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Report of the Hartree Centre CECAM Node Activities

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REPORT OF THE HARTREE CENTRE CECAM NODE ACTIVITIES

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cecam
Centre Européen de Calcul Atomique et Moléculaire

Prologue

This report describes the activities which took place in the first year of CECAM's Hartree node based at the STFC Daresbury Laboratory. At the CECAM Council meeting of January 21-22,2010 the Hartree node was formally accepted as one of CECAM's nodes and Walter Temmerman was accepted as its Director for a period of four years.

The governance of the Hartree node is its Director assisted by a steering committee consisting of James Annett (University of Bristol), Mike Ashworth (Advanced Research Computing ,Daresbury), Paul Durham (Vice-President CECAM Council, Daresbury), David Emerson (Computational Engineering, Daresbury), Mike Payne (University of Cambridge), Paul Sherwood (Computational Chemistry, Daresbury), Bill Smith (Computational Chemistry, Daresbury), Zdzislawa Szotek (Band Theory Group, Daresbury), Walter Temmerman (Director CECAM Hartree node), Stanko Tomic (Computational Material Science, Daresbury), Martyn Winn (Computational Biology, Daresbury). A budget of 70 kEuro provided by the STFC was at the Director's disposal.

During its first year of operation, three highly successful workshops were organized, one tutorial and one hands-on course. Regrettably CECAM felt unable to sponsor the following two workshops: The databases for quantum chemistry workshop, joint activity with the CECAM's Zaragoza node, which will be funded by the Hartree node in 2011. The KKR hands-on course was funded by the Hartree node in 2010, but not as a CECAM activity. These were two cases where the priorities of the Hartree node did not coincide with CECAM's priorities. It is unavoidable that such cases will keep occurring in the future.

The hands-on KKR course was the only event taking place in Daresbury with participants being bussed in from Chester. To make hands-on tutorials possible, it was requested that the participants provided their own laptops and nearly all students did. This simplified matters enormously and also had the added advantage that students could continue their calculations in the hotel where wireless was available. This was a formula which worked very well. The other events took place in Manchester (two workshops), London and Belfast.

The five meetings were a success. They led to five new collaborations and to an expansion of the subjects involving the quantum chemists and the computational biologists. CECAM's core activities such as code interoperability and code validation and verifications have a strong Daresbury input with no less than three members of the Computational Science and Engineering (CSE) Department involved.

To finish, I would like to thank all members of the CSE Department for their enthusiasm and support to make this a successful launch of CECAM's Hartree node. In particular, I would like to acknowledge Richard Blake, the CSE director, for providing the finances and Shirley Miller and Wendy Cotterill for the exemplary organization of the workshops and so much more.

Walter Temmerman
Daresbury
October 25, 2010

Report -2010

I/WORKSHOPS

1. Actinides: Correlated Electrons and Nuclear Materials Manchester June 14-16, 2010. Organizers: Leon Petit and Bernard Amadon

The workshop was attended by 50 people, with the purpose of theoreticians in the field of correlated electrons having discussions with people in nuclear materials fields. An important theoretical issue was the treatment of relativity and how it was described in our codes.

The workshop produced lively discussions and a final round table meeting. There was interest in a follow up collaboration which would be submitted together with CEA, France. The venue was ideal in the centre of Manchester – easily accessible and close to good restaurants, pubs within walking distance for a social programme. (Full report at Appendix A)

2. Empirical Methods in Semiconductor Nanostructures Design and Modelling. Manchester 21 June - 25 June 2010. Organisers: Stanko Tomic, Max Migliorato, Eoin O'Reilly, Gyaneshwar Srivastava

This was a joint workshop with the Dublin node. Whilst the ACAM (Dublin) Workshop focused primarily on computational/technical issues, numerical implementations and parametrisation strategies, this was followed immediately by the second (STFC Daresbury) Workshop highlighting the scientific issues and demands related to empirical nanostructure design and modelling. There was a round table discussion on Open Innovation in Scientific Software Engineering and code interoperability and code communication

The overall feeling of the community is that it would be ideal to submit a proposal for a further meeting in two years time on the same subject and a summer school or tutorials to be run in Rome next year. The Proceedings will hopefully go to the Journal of Physics-Conference Series. (Full report at Appendix B)

3. Advances in Strong Field and Attosecond Physics London 23- 25 June 2010. (Organisers: Paul Durham, Carla Faria, Maciej Lewenstein, Jens Biegert, Wolfgang Sandner, Misha Ivanov)

The meeting had been a success with more than 100 participants. It was not a traditional CECAM workshop but rather a mini research conference. The majority of attendees were in the laser field with quite a few experimentalists and the remainder were theorists. Hardy Gross, Peter Littlewood, Andrew Fisher and Paul Durham represented the Condensed Matter area.

The meeting included a panel discussion to assess the field and it was suggested that sights needed to be raised from Atomic and Molecular Physics to consider other more interesting applications. It was anticipated that this meeting would be written up in a special edition of Journal of Optics. The editorial page would act as a report of this meeting. The web pages would be retained and a report would be posted. (Full report at Appendix C)

II/TUTORIAL

CCP5 Summer School in Molecular Simulation Belfast 18 July - 27 July 2010 (Organisers: John Harding, John Purton, Mario G. Del Popolo)

This School is intended for newcomers to the science of molecular simulation and provides a comprehensive introduction to the methodology, practical sessions on computational methods and

examples of the power and versatility of simulation methods. These Schools are a yearly event following an extremely successful formula and the Hartree node envisages continued support for this series. (Full report at Appendix D)

III/OTHER RESEARCH MEETINGS

KKR Hands-On Course STFC Daresbury Laboratory and Chester Mill Hotel 4-6 October 2010 (Organizers: Hubert Ebert and Zdzislawa (Dzidka) Szotek)

The course took place in the Tower Seminar Room in Daresbury. The code was accessed via DL WiFi and NXClient, and run on the Munich University workstations. The participants used their own laptops to run NXClient on them. Daresbury Laboratory provided the wireless access to the internet and three spare PCs, supplied by the PC Support Group, which were on standby for those who might have had temporary problems with netbooks/laptops or had no laptops with. In the end all the PCs provided were used on occasions. . (Full report at Appendix E)

IV/VISITORS PROGRAMME

None

V/RESEARCH collaborations between Nodes/HQ

Code interoperability : This is a collaboration between the Hartree node (Dzidka Szotek and Walter Temmerman) with the Swiss CECAM node in Zurich (Thomas Schulthess and Anton Kozhevnikov). The collaboration is for the Daresbury/Oak Ridge LMTO-ASA package and the Ekaterineburg LMTO-ASA code to have common inputs.
Anton Kozhevnikov visited DL from 22 Feb to 6 Mar 2010, Thomas Schulthess visited DL on 1-2 Mar 2010, Dzidka & Walter visited Zuerich on 30-31 Mar 2010
The collaboration has put a functionality to construct a minimal tight binding Hamiltonians in the Daresbury/Oak Ridge code for the SIC-LSD Hamiltonian. This is a facility needed by both partners.

APPENDIX A

ACTINIDES: CORRELATED ELECTRONS AND NUCLEAR MATERIALS

Leon Petit (Daresbury Laboratory)
Bernard Amadon (CEA)

SCOPE OF THE WORKSHOP:

The workshop was held at the Ramada Jarvis hotel in Manchester from the 14-16 of June 2010. Altogether 47 participants were registered for the workshop. 27 invited talks were presented. Of the 18 delegates, 10 were students. Plenty of time was given for discussions, including a round table. The focus of the workshop was on investigating the impact that the study of correlations in the actinides can have on our understanding of the materials of the nuclear cycle. Whilst the main thrust was on the theoretical first principles tools that are currently being developed, close contact was made to current experimental investigations, including presentations on the state of the art of developing improved nuclear fuels, as well as new approaches to nuclear waste disposal.

Understanding the materials related problems requires understanding their electronic structure, and given the strongly correlated nature of the actinide 5f electrons, theories that go beyond the LSD approximation have to be developed and applied. The goal of the workshop was to present up to date software developments in the field, and the results obtained with these tools. These results range from electronic and magnetic structure of the stoichiometric compounds to the formation and diffusion energies of impurities and vacancies in actual reactor materials.

