter Temmerman (*Daresbury*): CECAM Daresbury Node Director
          Opening Remarks

          Chair: Thomas Schulthess (*Zurich*)

09:00   John Perdew (*Tulane*)
          "Rethinking the Perdew-Zunger Self-Interaction Correction, after 30 Years"

09:45 Alex Zunger (Colorado)
"Predicting localization, delocalization and polaron behaviour in insulators via restoration of the proper energy vs. occupation (linear) dependence to DFT"

10:30 Coffee/Tea

11:00 Mark Pederson (*Washington DC*)
"Computational Challenges for Wide-Spread Use of Self-Interaction-Corrections:A retrospective"

11:45 Nicola Marzari (*Lausanne)*
"Nothing works! Electronic-structure challenges in modelling materials for energy applications" *("Three perspectives on self-interaction - long-range charge transfer, short-range hybridization, and photoemission levels")*

12:30 Lunch

Chair: John Perdew *(Tulane)*

14:00 Klaus Capelle (*Sao Paulo*)
"Model Hamiltonians: A Theoretical Laboratory for DFT"

14:45 Stephan Kuemmel (*Bayreuth*)
"Kohn-Sham Self-interaction correction - a route to physically meaningful orbitals?"

15:30 Coffee/Tea

16:00 Peter Klüpfel, S Klüpfel, Hildur Guðmundsdóttir and Hannes Jónsson (*Reykjavik*)
"Perdew-Zunger SIC and other orbital density dependent functionals"

16:45 Olle Eriksson (*Uppsala*)
"Recent attempts of self-interaction"

19:00 - 22:00 Food and Posters

Tuesday 20 September 2011

Chair: Olle Eriksson (*Uppsala*)

09:00 Axel Svane (*Aarhus*)
"Self-interaction corrections of solids in the LMTO formalism"

09:45 Thomas Schulthess (*Zurich*)
 "Non-spherical self-interaction corrections implemented within the all-electron LAPW method"

10:30 Coffee/Tea

11:00 Björn Baumeier (*Mainz*)
"Self-interaction corrected pseudopotentials for crystalline systems"

11:45 Alessio Filippetti (*Cagliari*)

"A variational approach to the study of strong-correlated oxides based on the self-interaction removal from local density functional"

12:30   Lunch

Chair: Nicola Marzari (*Lausanne*)

14:00   Hisazumi Akai (*Osaka*)
"A pseudo-SIC implementation in the KKR code and applications"

14:45   Julie Staunton (*Warwick*)
"Magnetic and electronic structure at finite temperatures described ab-initio: disordered local moments and the self-interaction correction "

16:00   Walk around Chester & Workshop Dinner

Wednesday 21 September 2011

Chair: Mark Pederson (*Washington DC*)

09:00   Adrienn Ruzsinszky (Tulane)
"Nonempirical Fully-Nonlocal Density Functional for Correlation, Compatible with Self-Interaction Free Exact Exchange"

09:45   Eric Suraud (*Toulouse*)
"The Self Interaction Correction revisited"

10:30   Coffee/Tea

11:00   Takao Tsuneda (*Yamanashi*)
"Regional self-interaction corrections of long-range corrected DFT"

11:45   Aron Cohen (*Cambridge*)
"Connection between self interaction and strong correlation"

12:30   Lunch

Chair: George Malcolm Stocks (*Oak Ridge*)

14:00   Stefano Sanvito (*Dublin*)
"The self-interaction error in electronic transport across nanodevices"

14:45   Nikitas Gidopoulos (*Didcot*)
"Constraining density functional approximations to yield self-interaction free potentials"

15:30   Coffee/Tea + Round Table Discussion: George Malcolm Stocks (ORNL) – Moderator

17:30   Closing Workshop

Poster Session

Markus Daene
Computationally Simple, Analytic, Closed Form Solution of the Self-Interaction Problem in Kohn-Sham Density Functional Theory

Guntram Fischer
Magnetic Properties of Polar ZnO Surfaces: Application of SIC.