MAIN OUTCOMES:

The workshop was opened by Claude Guet, who presented an outlook on the role that nuclear energy will play in guaranteeing the future sustainable energy mix. The speaker emphasized the need for substantial R&D into nuclear materials, both with respect to experiment and computer simulations. The goal is among others to develop materials capable of sustaining intense irradiation in order to extend the lifetimes of reactors, fuels for the next generation of reactors, fuels that incorporate the minor actinides to achieve improved recycling, and glasses for long term safe waste disposal. Rudy Konings presented results on the performance of nuclear fuels under extreme conditions. The talk gave a comprehensive insight into the fuels for the next generation of nuclear reactors, and the modeling and experimental investigations that will be required for improving their performance under reactor conditions. Gerry Lander presented an overview of experiments over the years studying the behavior of actinide metals, and the change in bonding properties under pressure.

One of the most studied and still not fully understood problems in actinide physics, is nature of the ground state in δ-Pu, and which was also the subject matter of several presentations at the workshop. On one hand it was argued that the absence of magnetic moment might be explained in terms of the cancellation of the spin and orbital moments, on the other hand, given the strong indications from experiment that both spin and orbital moments in δ-Pu are individually zero, it was proposed that the non-magnetic ground state in some of the actinides can be obtained if the exchange enhanced spin-orbit coupling is correctly taken into account. The double-well potential that occurs in the DMFT approach to δ-Pu was instead derived by solving the periodic Anderson model within Hartree-Fock, and the LDA+Hubbard-I (HIA) approximation, studying the spectroscopy of actinide metals Pu, Am and Cm, found good agreement between theory and PES studies.

The actinide oxides remain the most used fuel form in current nuclear reactors, and a considerable number of presentations focused on giving an improved description of AO2 with the actinide A ranging from U to Cf. Results obtained with respectively, hybrid functional, GW, LDA+U, and SIC-LSD were presented, showing overall excellent agreement with available experimental data (energy gap, groundstate, crystal field excitations, Hubbard bands). New insight into the nature of the bonding in actinide oxides was presented. The experimentally observed stability of the Jahn-Teller distortion in UO2 was investigated as was the charge state, and formation and migration energies of interstitials and vacancies in a range of actinide dioxides. It was furthermore shown that the localized 5f electrons are required to describe the electronic structure and complex multipolar ordering in the actinide oxides, and that the dynamics observed in UO2 results from the complex interplay of spin, phonon and quadrupole degrees of freedom.

At the workshop, a number of presentations were given, addressing all aspects of experimental investigation into the actinide materials. Recent results on the surface reactivity of nuclear systems addressed issues such as the corrosion of spent nuclear fuel and the radiation assisted reduction of PuO2 by water. Based on susceptibility measurements and XPS studies it was concluded that the details of the 5f occupancy, rather than the Pu-Pu distance are relevant for magnetic properties. It was shown that the actinides show strong

5d-5f electric-multipole transitions that can be probed bulk sensitive using non-resonant inelastic scattering (NIXS) experiments. Insights gained from applying X-ray and electron spectroscopy to nuclear materials were discussed, as were the recently observed intrinsic localized modes (ILM) in metallic Uranium, and the impact they have on thermal and electrical conductivity, and interstitial diffusion among others.

The workshop provided interesting potential for future cross-field collaborations. A presentation on the use of molecular dynamics in nuclear materials investigated radiation damage in Gadolinium pyrochlores, a potential storage material for nuclear waste, and a talk on actinide chemistry, investigated the effect of spin-orbit coupling and the oxidation state in f-element organo metallics.

REPORT ON SELECTED DISCUSSIONS:

Round Table: 'The challenges of linking fundamental theoretical modeling to practical applications in reactor core materials' moderated by Malcolm Stocks (ORNL). The purpose of the round table was to establish what kind of difficulties the community encounters when trying to obtain insight into nuclear materials, and how these difficulties can be overcome. The discussions pointed out a number of issues:

- Energetics, how important is the ground state electronic structure for real materials at reactor operation temperatures?
- Radiation damage implies huge kinetic energies, what relevance has the ground state.
- Methodologies well suited for studying the effect of correlations are not necessarily adequate for calculating the structural properties of materials. One might therefore consider using a combination of methodologies to study the different aspect of the nuclear materials.
- Benchmark for condensed matter results. Different LDA+U calculations for example depending on the double counting term used, or whether one uses Dudarev's Ueff=U-J compared to Liechtensteins independent U and J.
- Are pseudopotentials approaches useful for benchmarking, is FLAPW? Do we have good pseudopotentials for the actinides?

- VASP. Pseudopotential is a problem, as we loose accuracy since we are not solving the all-electron relativistic problem.
- Is it relevant to create a database for our results?
- How well is relativity accounted for in the different codes, and is it important to solve the Dirac equation as is done in molecular calculations? As far as the quantum chemists are concerned, the solid state community seems to be satisfied with a moderate level of accuracy.
- LSDA, GGA, have a non relativistic exchange correlation squeezed into relativistic code.
- The multiple minima that occur in LDA+U calculations, do they have a specific meaning.
- What can be done to achieve a simple phase diagram? Is a multiscale approach realistic? Should one instead use the atomic information as reference in for example CALPHAD, i.e. go from ab-initio to the phase diagram without the need for MD.
- Much more experimental evidence is required. This is a considerable problem, given the high costs due to the associated security and safety concerns. Even more problematic is the fact that high quality crystals of Bk, Cm, Am, etc., are no longer available.
- Suggested future experiments:
* Most experimental tools investigate surface: need more bulk measurements.
* Theoretical support for surface phenomena: leaching, surface reactions, absorption.
* Energy gaps of the dioxides: plenty of theory but no experiments!
* Need well defined surfaces before doing calculations.
* Magnetism of strongly disordered actinide systems. Are the observed effects due to the loss of periodicity or frustration?
* Theoreticians need pair correlation functions of the disordered structure.
* Bond energies and cohesive energies: no calorimetric results available.
* ARPES measurements on delta-Pu single crystals

From the talks it emerged that considerable progress has been made in the last couple of years concerning the fundamental description of correlations in nuclear materials. It also became clear however that the next step will have to involve a certain level of validation and verification of the different methodologies, both compared to each others and compared to experiment. With respect to experiment, it would appear that not enough capabilities exist worldwide to guarantee, that on one hand the required crystals can be grown, and on the other hand, due to the prohibitive costs associated with security arrangements around actinide experiments, crucial experiments can no longer be performed within an overseeable future. Rudy Konings especially underlined the need for experimental investigations for actinide materials under extreme conditions.

TO WHAT EXTENT WERE OBJECTIVES ACHIEVED:

The workshop largely fulfilled the outcomes it set out to achieve. The atmosphere at the workshop was excellent with very animated discussions. A number of impressive new results were presented concerning the electronic structure of actinide materials, and the objective of bringing these data to the attention of the experimental community was successfully achieved. Indeed it emerged that the theoretical investigations are well ahead of experiment on a number of relevant issues, and it would be crucial for the sake of verification that new advanced experiments could be set up as soon as possible especially for simple systems. For complex systems, experiments are much ahead of theory. Accordingly one of the main outcomes of the workshop was the suggestion by the experimentalist for theoreticians to become much more involved in proposing new experiments.

There was also a lot of interactions between theoreticians, namely developers of methods and users who want to have a good description of some specific properties. Due to a couple of rather late

cancellations, DMFT was underrepresented at the meeting. This was unfortunate, as this very advanced methodology has previously been very successfully applied to actinide materials.

SUGGESTIONS FOR NEW WORKSHOPS ON THIS TOPIC:

As can be seen from the roundtable discussion, despite some considerable progress the description of correlations in actinide materials is still far from complete, and a number of important stepping stones remain to be removed.

It became clear during the workshop that there is still not straightforward way for connecting completely the electronic structure calculations to the actual properties of nuclear materials. Whilst this subject matter was discussed in connection with the molecular dynamics and multiscale computing, no conclusions were reached on the subject matter. It would be highly relevant to have a follow up workshop, including additional focus on connecting electronic structure data to the properties of nuclear materials, by seeking contact with the thermodynamics modeling community.

APPENDIX B

JOINT CECAM WORKSHOP "EMPIRICAL METHODS IN SEMICONDUCTOR NANO-STRUCTURES DESIGN AND MODELLING"

S. Tomić, E.P. O'Reilly, M. Migliorato, and G.P. Srivastava

SCOPE OF THE WORKSHOP

Ab-initio calculations, although very reliable in prediction of structural properties of matter, still lack predicting power for material properties such as the energy gap, excited states and spin-orbit interaction, all of which are crucial for designing devices. Even on supercomputers the simulation box sizes are still limited to a maximum of a few 10^4 particles, whereas a typical nanocrystal or self assembled quantum dot can contain of order 10^6 atoms.