Hildur Guðmundsdóttir
Self-interaction correction within the PAW formalism: implementation and applications

Dirk Hofmann
Self-interaction correction in the time-dependent Kohn-Sham scheme

Simon Klüpfel
More complex than expected: The Self-interaction corrected ground state of atoms and molecules

Anton Kozhevnikov
Full-potential SIC implementation

Martin Lueders
Flavours of SIC

Keld Lundgaard
Exchange correlation functionals including non-local correlation and error estimation

Abstracts of Invited Talks: Monday 19 September

Rethinking the Perdew-Zunger Self-Interaction Correction, after 30 Years

John P. Perdew

Department of Physics, Tulane University, New Orleans, Louisiana 70118, USA

The Perdew-Zunger self-interaction correction (PZ-SIC) [1] to a semi-local density functional for the exchange-correlation energy of a many-electron system, which ensures exact results for all one-electron densities, has had dramatic successes and failures. Among the successes are strongly improved descriptions for atoms, for open systems of fluctuating electron number, and for strongly-correlated solids. Among the failures are worsened descriptions of the equilibrium geometries and atomization energies of typical molecules and solids. Another disturbing fact is that PZ-SIC performance deteriorates as the underlying semi-local functional improves from the local to the gradient-corrected level. In an attempt to understand this situation, the satisfactory and unsatisfactory formal properties of PZ-SIC are reviewed. Then two variants of PZ-SIC are proposed, which avoid the unsatisfactory formal property that may be responsible for worsening SIC performance under improvement of the underlying semi-local functional. One variant has a more intuitive interpretation than the original PZ-SIC. Whether either variant will perform better in numerical applications remains

to be seen. Finally, a physical explanation is given of SIC's need for localized orbitals. (Work supported by NSF-DMR.)

[1] J.P. Perdew and A. Zunger, Self-Interaction Correction to Density-Functional Approximations for Many-Electron Systems, Phys. Rev. B **23**, 5048 (1981).

Predicting localization, delocalization and polaron behaviour in insulators via restoration of the proper energy vs. occupation (linear) dependence to DFT

Alex Zunger,

NREL and University of Boulder, Colorado, USA

 One of the main tragedies faced by DFT practitioners of the theory of insulators is the systematic exaggeration of delocalization characteristics. In the world of defects, this leads, for example, to very optimistic predictions of 'shallow levels', creating (false positive) excitement among experimentalists who take such prediction seriously and expect to find conducting insulators such as ZnO:N, but are repeatedly frustrated by disagreement with theory.

Another manifestation of this problem is the failure of DFT practitioners to systematically find bound polaron when they are expected, creating somewhat of a gap with the model-Hamiltonian practitioners that build-in polaronic behaviour "by hand" (say, Zhang-Rice) but cannot derive it from the electronic structure itself. A simple fix that restores to the DFT total energy the proper linear dependence on occupation number (" generalized Koopmans relation"), due to SIC .This produces systematically correct localization/delocalization in a wide range of insulators .This predicts very different results than scores of DFT or hybrid functional papers published over the last few years, while hopefully restoring some of the friendship and credibility between experimentalist and Theorists.

Computational Challenges for Wide-Spread Use of Self-Interaction-Corrections: A retrospective

Mark R. Pederson

Naval Research Laboratory, Washington DC 20375-5345

The original paper on self-interaction corrections (SIC)[1] provided a very complete description of the problem and potential solutions for addressing this issue and, with hindsight, identified future technological areas that could be impacted by SIC.   As noted in the original paper by Perdew and Zunger [1] orbital-dependent potentials such as those that arise within SIC functionals requires the practitioner to "*perform a unitary transformation of the Kohn-Sham fully occupied orbitals to a second set of (more localized) orbitals*" especially in multi-center problems such as molecules and solids. This talk will review the