The scope of these Joint CECAM Workshops was:

1) The design and modelling of semiconductor nanostructured materials on length scales that are currently not accessible by ab-initio methods.

2) To review the state of the art of a variety of alternative semi-empirical modelling implementations, e.g. multiband k·p, empirical tight-binding (TB), valence force field (VFF), empirical pseudopotential method (EPM), etc..

3) To review parametrization strategies for semi-empirical methods and possibilities for interfacing with ab-initio methods.

Those semi-empirical methods that are being employed commonly in the research of the semiconductor nanostructures, exploit not just the accumulated knowledge of existing high quality experimental and ab-initio results, but also exploit the increased computational power and advanced computational methods available nowadays. As such, development of semi-empirical methods inherently facilitates synergy between experiment and theory. It was shown that proper implementations of semi-empirical methods are capable of delivering new levels of understanding and design for both materials and devices alike. Applications of such schemes span from designing emitters and absorbers used in conventional optoelectronics, through new architectures proposed in quantum information processing, to investigation of novel concepts for the design of future high efficiency solar cells.

The workshop convened a group of world leaders in the field of theory and computation (North America, Asia, and Europe) and invited them to present an overview of state-of-the-art advanced computation methods, parametrisation and parallelisation strategies (ACAM). Participants in this workshop were engaged in the intense discussion of the fundamentals and theory underlying the simulation methods used in this area of research. After this critically important methodological ground work was laid in the ACAM workshop, the participants travelled to Manchester to meet up with other researchers for the second workshop (STFC-Hartree). Participants at the second workshop reported state-of-the-art scientific results of simulations using the methods reviewed in the first workshop to analyze recent experiments and put forward new designs for advanced photovoltaic and other optoelectronic device applications. The interaction between the two workshops led to improved understanding of the approximations underlying these state-of-the-art simulation methods and new ideas on how they may be improved to provide a more realistic

representation of the experimental results and applications. The workshop included Post-graduate students, Post-doctoral researchers, as well as other researchers, e.g., experimentalists from academia and people from computational industry.

MAIN OUTCOME OF KEY PRESENTATIONS:

Main general outcomes of the Dublin event:

The Dublin meeting included presentations of the main semi-empirical methods for nanostructure electronic structure calculations from leading exponents of each of the techniques.

Gabriel Bester (MPI, Stuttgart) gave an overview of the capabilities both of empirical and semi-empirical pseudopotential techniques, describing how the method can fill the gap existing between ab initio approaches and continuum descriptions. Current challenges include the development of pseudopotentials based on DFT-LDA but corrected for the band gap and effective masses using empirical functions. Such methods are giving access to an accurate electronic quasiparticle structure and good agreement with a wide range of experiments.

Two presentations overviewed details of the tight-binding method. Mikhail Nestoklon overviewed the development of accurate parameterisations and their application to specific electronic structure issues, while Tim Boykin discussed several aspects concerning the physical and numerical aspects of tight-binding implementations, with special reference to the NEMO-3D and OMEN simulation packages.

Four talks discussed **k.p** methods. Firstly, Bradley Foreman described the construction of Nanostructure Envelope-Function Models from First Principles, justifying the accuracy of **k.p** models for a wide range of applications. Lok Lew Yan Voon and Stefan Birner addressed the Physics and Numerics of Multiband k.p Nanostructure Models, with Birner illustrating the use of the *nextnano3* simulation package to investigate Type-II Broken-Gap Superlattices. From a different perspective, Marc-André Dupertuis described how empirical methods can naturally take advantage of Symmetries in Nanostructures, linking the Physical Aspects to the Computational Aspects. Two final presentations addressed the implementation of highly efficient and scalable parallel eigensolver methods (Andrew Sunderland) and also the issues in approaching *ab-initio* electronic transport calculations in nanostructures (Giorgos Fagas).

Overall, the workshop satisfied well its aim to present an overview of state-of-the-art advanced computation methods, parametrisation and parallelisation strategies, providing a comprehensive overview and discussion of semi-empirical techniques and their implementation in advance of the Manchester meeting.

MAIN GENERAL OUTCOMES OF THE MANCHESTER EVENT

1) Need to change thinking in the community from "*my method is fast and with small memory footprint* that allows me to describe current systems of interest even on the desktop PC" to more adventurous such as "*my method is fast and with small memory footprint* that allows me to describe much larger systems on advanced computer architectures". In that context the codes used in the community have to more vigorously exploit available possibilities inside HPC solutions.

2) Clearly identified need for multi-length-scale approach in the modelling of semiconductor nanostructure devices.

3) Clearly identified need, and very positive and enthusiastic response, for regular CECAM workshops/tutorials in the area of the empirical methods in semiconductor nano-structures design and modelling. General consensus was that workshops and tutorials should alternate each year. Scientific outcomes:

F. Aniel, “k.p theory beyond standard 8-band theory parametrization strategies and its applicability in electronic and optoelectronic devices design” the main outcome was the development of continuum method, based on the envelope k.p method, that for the first time can describe entire first Brillouin zone with the same quality as the ab-initio GW theory

P. Hawrylak, “QNANO: Computational platform for electronic properties of semiconductor nanostructures” description of the methodologies used in the development of the empirical tight binding based QNANO code for electronic structure of semiconductor QDs. Particular strength was explanation of the surface effects as they were implemented inside TB and large configuration interaction (CI) based calculations of the charged excitons and multi-exciton complexes.

B. Witzigmann. “The non-equilibrium Green’s function formalism for optoelectronic devices”. Description of the quantum mechanical transport model based on the Green’s function formalism that goes beyond commonly adopted drift-diffusion model. The model is capable of describing many-body quantum system out of equilibrium, taking into account relevant scattering and coherence effects in the active region, as well as the effect of contacts that surrounds the active region. Model was demonstrated on the QW structure, while the challenging task remains to be expanded for QD structure and to include other nonradiative scattering processes like Auger recombination. Clear potential of the HPC solution for such demanding task was recognised here. Prof Michael Flatte. of Iowa University presented comprehensive review of his research which focussed on the application of the tight binding and k.p approach to the study of materials for spintronics applications. In particular it was refreshing to see how strong interaction between his group and the Scanning Tunnelling Microscopy group in Eindhoven worked closely on a project related to imaging of Mn impurities in GaAs hosts. Their combined theoretical and experimental work produced some very high impact factor publications in e.g. Nature (vol 442, p 436, 2006 & vol 462, 419-420 (25 November 2009)). It shows how close interaction among modelling and experimental groups is able to benefit both aspects of the research and produce internationally leading findings.

G. Allan. “Carrier multiplication in bulk and nanocrystalline semiconductors Mechanism, efficiency, and interest for solar cells”. Presentation discusses combined experimental/theoretical work on complex dielectric function of colloidal PbS, PbSe, and PbTe QDs. Based on ab initio GGA method he shown that values for lead chalcogenide QD remain close to the bulk dielectric constant. Based on this findings he examine carrier multiplication in led containing QD SCs. Carrier multiplication is known to occur in bulk semiconductors, but has been thought to be enhanced significantly in nanocrystalline materials such as quantum dots, owing to their discrete energy levels and enhanced Coulomb interactions. Contrary to this expectation, he demonstrate here that, for a given photon energy, carrier multiplication occurs more efficiently in bulk PbS and PbSe than in quantum dots of the same materials. Measured carrier-multiplication efficiencies in bulk materials are reproduced quantitatively using tight-binding calculations, which indicate that the reduced carrier-multiplication efficiency in quantum dots can be ascribed to the reduced density of states in these structures. Their combined theoretical and experimental work produced some very high impact factor publications in e.g. Nature Physics (vol 5, p 811, 2009).

REPORT ON SELECTED DISCUSSIONS, EG WERE THERE INTERESTING HINTS FOR NEW RESEARCH, NEW DEVELOPMENTS OR COLLABORATIONS?

The Round Table Discussion was opened with a brief presentation by Tomic on the aims and achievements of the Dublin-Manchester nodal CECAM Workshop. That led to a Round Table Discussion of following four main issues.

•Empirical methods for electronic structure calculations:
Successful empirical methods include (1) multi-band k.p methods, (2) envelop function methods, (3) tight-binding methods, (4) pseudopotential method, (5) molecular dynamics, (6) atomic-scale finite-element methods, and (7) hybrid methods, such as envelop function + CI, tight-binding + envelop function, tight-binding + k.p, tight-binding + MD, and DFT + Wigner function + non-equilibrium Green's function, etc.

• Software development:
Two important issues were raised. Firstly, different groups have been developing similar codes independently, without specifically aiming to make them portable. Secondly, with a few exceptions, most groups have been developing their codes on their local Windows environment, or Linux machines, or Linux clusters. The Workshop agreed for the need of (1) developing codes that can be cross-checked and utilized by other groups. The need for graphical interface capabilities was considered very important, particularly for use by industrial applicants. It was also felt that appropriate citations of codes would encourage, and prove beneficial to, program developers.

• Code interfacing for different length scales:
It was noted that programmers should adopt a standard scheme, with clear description, for (i) structure of system for study, and (ii) code inputs and outputs. It was also felt that a strategy should be developed for interfacing different codes, particularly codes written at different length scales. The Workshop agreed that there is a need for a motivated and dedicated group within CECAM or European Community to achieve these.

• Open innovation in scientific software engineering:
It was felt that the community should look forward to an open innovation in scientific software engineering. To make it a reality it would be important to (i) develop interface standards for linking various available codes, (ii) produce a data base, including version control, parameters, test runs, license, etc, (iii) produce bench marks and declare computational environment, and (iv) set up a network of spin-off companies and academic communities. The community should consider making an application under the FP7 scheme.

• Challenges ahead and role of CECAM
At the heart of all this is clear recognition of essential and specific physics problems with multiscaling being the important objective. The Workshop recognized the important role CECAM can play in assisting the academic community to achieve its objectives. In other words, financial support from CECAM is required to produce scientific and engineering innovation in multiscale collaborative research effort for technologically important applications for nanostructured materials. The Workshop identified two routes for making progress in this direction: (i) training of postgraduates and postdoctoral research fellows, and (ii) scientific meetings and exchanges of scientific personnel to discuss theories, algorithms, computational techniques, and development of collaborative computational projects and codes. CECAM meetings should be held in alternate years to make progress in these two directions.

TO WHAT EXTENT WERE THE OBJECTIVES OF THE WORKSHOP ACHIEVED (STRONG AND WEAK POINTS)

Our impression is that, overall, both meetings were generally well received. We believe however that the idea of a joint workshop, divided between two locations, is not a format to be recommended. There was a reasonable overlap in attendance between the two meetings – about 15 delegates attended both. This provided some continuity. However one Dublin invited speaker commented that some of the discussion in Manchester would have been a lot better informed if the Manchester delegates had heard all Dublin presentations. In addition, the joint meeting ran over 5 days, whereas if organised as a single workshop it would have been a 3- or 4-day meeting. Nevertheless it could still be worthwhile to organise further joint events in future between ACAM and CECAM-Daresbury, but it would probably be more appropriate to do so by holding meetings led in consecutive years by ACAM and by CECAM-Daresbury.

APPENDIX C

ADVANCES IN STRONG FIELD AND ATTOSECOND PHYSICS

Carla Faria (University College London)
Paul Durham (STFC Daresbury Laboratory)
Misha Ivanov(Imperial College London)
Wolfgang Sandner (MPI Berlin)
Jens Biegert and Maciej Lewenstein (Institute for Photonic Sciences Barcelona)

SCOPE OF THE WORKSHOP:

This workshop, sponsored by the Hartree Node of CECAM, aimed to bring leaders in the fields of quantum chemistry and condensed matter physics together with pioneers in strong field laser physics to assess where we are with the various theoretical and computational approaches to short pulse problems and discuss the best ways to progress from atoms to the more complex systems of current interest. In the past few years, considerable progress has been made in the attosecond imaging of matter and in the understanding of how complex systems interact with strong laser pulses. There exists, however, a great deal of controversy, especially with respect to an accurate treatment of the targets in intense fields. This discussion goes beyond the current scope of strong-field laser physics and moves towards the fields of quantum chemistry and condensed-matter theory.

The workshop ran for three full days, with over thirty speakers and approximately 100 participants. Full details of the workshop (including the programme and talks) can be found on the website: http://www.cse.scitech.ac.uk/events/Attosecond_Physics/ which will be preserved by the Hartree Node of CECAM and will be accessible through its own website.

MAIN OUTCOMES:

Overall outcomes

The workshop included most leading scientists worldwide in strong-field and attosecond physics. We also managed invite several reputed quantum chemists and condensed-matter theorists. We focused on theory, but also invited key experimentalists. From the presentations, it was possible to identify the following trends:

1) Molecular systems in strong fields: this topic consisted of a large percentage of the talks. In particular multielectron effects in molecules, their internal degrees of freedom, excitations, shape resonances and the treatment of molecules in strong fields beyond the single-orbital, single-electron approximation have been discussed. An appropriate treatment of heteronuclear molecules and the limitations of existing theories in these systems has also raised considerable debate.

2) Electron-electron correlation, laser-induced double and multiple ionization (NSDI, NSMI): this was in particular discussed in the context of attosecond streaking and free-electron lasers. Some talks also addressed physical mechanisms in NSDI, NSMI, such as excitation.

3) Novel strong-field approaches: currently, several groups worldwide are trying to develop new approaches in order to face challenges such as an adequate treatment of the binding potentials, the solution of the time-dependent Schroedinger equation with less numerical effort, or how to deal

with multielectron effects. Concrete examples are electron trajectories in a coupled coherent-state basis, complex scaling in order to solve the time dependent Schrodinger equation, Bohmian trajectories and several Coulomb-corrected versions of the strong-field approximation.

There was also a section on condensed-matter theory, which was largely acknowledged by the strong-field community. The interaction with condensed-matter physicists is viewed as a necessary step in order to make the transition to more complex systems.
The proceedings of the workshop will be published as a special edition of the Journal of Modern Optics.

The presentations are also accessible from the workshop website:

http://www.cse.scitech.ac.uk/events/Attosecond_Physics/

Computational Aspects

This workshop covered a problem in quantum dynamics where perturbation theory is inadequate and accurate computations are essential but difficult. The real computational issue facing the field lies in handling many-electron effects in realistic complex systems. The workshop addressed the question of whether a collaborative effort to assist in the development of the required new codes would be useful.

Training and Collaboration

We also intended that this workshop should provide training for young researchers. We succeeded in this this and managed to attract a large percentage of young researchers from all over Europe, and, to a lesser extent, from Asia and the US. They consisted of almost 70% of the overall participants. We held a large and lively poster session in which young researchers were able to exhibit and discuss their work.

Apart from that, we observed a very strong interaction between young researchers and leading lights in the field, which was favored by the informal atmosphere of the workshop. There was also a great deal of discussion between scientists of different European countries, which may lead to international collaborations in the future.

REPORT ON SELECTED DISCUSSIONS:

At the end of the workshop there was a wide-ranging panel discussion covering inter alia but in particular the following issues:

1) The need for strong field and attosecond techniques to be applied outside the domain of atomic and molecular physics, even though the problems within that field are fascinating in themselves and not yet solved.

2) The state of computational work in the field, ranging from semi-analytical and semi-phenomenological calculations to fully ab initio, multi-electron calculations requiring the most powerful parallel supercomputers. All parts of this computational spectrum are important and feed off each other.

Issue (1) shows the necessity of attosecond physicists, quantum chemists, and condensed-matter scientists working together in order to tackle the challenges ahead. Systems of interest have been identified as biomolecules, clusters and nanostructures, among others. An interdisciplinary effort between the above-stated communities will be necessary in order to describe and understand the interaction of such systems with strong fields.

Issue (2) implies that the two main schools of thought in theoretical strong-field phsyics, which prefers either the former or the latter approaches, must work together in order to make the field progress.

Apart from that, there was a high level of discussion throughout the workshop. Several speakers brought new and unpublished results in a highly informal atmosphere. This provided junior researchers with the great opportunity of having access to cutting-edge work. It also contributed to a strong interaction among scientists of different disciplines and European countries.

TO WHAT EXTENT WERE THE OBJECTIVES ACHIEVED:

We believe our objectives were met. The workshop itself was a very lively affair and was acknowledged by participants to be an exceptionally interesting one. Indeed, the number of participants was much higher than we originally expected and included many leading experimentalists as well as theoreticians. We also held a stimulating session in which leading condensed matter theoreticians talked about the ways in which strong field and attosecond physics could have an impact in their field. These condensed matter people found the workshop stimulating and their presence was appreciated by the strong field community.