SIC localization equations[2] that arise from the variational principle, discuss the physical significance of both localized and canonical orbitals[2] in molecules and solid-state systems, and review applications to molecules, clusters and solids that occurred during the first decade of effort. In addition I will discuss why the yet-to-be commonly realized full-scale implementation and use of a self-interaction corrected quantum methods could impact many application-oriented fields of science that I have participated more recently.   This includes molecular magnetism and technological areas, especially to those related to light harvesting, where efficient and effective descriptions of localized excitations and charge transfer are needed to make progress.

[1] J.P. Perdew and A. Zunger, *Self-Interaction Correction to Density-Functional Approximations for Many-Electron Systems*, Phys. Rev. B **23**, 5048 (1981).
 [2]M.R. Pederson, R.A. Heaton, C.C. Lin, *Density-Functional Theory with Self-Interaction – Application to the Lithium Molecule*, J. Chem. Phys. 82 2688-2699 (1985); *Local-Density Hartree-Fock Theory of Electronic States in Molecules with Self-Interaction Corrections*, J. Chem. Phys. **80**, 1972-1975 (1984).

Nothing works! Electronic-structure challenges in modelling materials for energy applications

("Three perspectives on self-interaction - long-range charge transfer, short-range hybridization, and photoemission levels")

Nicola Marzari

Department of Materials, University of Oxford, U. K.[(*)]

Density-functional theory has become a very powerful tool to understand, predict, or design the properties of complex materials and devices. It is also an imperfect tool, with open and urgent challenges in our quest towards qualitative and quantitative accuracy, and in our ability to perform quantum simulations under realistic conditions.

Several of these challenges stem from the remnants of self-interaction in our electronic-structure framework, leading to qualitative failures in describing especially some of the fundamental processes involved in energy applications - from charge-transfer excitations, to photoemission spectra, to structure and reactivity of transition-metal complexes.

I'll discuss these challenges in realistic case studies, and suggest possible solutions based on constrained DFT, on extended Hubbard functionals, or on imposing a generalization of Koopmans' theorem. I'll also highlight how the calculation of magnetic properties (NMR/EPR) or the use of wavefunction techniques can provide stringent validation criteria for novel developments.

(*) Present address: Theory and Simulations of Materials, EPFL, Switzerland.

Model Hamiltonians: A Theoretical Laboratory for DFT

Klaus Capelle

UFABC, Sao Paulo, Brazil

The density-functional approach and the model-Hamiltonian approach each constitute one of the pillars of modern many-body theory. In the past, crosslinks between both pillars have been forged in various different ways. In this talk I first review some of these connections, highlighting the many possible benefits that arise from using insights from DFT to study model Hamiltonians, and ideas arising from model Hamiltonians to improve functionals for DFT. Next, I address one particular connection: the use of the Hubbard model as a theoretical laboratory for investigating concepts and computational tools of DFT for a well-controlled model Hamiltonian. Specifically, I consider an orbital-dependent functional, the Perdew-Zunger self-interaction correction, and compare results from six different levels of approximate implementation, ranging from simple post-LDA strategies to a full OEP, to available exact results. It turns out that sometimes simpler is better.

Kohn-Sham Self-interaction correction - a route to physically meaningful orbitals?

Stephan Kuemmel, Matthias Dauth, Thomas Koerzdoerfer

Bayreuth University, Germany

The original self-interaction correction (SIC) scheme of Perdew and Zunger, and many works since then, minimized the SIC energy with respect to the orbitals. In this contribution the Kohn-Sham approach to the SIC using one global multiplicative potential is discussed. The effects of orbital localization and the physical reliability of the thus obtained eigenvalues are studied. In particular we investigate the reliability of orbital densities as predicted by Kohn-Sham SIC in comparison to "measured orbital densities" that are available from photo-emission experiments for organic semiconductor molecules.