SUGGESTIONS FOR NEW WORKSHOP ON THE TOPIC:

This is a "hot" field which will undoubtedly need further workshops as the range of applications expands.

APPENDIX D

REPORT ON THE METHODS IN MOLECULAR SIMULATION SUMMER SCHOOL 2010

1. ORGANISERS

The Methods in Molecular Simulation Summer School 2010 was held at Queen's University Belfast from 18 -27 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, P.M. Rodger, M. del Popolo and D. Willock. The local organisation was handled by M. Del Popolo, from the Atomistic Simulation Centre at Queen's University.

2. LOCATION AND FACIITIES

The School was held on the University campus, mostly at the Elmwood Learning and Teaching Centre (ELTC), with some sessions at the Peter Froggatt Centre. 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 XX 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. The numbers were significantly better than in 2009 – suggesting that some of the effects of the Credit Crunch had abated.

69 students attended. Those attending originated from 29 countries: 20 were from the host nation (UK) and 32 were from elsewhere in Europe.17 students were from outside Europe. A full list of participants, their nationalities and home institutions, is presented in Appendix 1.

4. SUPPORT

A registration fee of £390 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 the ELTC. 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 2009 and the student responses were taken into account, as far as was practical, in 2010.

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) Optimization methods. J. Harding
- (1) Potentials. J Purton
- (1) An overview of molecular simulation. M. Rodger.
- (2) Statistical mechanics. M. del Popolo.
- (4) Molecular dynamics. D. Willock.
- (1) Non equilibrium molecular dynamics. M. Rodger.
- (4) Monte Carlo. P. Camp.
- (1) Long range forces. J. Purton.
- (1) Hyperdynamics. J. Harding
- (2) Free energy methods. M. Rodger

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 2.

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:

Xavier Periole, University of Groningen: *Coarse grained molecular dynamics simulations of biomolecular systems.*

Emanuele Paci, University of Leeds: *Protein landscapes and mechanics*.

Syma Khalid, University of Southampton: *Coarse grained molecular dynamics simulations of DNA-lipoplexes.*

Christian Holm, University of Stuttgart: *Simulating charged macromolecules - what are the current challenges?*

Graeme Watson, Trinity College Dublin: *Periodic DFT modelling of defects in solid state materials.*

Michiel Sprik, University of Cambridge: *Design for a computational normal hydrogen electrode.*

A plenary session was also dedicated to short (15 min.) talks given by the students. The four talks selected this year were:

- **Matthew Bano** , University of Warick, UK: *A molecular simulation study of nano-particles of tricalcium phosphate.*
- **Sebastien Lectez**, IPNO, France: *Uranyl behaviour at the gibbsite-water interface: a Car Parrinello molecular dynamics study.*
- **Anikó Udvarhelyi**, MPI Medical Research, Germany: *Hydrogen bond dynamics in BLUF blue light photoreceptor proteins.*
- **Szilard Pall**, Stockholm University, Sweden: *Optimizing and Automating Parameter Selection for Free Energy Calculations Using Entropy Measures.*

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. Anikó Udvarhelyi (Max-Planck-Institute for Medical Research, Germany) for best short seminar, and Mr. Sela Samin (Ben-Gurion University of the Negev, Israel) 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).
- 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, 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.

8. THE FUTURE

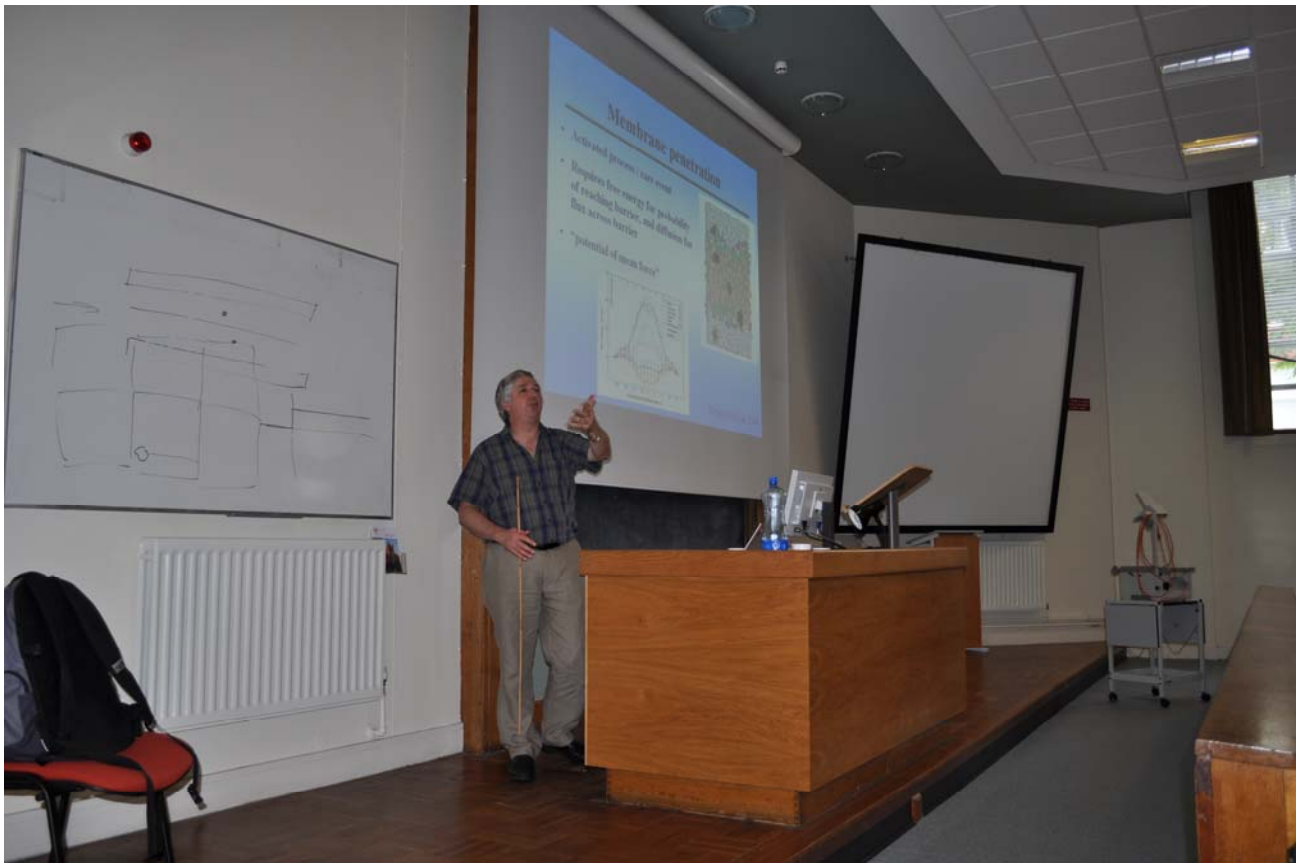
The Summer School in 2011 is also planned for Queen's University of Belfast. CCP5 will provide some funding and additional funding will be requested from CECAM.

9. GALLERY

The Summer School 2010 group photograph

Anikó Udvarhelyi receiving the award for best student lecturer

At the computing workshops



Mark Rodger, Lecturer

Appendix A -. Attendance List

Mr	Yahia	Chergui	Badji Mokhtar Annaba	Algerian
Ms	Lauren	Abbott	Pennsylvania State University	American
Mrs	Edita	Sarukhanyan	University of Salerno	Armenian
Mr	Aleksandr	Sahakyan	University of Cambridge	Armenian
Mr	Reinhard	Maurer	Karl-Franzens-Universität Graz	Austrian
Mr	Thomas	Lion	University of Edinburgh	British
Mr	Jeffrey	Armstrong	Queens University Belfast	British
Mr	James	Miller	University of Strathclyde	British
Ms	Laura	Leay	University of Manchester	British
Mr	Michael	Doig	University of Edinburgh	British
Mr	Christopher Andrew	Lee	Cardiff University	British
Ms	Selina	Nawaz	University of Manchester	British
Ms	Kate	Meadows	University of Warwick	British
Ms	Bruck	Taddese	University of Essex	British
Mr	Matthew	Bano	University of Warwick	British
Mr	Adam	Rigby	University of Manchester	British
Mr	Charles	Matthews	Edinburgh University	British
Mr	Hlengisizwe	Ndlovu	University of Leeds	British
Mr	James Alexander	Dawson	University of Sheffield	British
Mr	Chris	Pittock	University of Southampton	British
Mr	Luke	Debono	University of Bristol	British
Mr	Oliver	Warr	University of Manchester	British
Ms	Melissa	Cutler	University College London	British

Mr	Michael	Carter	University of Southampton	British
Mr	Jordan	Muscatello	Imperial College London	British
Mr	Wei	Ke	University of Stavanger	Chinese
Mr	Liang	Wu	Imperial College London	Chinese
Mr	Linjiang	Chen	The University of Edinburgh	Chinese
Ms	Lixian	Zhang	University of Basel	Chinese
Mr	Michal	Kolar	Academy of Sciences of the Czech Republic, v.v.i.	Czech
Ms	Rosanne	Zeiler	Universiteit van Amsterdam	Dutch
Mr	Hailu Kebede	Abay	Stavanger University	Ethiopian
Mr	Sébastien	Lectez	IPNO	French
Mr	Bastian	Ohler	University of Greifswald, Institute for Biochemistry	German
Mr	Manolis	Vasileiadis	Imperial College London	Greek
Ms	Maria	Anagnostopoulou	National Kapodistrian University of Athens	Greek
Ms	Anikó	Udvarhelyi	Max-Planck-Institute for Medical Research	Hungarian
Mr	Ramachandra Moorthy	Bhaskara	Indian Institute of Science	Indian
Mr	Rameshwar U.	Kadam	University of Berne	Indian
Mr	Gavin	Melaugh	Queen's University Belfast	Irish
Ms	Caoimhe	de Frein	University College Dublin	Irish
Mr	Sela	Samin	Ben-Gurion University of the Negev	Israeli
Dr	Simone	Sturniolo	University of Pavia	Italian
Mr	Filippo	Marozzelli	Cardiff University	Italian
Mr	Salvatore Mario	Cosseddu	University of Warwick	Italian
Ms	Carla	Jamous	Université d'Evry-Val-d'Essonne	Lebanese

Mr	Mantas	Gabrielaitis	Lancaster University	Lithuanian
Mr	Grisell	Diaz Leines	University of Amstedam	Mexican
Mrs	Katarzyna	Bartus	University of Silesia	Polish
Mr	Szymon	Daraszewicz	University College London (UCL)	Polish
Mr	Miroslaw	Cwiok	University College London	Polish
Mr	Krzysztof	Gorny	University of Silesia	Polish
Ms	Ana Catarina	Mendonça	Université Blaise Pascal	Portuguese
Ms	Mariana	Oliveira	Universidade de Aveiro	Portuguese
Ms	Marta	Batista	University of Aveiro	Portuguese
Mr	Szilard	Pall	Stockholm University	Romanian
Mrs	Uliana	Alekseeva	Forschungszentrum Juelich	Russian
Mr	Dmitriy	Rozhkov	Ural State University	Russian
Mrs	Milica	Lukic	RWTH Aachen University	Serbian
Mr	Stas	Bevc	National Institute of Chemistry	Slovene
Mr	Ausias-March	Calvo Minguillón	Universitat Politecnica de Catalunya	Spanish
Mr	Jordi	Ortiz de Urbina	Universitat Politecnica de Catalunya	Spanish
Mrs	Maria	Aznar Palenzuela	Universidad de Barcelona	Spanish
Ms	Gabriella	Jonasson	Université de Paris-Sud	Swedish
Mr	Kai-Ming	Tu	Academia Sinica	Taiwanese
Mr	Hung-Ru	Chen	University of Sheffield	Taiwanese
Ms	Nina	Ramrattan	Imperial College London	Trinidadian
Mr	Batu	Hunca	Trakya University	Turkish

	18 July	19 July	20 July	21 July	22 July	23 July	24 July	25 July	26 July	27 July
09.00		Overview of Molecular Simulation	Statistical Mechanics 2	Monte Carlo 2	Monte Carlo 3	Molecular Dynamics 4	Molecular Dynamics 5	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	Long Ranged Forces		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	Hyper - -dynamics Methods		Practical Session FPS BIO MESO	Practical Session FPS BIO MESO
12.30		*Lunch*								
14.00		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	Arrival	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 X. Periole	Research Seminar E. Paci	Student Research Seminars -> Posters	Research Seminar S. Khalid	Research Seminar C. Holm		Research Seminar G. Watson	Research Seminar M. Sprik	

APPENDIX E

Report on the KKR Hands-on Course STFC Daresbury Laboratory and Chester Mill Hotel
4-6 October 2010

This KKR Hands-on Course was already the 7th in the series of workshops organized since 2002, with three in Munich (Germany), two in Daresbury, one in Poznan (Poland) and one in Chicago (USA). The present course attracted 21 participants; four more potential participants had to cancel their attendance in the last week prior to the course, because the U.K. authorities refused to grant visas to them (two were from Russia, one from Ukraine and one of a Korean/Chinese origin, but working at Soleil in France). Among the participants there were both theoreticians and experimentalists, in approximately equal proportions, thus reflecting substantial interest in and demand for this workshop series. The participants were a very interesting bunch, with nine from Germany, three from the U.K., two each from France, Poland and Switzerland, and one each from Hungary, India and Slovenia.

The aim of the present course was to introduce theoreticians as well as experimentalists into the KKR band structure method and its use to calculate spectroscopic properties of magnetic solids (see the recent scientific highlight articles of the Psi-k Newsletter Numbers 97 and 101: http://www.psi-k.org/newsletters/News_97/newsletter_97.pdf and http://www.psi-k.org/newsletters/News_101/newsletter_101.pdf).

Accordingly, there were five one hour lectures dealing with the formal background and technical details of the KKR method (and its CPA extension). As seen in the programme and from abstracts, the lectures were selected so as to cover most broadly the whole range of topics underlying the theory and development of the code as well as to demonstrate a wide range of observables that can be calculated with it for a variety of complex materials. Specifically, they covered Density Functional Theory, multiple scattering theory and Green's functions, relativistic and many-body effects, spectroscopies, response functions, relaxations, forces and phonons, etc. The emphasis was put on a fully relativistic formulation supplying the basis for a treatment of dichroic effects in spectroscopy. The corresponding theory for magnetic dichroism in x-ray absorption, photoemission and related spectroscopy was reviewed. The tutorial lectures were also displayed on the posters, giving participants the opportunity to go once more through them and ask detailed questions. In addition, at the coffee breaks, the participants could also present posters on their own research projects and quite a few did, so there were some lively discussions around them.

The lectures were supplied with 10.5 hours of practical, hands-on, tutorials, divided in six individual sessions. They were devoted to applications making use of the Munich SPR-KKR program package that includes a graphical user interface called xband. The various calculations on clusters and ordered as well as disordered solids, which were meant in particular to introduce inexperienced users to the field, were guided by tutors. There were 10 lecturers and/or tutors available to provide participants with the theoretical and hands-on support.

The course took place in the Tower Seminar Room and the code was accessed via DL WiFi and NXClient, and run on the Munich University workstations. The participants used their own laptops to run NXClient on them. Daresbury Laboratory provided the wireless access to the internet and three spare PCs, supplied by the PC Support Group, which were on standby for those who might have had temporary problems with netbooks/laptops or had no laptops with. In the end all the PCs provided were used on occasions.

The course was run in a very relaxed manner. Every participant had a sheet of detailed exercises to go through at his/her own pace and explore the capabilities and difficulties with setting up the runs and analysing results. The graphical user interface xband was used for running the package for a variety of problems and processing results in a pictorial form. In case of difficulties or when anybody was interested to run some specific tasks of their own, tutors and lecturers were available to provide help. In fact, a couple of participants came to the course with specific projects in mind and were helped by the Munich group in setting up and starting the relevant, more complex, calculations as well as collaborations.

The accommodation was at the Mill Hotel and Spa in Chester and the bus transportation between Chester and Daresbury was managed by Anthony's Travel. The hotel was comfortable, situated on the canal, in close proximity to the Chester cathedral, and the hotel staff was very helpful and friendly. Altogether, it was a nice experience, especially that considering its location, the hotel was not too expensive and we would not hesitate to recommend it for similar events in future.

The workshop was very successful and its organization highly praised by all the participants. The organization was a common effort of the Munich group of Hubert Ebert and the Band Theory Group of CSE department, with Hubert Ebert and Zdzislawa (Dzidka) Szotek responsible for the general and scientific organization of the event. The whole administrative, local, organization was taken care of mainly by Shirley Miller and Wendy Cotterill. The registration process, hotel matters, transportation, workshop materials, and special care of participants (one was severely handicapped), restaurant meals, coffees and refreshments, etc., were very efficiently organized by Shirley and Wendy. We are very grateful to them for their professional help and dedication which greatly contributed to the overall success of the workshop.