Perdew-Zunger SIC and other orbital density dependent functionals

Peter Klüpfel, Simon Klüpfel, Hildur Guðmundsdóttir and Hannes Jónsson

Science Institute and Faculty of Science, University of Iceland, 107 Reykjavik, Iceland

Results of self-consistent calculations of PZ-SIC applied to GGA and LDA functionals will be presented for atoms, molecules and solids. The calculations make use of an efficient method to minimize the energy with respect to the orbitals, involving explicit unitary optimization.

Symmetry breaking at the single-particle level, including time-reversal symmetry, is found to be essential. The PZ-SIC based on the PBE functional gives significant improvement in the total energy of atoms and orbital energies agree well with ionization energies. For other GGA functionals no improvement is obtained and thus PZ-SIC can not be considered a general correction scheme.

Another severe problem of the PZ-SIC is the lack of size consistency. It always arises when the PZ-SIC of an orbital is positive, which is the typical case for valence electrons in the GGA framework but can also be observed in LDA-SIC. In periodic systems, the positive contribution to the energy can be avoided by complete delocalization of such orbitals. However, in numerical PZ-SIC calculations no continuous transformation from localized to delocalized states can be modeled in a finite simulation box. This makes self-consistent calculations of periodic systems impossible, unless prior assumptions are made regarding the level of localization of the orbitals.

Both problems can possibly be overcome within the more general framework of orbital density dependent (ODD) functionals. We are developing a size-consistent, self-interaction free and numerically stable ODD functional. First steps towards this functional and its application will be presented.

Recent attempts of self-interaction

Olle Eriksson

Department of Physics and Astronomy, Uppsala University, Sweden

In this presentation I will discuss attempts of self-interaction correction, both using the approach of Ref. 1 as well as recent PZ-SIC in a full charge density implementation. Problems but also opportunities in general with reproducing a many-electron charge density from an effective one-electron theory will be discussed [2] and compared to recent developments using dynamical mean field theory.

References:
1. U. Lundin and O. Eriksson, Int. J. of Quant. Chem. **81**, 247 (2001).
2. O. Eriksson, J.M. Wills, M. Colarietti-Tosti, S. Lebegue and A. Grechnev, International Journal of Quantum Chemistry **102** 1046 (2005).

Self-interaction corrections of solids in the LMTO formalism

Axel Svane

Department of Physics and Astronomy, Aarhus University, Denmark

The implementation of the Perdew-Zunger self-interaction corrected (SIC) energy functional for solids is discussed. Applications using the LMTO method are presented. The one-particle states which benefit from the self-interaction correction necessarily must be localized, which contrasts the conventional Bloch picture of periodic solids. The localized picture is however the more appropriate for certain cases, e.g. the 4f states in rare earth compounds, the 5f states in actinides, and the 3d states of many transition metal compounds. The SIC therefore leads to a mixed picture with some electron states being localized and some being itinerant. The SIC allows the study of delocalization under pressure, e.g. the spectacular phase transitions observed in cases like elemental Ce, CeP, SmS, and YbS. For the actinides the delocalization proceeds by delocalizing the f-electrons one at a time, and the volume range over which the transition from the localized to the itinerant scenario takes place may be identified.

[1] L. Petit, R. Tyer, Z. Szotek, W. M. Temmerman and A. Svane, New J. Phys. 12, 113041 (2011).
[2] L. Petit et al.: PRB76, 115116 (2007); ibid. 80, 045124 (2009); ibid 81, 045108 (2010).