Finally, we would like to acknowledge the sponsorship of the workshop provided by the Hartree Centre/CSE/CECAM node training and networking fund. The money received covered travel and accommodation for the lecturers/tutors, the conference dinner and lunches for everybody, coffee and refreshments, and bus transportation for the duration of the course. In addition, in order not to differentiate between the participants, we covered the difference in price between the two available hotel room types, namely the standard and executive ones, especially that we had no influence on the choice of the rooms. In reality, only 14 standard rooms were provided, with the rest of the executive type. The remaining costs were the administrative ones, covering workshop materials and times spent on the organization by Shirley Miller and Wendy Cotterill. On balance, the financial side of the course was well managed and we finished with a couple of hundred pounds still in pocket.

For completeness, below we supply a detailed programme of the workshop, abstracts of talks and posters, plus the lists of participants and lecturers and tutors.

Programme

Sunday, 3 October 2010

17:00-19:30 Arrival at the Mill Hotel & Spa, Chester and registration

Monday, 4 October 2010

08:00-8:45 Bus from hotel in Chester to Daresbury Laboratory

08:45-09:30 Preparation of Laptops and PCs

09:30-10:30 DFT: An Efficient Approach to the Quantum Many-Body Problem (E. Engel)

10:30-11:00 Coffee

11:00-12:00 Introduction to the KKR method (H. Ebert)

12:00-13:30 Lunch

13:30-15:30 Hands-on Session I
I
15:30-16:00 Coffee + Posters

16:00-18:00 Hands-on Session II

18:00 Return by bus to Chester Mill Hotel & Spa

19:00 Meet in Hotel Foyer for Conference dinner on the Cruising Hotel Boat

Tuesday, 5 October 2010

08:30-9:30 Bus from hotel in Chester to Daresbury Laboratory

09:30-10:30 Spectroscopy and many-body effects beyond LDA (J. Minar)

10:30-11:00 Coffee

11:00-12:00 Magnetic interactions and electronic transport (D. Ködderitzsch)

12:00-13:30 Lunch

13:30-15:30 Hands-on Session III

15:30-16:00 Coffee + Posters

16:00-18:00 Hands-on Session IV

18:00 Return by bus to Chester

Wednesday, 6 October 2010

08:30-9:30 Bus from hotel in Chester to Daresbury Laboratory

09:30-10:30 Calculation of Forces and Lattice Relaxations by KKR (P. Dederichs)

10:30-11:00 Coffee

11:00-12:00 Hands-on Session V

12:00-13:30 Lunch

13:30-15:00 Hands-on Session VI

15:00-15:30 Coffee

15:30-16:30 Future developments in SPRKKR/Closing remarks & licence issues, etc. (Hubert Ebert)

16:30 Workshop Close and Bus back to Chester

TALK ABSTRACTS

Density Functional Theory: An Efficient Approach to the Quantum Many-Body Problem

Eberhard Engel

Centre for Scientific Computing, J.W. Goethe-Universität Frankfurt am Main, Germany

After a brief introduction the foundations of density functional theory (DFT) are reviewed. This review starts with the Hohenberg-Kohn theorem, the basic existence theorem of DFT, which states that the (non-degenerate) ground state $|\psi_0\rangle$ of an interacting many-particle system is uniquely determined by the corresponding ground state density n_0, i.e. is a unique functional of n_0, $|\psi_0[n_0]\rangle$. As a consequence all ground state expectation values are uniquely determined by n_0, most notably the ground state energy $E_0=\langle\psi_0[n_0]|H|\psi_0[n_0]\rangle$.

The Ritz principle then leads to the statement that $E[n] := \langle\psi_0[n]|H|\psi_0[n]\rangle > E_0$ for all densities $n \neq n_0$. This allows the many-particle problem to be recast as a minimization of the energy functional E[n] with respect to n. In practice, this minimization is performed with the help of the Kohn-Sham (KS) procedure. In the KS approach an auxiliary non-interacting system with the same density as that of the actually interesting interacting system (i.e. n_0) is constructed by using a suitable effective, multiplicative, single-particle potential v_s (**r**). The crucial quantities of the KS method are the exchange-correlation (xc) energy functional E_{xc} [n] and the corresponding potential $v_{xc}[n](\mathbf{r}) = \delta E_{xc}[n]/\delta n(\mathbf{r})$. Together with the direct Coulomb potential produced by the density n (Hartree potential), it represents the electronic contribution to the total potential $v_s(\mathbf{r})$. If the exact functional $E_{xc}[n]$ is utilized, the resulting exact $v_{xc}[n](\mathbf{r})$ ensures that the non-interacting KS system reproduces the exact interacting density. Since the interacting density is not known a priori, $v_s(\mathbf{r})$ has to be calculated in a self-consistent fashion, in close analogy to the Hartree-Fock scheme. Once the exact density has been obtained by solution of the self-consistent KS equations, insertion of n_0 into $|\psi_0[n]\rangle$ in principle allows to evaluate any quantity of interest.

The talk will proceed with summarizing various extensions of the basic theorems, which allow the application of the KS method to magnetic and relativistic systems. The resulting (relativistic) spin-density functional theory (R)SDFT is based on additional density variables which are required for a

unique determination of the ground state, such as the magnetization density. Moreover, in the relativistic situations the KS equations are of Dirac type. Next, the standard approximations for $E_{xc}[n]$ are introduced, the local density approximation (LDA) and the generalized gradient approximation (GGA).

The derivation of these approximations starts from the homogeneous electron gas, for which the density dependence of E_{xc} is known. Corrections to the density dependence of the homogeneous system can then be constructed from the response of the electron gas to a weak perturbation.

Some prototype results obtained with the LDA and GGA will motivate a third line of approximations, the so-called implicit density functionals. In this case E_{xc} is expressed in terms of the KS single-particle states which, in turn, are unique functional of the density, so that one stays within the framework of standard DFT.

The multiplicative $v_{xc}[n](\mathbf{r})$ corresponding to such orbital-dependent functionals has to be calculated by solution of an integral equation, the so-called optimized (effective) potential method (OPM). The prototype orbital-dependent functional is the exact exchange of DFT, which is nothing but the Fock expression written in terms of KS states. Use of the exact exchange resolves several long-standing problems of the LDA and GGA. As an example the talk will address the anti-ferromagnetic (type II) phases of the transition-metal monoxides MnO, FeO, CoO and NiO at T=0K. In contrast to the local density (LDA) and generalized gradient approximation, the exact exchange (combined with LDA correlation) correctly yields insulating ground states for all four compounds. The values for the band gaps and magnetic moments obtained with this parameter-free first principles method are in good agreement with the experimental data, in spite of the single-particle approach used. Finally, it will be shown that orbital-dependent functionals also yield much improved correlation potentials.

Introduction to the KKR method

Hubert Ebert

Ludwig-Maximilians University of Munich, Germany

The talk will give a first introduction to the Korringa-Kohn-Rostoker (KKR) method for electronic structure calculations. The method differs from most other methods as it describes the electronic structure not in terms of energy eigenvalues and eigenfunctions - i.e. band structure E(k) and Bloch wave functions in case of ordered solids - but in terms of the electronic Green's function, that can be seen as a generalized, spatial dependent density of states function. This has many advantages that can be exploited when dealing with systems without three-dimensional translational or Bloch symmetry as surfaces, lattice imperfections or impurities, clusters deposited on surfaces, disordered alloys and so on. In addition it supplies a very powerful basis to deal with any kind of response function as for example electric conductivity or magnetic susceptibility that can be expressed in a very clear and flexible way in terms of the electronic Green's function. This also applies when one is dealing with spectroscopy properties or many-body corrections to the local density approximation. In practice the KKR method implies application as multiple scattering theory, essentially as it is used for example to discuss EXAFS. Accordingly, the major ideas of multiple scattering theory will be explained together with its use for calculating the electronic Green's function. These will be illustrated by corresponding examples. In addition results of a number of applications of the KKR method will be shown that demonstrate the extremely wide applicability of this method.