Non-spherical self-interaction corrections implemented within the all-electron LAPW method

Thomas C. Schulthess (1,2), Anton Kozhevnikov (1), Walter Temmerman (3), and Zdzislawa Szotek (3)

1.   *Institute für Theoretische Physik, ETH Zürich, Switzerland*
2.   *Center for Nanophase Materials Science, Oak Ridge National Laboratory, USA*
3.   *STFC Daresbury Laboratory, UK*

Perdew-Zunger self-interaction corrections to the local spin-density (SIC-LSD) approximation seem appealing for electronic structure studies of strongly correlated systems that exhibit a Mott transition, as the method is capable of describing localized and delocalized electrons within the same theoretical framework. Such studies have so far been implemented within the LMTO-ASA method and applied with success to numerous transition metals oxide and rare earth systems. However, a question remains as to whether the ability of the SIC-LSD method to describe localization-delocalization transition is an artifact of the spherical approximation used within the LMTO-ASA approach. We have thus set out to implement the SIC-LSD within the full-potential LAPW method. With the new method, we reproduce rather well the LMTO-ASA results for NiO and solid Hydrogen, as well as the total energies in the atomic limits of several elements for which exact and state of the art SIC results are known.

A number of numerical challenges to do with the non-spherical implementation had to be addressed and will be discussed in the presentation.

Self-interaction corrected pseudopotentials for crystalline systems

Björn Baumeier

Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

It is well known that the use of local or gradient-corrected exchange correlation functionals in density-functional theory calculations introduces a spurious electronic self-interaction to both total energy functional and, concomitantly, the effective potential. Therefore, structural, electronic, and optical properties of solids calculated based on the Solution of the Kohn-Sham equations show systematic errors, for instance the over-delocalization of (strongly) correlated electrons or the underestimation of fundamental band gaps in semiconductors and insulators. The atomic self-interaction correction scheme heuristically introduced by Perdew and Zunger [1] turns out to be notoriously difficult to adapt directly to polyatomic environments, such as bulk crystals or crystal surfaces (cf. e.g. [2-4]). In this talk, I will review the pragmatic method, developed in Prof. Pollmann's group at WWU Münster, of transferring atomic self-interaction corrections to solids via inclusion into angular- momentum dependent atomic pseudopotentials [5,6]. After an overview about its concept, it will be demonstrated that for a large number of compounds with partially ionic characteristics, e.g. silicon carbide or alkali-metal oxides, this approach can be used to predict structural data, electronic band structures, as well as optical spectra in a quantitatively reliable fashion without being more demanding computationally than standard local-density calculations. The method is also useful to study magnetic properties, as e.g. in the case of N-doped MgO, a dilute magnetic semiconductor exhibiting $d0$-magnetism.

[1] Perdew, Zunger, Phys. Rev. B 23, 5048 (1981)
[2] Svane, Gunnarsson, Phys. Rev. B 37, 9919 (1988)
[3] Szotek et al., Phys. Rev. B 47, 4029 (1993)
[4] Stengel, Spaldin, Phys. Rev. B 77, 155106 (2008)
[5] Vogel et al., Phys. Rev. B 52, R14316 (1995)
[6] Baumeier et al., Phys. Rev. B 73, 195205 (2006)

A variational approach to the study of strong-correlated oxides based on the self-interaction removal from local density functional

Alessio Filippetti

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The ever growing applicative importance of strong-correlated materials, such as magnetic and superconducting oxides, requires an accurate and at the same time computationally affordable description based on First-Principles. The pseudo-self-interaction corrected local spin density functional theory (PSIC) [1] introduced few years ago matches these requirements: it is based on a straightforward atomic-like parametrization of the self-interaction potential; it is conceptually simple and computationally manageable almost as a local-density functional approach. Furthermore, it does not make use of adjustable parameters and is applicable to Mott insulators and metals alike. Recently the method has been reworked in a fully variational form (VPSIC) [2] thus extending its applicability to structural optimization, phonon calculations, and higher-order total energy derivatives. Here we illustrate the background of the theory and present results of recent applications to different classes of materials: non-magnetic oxides (bulk $SrTiO_3$, $LaAlO_3$, $SrTiO_3/LaAlO_3$ interfaces), magnetic t_{2g} systems ($LaTiO_3$, $YTiO_3$), magnetic e_g systems (transition metal monoxides, manganites). Overall the method shows a satisfying accuracy for a remarkable generality of systems.

References
1. A. Filippetti and N. Spaldin, *Phys. Rev. B* **67**, 125109 (2003).
2. A. Filippetti *et al*, to be published.

A pseudo-SIC implementation in the KKR code and applications

Hisazumi Akai

Department of Physics, Osaka University, Japan

Implementations of the pseudo-SIC proposed by Filippetti and Spaldin have some advantages over the implementations of original SIC. First, it is rather easy to implement and to perform pseudo-SIC calculation. Also it can produce the same results as a normal SIC as for localized atomic states. The disadvantage on the other hand is that using the pseudo-SIC is less justifiable. Putting this point aside for a moment, I first will explain the implementation of the pseudo-SIC in the KKR code. Instead of using a fixed atomic orbital and the projection on it, in the KKR code we use energy functions. For all energy functions of a given angular momentum (l, m) and a spin, we use a common SIC potential. As an example of using this implementation, I will present some results of calculation of MCD spectra of diluted magnetic semiconductors (DMS's). The analyses of the MCD spectra of DMS's caused many controversies in the past. Our calculation confirmed that exploiting SIC seemed to provide a better framework for the descriptions of the spectra.

Finally, I will discuss the possible justification of using the pseudo-SIC. It seems that using the pseudo-SIC can be regarded as one of the ways to improve the treatment of the exchange energy of electrons in narrow bands rather than to eliminate the self-interaction that anyway does not exist for extended states.

Magnetic and electronic structure at finite temperatures described ab-initio: disordered local moments and the self-interaction correction

Julie Staunton

University of Warwick, U.K.

Density functional theory is extensively used in ab-initio materials modelling. This talk will show how this is extended by the identification of different time scales amongst the collective electronic degrees of freedom. For example, it provides the starting point for the description of temperature dependent magnetic properties. Magnetic excitations, which trigger the loss of magnetic order with rising temperature, are incorporated by attaching to all atomic sites local spin-polarisation axes, whose orientations vary very slowly on the time-scale of site-to-site electronic propagation. Averaging over these `local moment' degrees of freedom provides a quantitative description of the type and onset of magnetic order, high temperature paramagnetic phases and indeed magnetic phase diagrams. In many magnetic materials the standard LDA treatment of electron exchange and correlation is inadequate. Recently we have incorporated the effects of strong electron correlations using the local-SIC [1] approach into our disordered local moment (DLM) theory of finite temperature magnetism. Here a brief overview of this theoretical approach will be given followed by an application to the magnetic phase diagram of gadolinium and the other heavy rare earths [2]. Findings reveal a delicate competition between conflicting magnetic interactions in heavy rare-earth systems and their link to the hexagonal close packed lattice parameters. In particular there can be a near degeneracy between ferromagnetic ordering and Fermi surface nesting driven incommensurate anti-ferromagnetism. We will also describe results for the transition metal oxides Mn0, FeO, Co0 and NiO which have anti-ferromagnetic order at low T. We will show how the DLM-SIC picture explains the persistence of the large insulating gap into the paramagnetic state [3].

[1] M.Lueders et al.,Phys. Rev. B**71**:205109, (2005).
[2] I.D. Hughes,M. Daene, A. Ernst, W. Hergert, M. Lueders, J. Poulter, J. B. Staunton, A. Svane, Z. Szotek and W. M. Temmerman, Nature, **446,** 650-653, (2007).
[3] I. D. Hughes, M. Daene, A. Ernst, W. Hergert, M. Lueders, J. B. Staunton, Z. Szotek and W. M. Temmerman, New J. Phys. **10**, 063010, (2008).