Spectroscopy and many-body effects beyond LDA

Jan Minar

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Spectroscopy (like for example photoemission) is an extremely important experimental tool providing information on the electronic structure of the probed system. A strong feature of the SPR-KKR package is the possibility to calculate various spectroscopies like for example X-ray photoemission, X-ray absorption, magnetic Compton profiles etc., including in particular matrix

elements and spin-orbit coupling induced effects. In this lecture we will introduce the basic ideas and overview the various spectroscopic features of the SPR-KKR package. Some of the spectroscopies are surface sensitive, like for example angle-resolved photoemission. Here, we will also introduce the tight-binding KKR mode which is suitable for calculations of 2D-structures and surfaces. In addition an introduction to the LSDA+U and LSDA+DMFT methods will be discussed because these methods are suitable for spectroscopical calculations of correlated materials.

Magnetic interactions and electronic transport within KKR

Diemo Ködderitzsch

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The lecture will focus on magnetism and transport properties of solids. In particular, these aspects will be treated in close conjunction with the spin-polarized relativistic version of the KKR. The talk motivates and introduces the relativistic formalism (Dirac equation, orbital magnetism, spin-orbit interactions) as implemented in the Munich KKR package. Using the former framework various applications will be given (magnetic interactions, mapping on Heisenberg-Hamiltonian, Liechtenstein approach, etc). Examples will be presented which demonstrate how the information gathered from the first principles calculation can subsequently be used. The second part of the lecture focuses on how to calculate transport properties of randomly disordered solids using a multiple scattering approach. A brief introduction to the Kubo formalism along with its implementation will be outlined. Again applications as, e.g., determining the anomalous- and spin-Hall conductivity, respectively, will illustrate the framework.

Calculation of Forces and Lattice Relaxations by KKR

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We review the calculation of forces and lattice relaxations using the KKR Green function method. We apply a modification of the Hellmann-Feynman theorem by rigidly shifting the core-electrons with

the nuclear coordinate and by calculating the valence electrons and semicore electrons self-consistently by the full potential KKR method with typically ℓ_{max} = 4. The results are in good agreement with forces calculated from total energy differences. For the calculation of relaxations basically two methods exist. For small relaxations an algebraic U-transformation can be used describing the shift of the structural Green function from the unshifted to the shifted position. For larger relaxations (> 5-10 % of nearest neighbour distance) one can start from a supercell which contains both the shifted and the unshifted positions. For larger relaxations the division of space into non-overlapping Voronoi cells around each atom has to be adjusted to the relaxations. We present calculations for metallic systems, where the relaxations are usually very small, as well as for semiconductor systems where much larger relaxations can occur.

POSTER ABSTRACTS

Theoretical Study of the Electron Spin Motion in MgO/Fe(001)

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Spin-dependent electron reflection measurements on MgO/Fe(001) show that the spin-polarization direction of the reflected electrons is very sensitive to small coverages of MgO . We think that a normal relaxation of the Fe surface due to formation of O-Fe bonds is responsible for this behaviour. Indeed, an Xray diffraction analysis of the MgO/Fe(001) interface showed that already sub-monolayer coverages of MgO are able to induce a significant relaxation of the Fe surface layer [1]. In order to support this hypothesis spin-dependent low energy electron diffraction calculations have been performed. By using a LMTO (Linear Muffin-Tin Orbitals) code and introducing the atomic potential in a SPRKKR model (Spin-Polarized Relativistic Korringa-Kohn-Rostoker) we were able to simulate the spin-dependent electron reflection experiments. An increase in relaxation, i.e. the first Fe interlayer distance is increasing, corresponds to an increase in MgO coverage. Although the

absolute values in the calculations differ quite significantly from the experimental ones at certain energies, the global structures as well as the tendency for increasing MgO coverage are reproduced.

[1] H.L. Meyerheim et al., Phys. Rev. B **65**, 144433 (2002).

Electronic structure of intermetallic Ti-Al: A First principle study

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We report the first principle study of the electronic structure in the intermetallic TiAl alloy. The calculations are performed using SPR-KKR and FP-LAPW methods. In order to examine the charge transfer, using SPR-KKR method theoretical momentum densities are also calculated for the alloy and constituent metals. The present study reveals a charge transfer from Al to Ti atom on alloy formation.

[1] V. Ragghavan, Al-Ti (Aluminum-Titanium), J. of Phase Equil. and Diff. 26 (2005) 171-72.

[2] C. Angeles-Chavez, G. Rosas, J. Reyes-Gasga and R. Perez, Structural characteristics of intermetallic Ti-Al-Cu alloys, ATM 3 (2001) 1-6.

[3] The Munich SPR-KKR package, version 5.4, H. Ebert et al., http://olymp.cup.uni-muenchen.de/ak/ebert/SPRKKR.

[4] P. Blaha, K. Schwarz,G. K. H.Madsen, D. Kvasnicka, J. Luitz (2001) WIEN2K, an augmented plane wave + local orbitals program for calculating crystal properties edited by KSchwarz, http://www.wien2k.at.

Near field corrections for total energy calculations

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Total energy calculations need an accurate treatment of the Madelung energy, especially for open systems and systems with strong atomic distortions. We want to consider such systems with our KKR-GF method. For this purpose we implemented three different schemes of near-field corrections: direct evaluation, shifting of the bounding sphere and solution of the Poisson's equation of Weinert. Therefore we discuss implementation and convergence problems and compare the results for different examples.

Implementation of nonequilibrium Green's functions in the screened Korringa-Kohn-Rostoker method

Steven Achilles

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Electronic structure calculations are nowadays an important tool for investigating and predicting physical effects of new materials on the nanometerscale. In particular, the electronic transport properties are of great interest. In experiments the electronic transport properties of quantum systems are investigated even under applied bias. The resulting voltage drop has a strong influence on the electronic properties and is sensitive to the geometry of the system. For example in a tunnel junction one expects a simple linear voltage drop over the barrier but for atomic-sized contacts, nanowires, or molecules the spatial dependence of the voltage drop is unknown. To account for systems under bias we extended our Korringa-Kohn-Rostoker Green's function method [1] to the Keldysh formalism [2]. The method was developed for two different types of geometries, planar junctions and embedded clusters. Both implementations include the self-consistent treatment of systems under external bias using the nonequilibrium charge density. We present ab initio results of voltage drops and current-voltage characteristics for the two different types of geometries.

[1] R. Zeller, P.H. Dederichs, B. Ujfalussy, L. Szunyogh, and P. Weinberger, Phys. Rev. B 52, 8807 (1995); P. Zahn, I. Mertig, R. Zeller, and P.H. Dederichs, Mat. Res. Soc. Symp. Proc. 475, 525 (1997).
[2] C. Heiliger et al., J. Appl. Phys. 103, 07A709 (2008).

Band structure calculations for $EuCo_2X_2$ (X=Ge,Si) and EuM_5 (M=Cu,Ni)

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Band structure calculations of metallic systems with known divalent and trivalent Eu have been performed using FP-LAPW and FPLO DFT band structure codes. In the case of $EuCo_2X_2$ valence band photoemission spectra are compared with calculation results. Correlations were taken into account within Around Mean Field (AMF) and Fully Localised Limit (FLL) approach. Several exchange-correlation potentials were compared in the case of EuM_5. Equilibrium lattice parameters in EuM_5 were calculated and magnetic properties at these lattice parameters were studied. Antiferromagnetic supercell has been constructed for $EuCo_2X_2$.

X-ray absorption spectroscopy, linear and magnetic circular dichroism in dilute magnetic oxides

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X-ray absorption spectroscopy (XAS) using linear (XLD) and circular (XMCD) polarized light offers a powerful toolbox of element-specific structural, electronic, and magnetic probes that is especially well suited for studying $Zn_{1-x}Co_xO$ (Co:ZnO) to unravel its intrinsic properties. We demonstrate that as long as phase separation or excessive defect formation is absent, Co:ZnO is paramagnetic and a combination of experiment and simulation of the XLD allows quantifying the amount of dopant atoms incorporated on substitutional lattice sites [1]. We can establish quantitative thresholds based on four reliable quality indicators using XAS; samples which show ferromagnet-like behaviour fail to meet these quality indicators, and complementary experimental techniques indeed prove phase

separation [2]. Careful analysis of XAS spectra is shown to provide valuable information of secondary phases in a highly sensitive, non-destructive manner.

[1] A. Ney et al., Phys. Rev. Lett. 100 (2008) 157201.

[2] A. Ney et al., New J. Phys. 12 (2010) 013020.

KKR Hands-on Workshop

4 - 6 October 2010

Chester and Daresbury

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