Abstracts of Invited Talks: Wed 21 September

Nonempirical Fully-Nonlocal Density Functional for Correlation, Compatible with Self-Interaction Free Exact Exchange

Adrienn Ruzsinszky

Adrienn Ruzsinszky[1], John P. Perdew[1], and Gábor I. Csonka[2] , [1]Department of Physics, Tulane University, New Orleans, LA 70118, and [2] Department of Chemistry,

Budapest University of Technology and Economics, Budapest, Hungary

On the ladder of density functional approximations, the three semi-local rungs are not self-interaction free. To be self-interaction free, we have to add exact exchange. The exact exchange becomes available only on the fourth rung of the ladder of approximations. A fifth-rung density functional, the random phase approximation, has the exact exchange, but its correlation is not self-correlation free.

The semilocal density functionals have nonempirical constructions, but so far the hyper-GGA or hybrid rung, which adds exact-exchange ingredients, does not. In an attempt to construct a nonempirical hyper-GGA correlation compatible with full exact exchange, we model the correlation hole density $n_c(\vec{r},\vec{r}')$ at $\vec{r}'$ around an electron at $\vec{r}$, using the same exact constraints used to construct early generalized gradient approximations. But we also add fully nonlocal constraints: the correlation hole density must vanish where $n(\vec{r}')$ does, and its long-range or large $|\vec{r}'-\vec{r}|$ part can cancel that of the exact exchange hole. We test this model on atomization energies of molecules, and in particular on the nonlocal correction (as treated differently in [1]) to the random phase approximation [2,3,4].

[1] A. Ruzsinszky, J.P. Perdew, and G.I. Csonka, J. Chem. Theory Comput. *6*, 127 (2010).
[2] F. Furche, Phys. Rev. B *64*, 195120 (2001). [3] P. Mori-Sanchez, A.J. Cohen, and W. Yang, *arXiv* 0903.4403.[4] A. Ruzsinszky, J.P. Perdew, and G.I. Csonka, J. Chem. Phys. *134*,114110 (2011).

The Self Interaction Correction revisited

J. Messud[1], P. M. Dinh[1], Eric. Suraud[1], P. G. Reinhard[2]

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[2]Institut fuer Theoretische Physik, Universitaet Erlangen Staudtstr. 7, D-91058 Erlangen, Germany

The Self Interaction Correction (SIC) is a long standing problem in Density Functional Theory (DFT). It causes several major difficulties especially with the universally used simple and efficient Local Density Approximation (LDA). The standard SIC approaches lead to the introduction of orbital dependent functional which exhibit several formal and technical problems. The Optimized Effective Potential (OEP) methods allow to deal with such difficulties but in an approximate manner. The fully time dependent cases remain especially problematic, which leads to significant difficulties for the treatment of ionization "on the fly".

We discuss an extension of time-dependent DFT including SIC. A strictly variational formulation is given taking care of the necessary constraints. A manageable and transparent propagation scheme using two sets of wavefunctions is proposed and applied to laser excitation with subsequent ionization of a dimer molecule. We also discuss the use of such an elaborate SIC formalism to the analysis of electronic emission in terms of energy

(Photoelectron Spectra, PES) and angles (Photoelectron Angular Distributions, PAD) with examples in the case of small metal clusters.

References

[1] J. Messud, P. M. Dinh, P. -G. Reinhard, E. Suraud, Phys. Rev. Lett. **101** (2008) 096404.

[2] J. Messud, P. M. Dinh, P. G. Reinhard, E. Suraud, Ann. Phys. (NY) **324** (2009) 955.

Regional self-interaction corrections of long-range corrected DFT

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In the talk, I will review our RSIC-series methods and will show their availabilities in core excitation calculations. I will also briefly review for the significance of self-interactions on orbital energies.

The connection between self interaction and strong correlation

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Many of the problems of one electron systems can be understood from the viewpoint of the self-interaction error. We will show some of the dramatic effects of self-interaction and the lack of it in approximate functionals in some simple one-electron systems.

We will also show the understanding from the viewpoint of strong correlation which will stress the connection between self-interaction and static correlation. For the two simplest molecules in the whole of chemistry this connection can be seen by the performance of a whole range of methods ranging from approximate functionals in DFT to RPA to Many-Body methods and RDMFT.

The self-interaction error in electronic transport across nanodevices

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Quantitative electron transport theory has made enormous progresses in the last decade, and today fully functional algorithms based on the non-equilibrium Green's function (NEGF) formalism implemented within density functional theory (DFT) are the workhorse for modelling material-specific nano-devices [1]. Such a computational scheme, however, has a number of fundamental and practical limitations [2], mostly related to the improper use of the Kohn-Sham eigenvalues as single particle levels. Still the theory, which enjoys relatively low computational overheads, can be transformed in an effective scheme capable of quantitative predictions. This is achieved by using self-interaction-free exchange and correlation functionals.

In this contribution I will discuss the most common pitfalls in the NEGF+DFT approach to electron transport and demonstrate that an approximated self-interaction scheme [3,4] can be used to obtain quantitative predictions for technologically relevant nano-scale devices. Examples will be drawn from transport in molecules, in multi-functional tunnel junctions and in organic systems in solution. Furthermore, I will show preliminary results where fully non-local exchange and correlation functionals will be combined with the NEGF scheme.

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Constraining density functional approximations to yield self-interaction free potentials

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The SI error present in the direct Coulomb or Hartree energy term is a quantity that cannot be defined unambiguously. This ambiguity is then reflected in the attempts to correct SI

errors in the total energy. On the other hand the effect of SI's in the Kohn-Sham (KS) potential can be determined unambiguously, and we have obtained a necessary condition for the local potential to be SI free, even though it still corresponds to an energy expression (like the local density approximation, LDA) that is not SI free. Implementing this necessary condition requires techniques from the Optimised Effective Potential (OEP) methodology. Calculations on simple atoms show that the resulting SI-corrected LDA potential decays correctly as 1/r. Crucial in our theory is the introduction of the notion of the screening charge density, whose properties will be discussed.

Participants

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APPENDIX E

Quixote Collaboration Meeting 22 - 23 March 2011, STFC Daresbury Laboratory
Organiser: Jens Thomas (STFC Daresbury Laboratory)

A collaboration meeting was held at Daresbury on the 22-23rd March. For background
information and programme, see here:

http://quixote.wikispot.org/First_Quixote_Conference_-_22nd-23rd_March_2010

There was a wide spread of participants from a range of disciplines and interests, including
representatives from molecular and solid-state communities. Rather than being a discussion
and planning meeting, the collaboration had a very distinct practical goal, to complete a
demonstration by which outputs from quantum chemistry calculations could be parsed and
the results stored in an searchable public database. This target was achieved, and since
then two data collections have been added to the database, which is available at
http://quixote.ch.cam.ac.uk/

Significant achievements arising from work following the meeting include

    I.   A manuscript on the project has been written and is in press
        http://www.dspace.cam.ac.uk/handle/1810/238392

   II.   A further meeting was held in Zaragossa, for details of this see

        http://sonexworkgroup.blogspot.com/2011/08/stm-research-data-management-and.html

  III.   There is a renewal bid for the COST D37 WG5 which includes the involvement of
        Quixote

  IV.   There were several presentations at the American Chemical Society (Chemical
        Information and Comp Chem divisions) on or referencing Quixote

   V.   Peter Muray-Rust is visiting PNNL in October 2011 to continue to develop quantum
        chemistry dictionaries

Future Plans

We are continuing to develop dictionary technology and Chempound. Both are now
accepted for publication.

PMR's visit to PNNL in October should establish a draft for the communal CompChem
dictionaries

We intend to apply for further funding under "Pathways to Impact".
We propose another workshop which we plan to fund from this collaboration budget.