Report on the first joint CECAM-PSI-k Tutorial
"Quantum Simulation of Liquids and Solids"
CECAM, Lyon,
November 07 2005 to Nov. 18 2005

http://www.cecam.fr/index.php?content=activities/pastTutorials&action=details&wid=23

This course aimed at giving an introduction in the simulation of electronic structure in condensed phase materials, solids and liquids. A first series of lectures was devoted to the basics of Density Functional Theory and to the solution of the electronic structure problem in solids using plane wave basis sets and Green's function technique. This part of the tutorial was based on the book by R. M. Martin "Electronic Structure. Basic Theory and Practical Methods" (Cambridge University Press, Cambridge, 2004). A second series of lectures was focused on the simulation of liquid systems using *ab initio* Molecular Dynamics. These also include an introduction to advanced techniques 1) to simulate reactive processes in liquids 2) to couple quantum simulations to classical molecular dynamics (so-called QM/MM).

The tutorial was organized by Evert Jan Meijer (University of Amsterdam, Netherlands), Igor Abrikosov (Linköping University, Sweden), and Rodolphe Vuilleumier (Université Pierre et Marie Curie, France). The invited lecturers include Sergei Simak, Sam Shallcross (Linköping University, Sweden), and Elske Leenders (University of Amsterdam, Netherlands). The morning sessions were lectures introducing the methods and in the afternoons there were computer exercises in which these methods were applied. During these practical classes the students run a few simulations using existing packages, like CPMD, KKR-ASA and VASP, to apply the techniques discussed in the morning lectures and be acquainted with these packages. In addition, a miniworkshop was organized, where 5 participants presented results of their research. Unfortunately, because of the unrests in Lyon, some evening classes and week-end sessions had to be shortened or even canceled. The course did not assume any previous knowledge in molecular simulations. However, elementary knowledge in quantum physics was assumed. Support for participation (travel and lodging) was available via the Marie Curie Action “MolSimu”.

The tutorial was heavily overbooked, by factor of two. In the end, 37 participants (42 including conference organizers and invited lectures) were selected, representing 12 European countries, Bulgaria (3), Czech Republic (5), France (5+1 organizer), Germany (2), Italy (3), Netherlands (organizer and lecturer), Russian Federation (3), Spain (1), Sweden (6 participants, 1 organizer, 2 lecturers), Switzerland (3), Turkey (2), United Kingdom (3).

The need for such type of tutorials is due to the fact that a distribution of computer codes for the electronic structure calculations goes much faster than the transfer of the corresponding knowledge for the underlying theory. Unfortunately, though the codes have become really user friendly, the theory on its own has not. Therefore using the codes is not fool proof. In particular, errors produced by non-experienced users, as well

as their unmotivated high expectations, may accumulate, and create overall negative impression for the possibilities of the electronic structure theory. The organizers see a real and clear necessity to **educate qualified experts in the field**. Important here is that the educational activities should be directed to qualified teaching of the underlying theory rater than (exclusively) to instructions for the use of particular codes (click this button, enter this parameter). As tutorial organizers, we were very pleased that most of participants shared this view point, showed real interest in both, lectures and computer classes, asked relevant questions, and followed the subject. Moreover, participants who had experience with the codes in question, acted very efficiently as instructors to their fellow students with less experience in the electronic structure calculations. In particular, help from Tobias Marten, Christian Göransson, Arkady Mikhaylushkin, and David Andersson is greatly appreciated by the tutorial organizers. In summary, as teachers, we were very pleased with audience responses. A student questionnaire carried out upon the completion of the tutorial also showed that the absolute majority of the participants gave positive evaluation to the tutorial. We note, that this is a remarkable result, as participants represented in approximately equal amounts two different communities, the solid state band theory (Psi-k) and molecular simulations (CECAM). Obviously, the experience gained in this first joint tutorial opens a new way for collaborations and contacts between these two communities.

Finally, we would like to acknowledge help from CECAM in organizing the tutorial, Berend Smit (CECAM Director), Emilie Bernard and Caroline Werlingshoff (administrative assistants), and Fred Barmes (computer administration). The BGFM code used for the present tutorial that implements the KKR-ASA method was developed by I. A. Abrikosov, A. V. Ruban, and H. Skriver. We are grateful to Prof. J. Hafner for the permission to using Vienna Ab initio Simulation Package (VASP) for our computer classes.

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Program

Session 1, Igor A. Abrikosov (IAA), Sergei I. Simak (SIS), and Sam Shallcross (SSh).

Monday, November 7

9.00 - 9.45 General information and introduction into the tasks of the tutorial (IAA)
10.00-10.45 Basics of the electronic structure theory (IAA)

10.45 - 11.15 Coffee

11.15-12.45 Periodic solids and electronic bands (SIS)

12.45 - 14.00 Lunch

14.00-14.45 Introduction into computational tasks (SSh and IAA)
15.00-18.00 Computer classes: calculations of lattice parameters, compressibilities, and structural energy differences across transition metal series using KKR-ASA method.

Tuesday, November 8

9.00 - 10.45 Many-body problem and density functional theory (IAA)

10.45 - 11.15 Coffee

11.15-12.45 Self-consistent band structure calculations for periodic solids (SIS)

12.45 - 14.00 Lunch

14.00-18.00 Computer classes: Calculations of mixing and ordering energies in alloys, changes of the electronic structure upon order-disorder transition, magnetic moments in alloys, band gaps in semiconductors, simple estimates of Curie temperature of bcc Fe, etc. using KKR-ASA method.

Wednesday, November 9

9.00 - 9.45 Introduction into the multiple-
10.00-10.45 scattering theory (IAA)

10.45 - 11.15 Coffee

11.15-12.00 Introduction into the pseudopotential
12.15-12.45 and PAW technique, part 1 (SIS)

12.45 - 14.00 Lunch

14.00-18.00 Computer classes: optimization of c/a ratio in hcp transition metals and calculations of total energy along the Bain path using VASP.

Thursday, November 10

9.00 - 10.45 Green's function technique and the coherent potential approximation (IAA)

10.45 - 11.15 Coffee

11.15-12.45 Introduction into the pseudopotential and PAW technique, part 2 (SIS)

12.45 - 14.00 Lunch

14.00-18.00 Computer classes: determination of interatomic interactions in random alloys using KKR-ASA-CPA method and estimation of the contribution due to local lattice relaxations to the alloy total energy using special quasirandom structure method and VASP.

Friday, November 11

9.00 - 10.45 Linear scaling methods within the Green's function approach (IAA)

10.45 - 11.15 Coffee

11.15-12.45 Alloy phase stabilities from Monte-Carlo simulations (SSh)

12.45 - 14.00 Lunch

14.00-18.00 Computer classes: calculation of order-disorder transition temperature by means of Monte-Carlo simulations

Session 2, Evert Jan Meijer (EJM), Rodolphe Vuilleumier (RV) and Elske Leenders (EL).

Monday 14th

09h00-09h45 Recapitulation on DFT, Plane Waves, Pseudo-Potentials… simple CPMD examples - Part 1 - (Evert Jan Meijer)

10h00-10h45 Recapitulation on DFT, Plane Waves, Pseudo-Potentials… simple CPMD examples - Part 2 -

10h45-11h15 *Coffee*

11h15-12h00 Optimization - Part 1 - (Rodolphe Vuilleumier)

12h15-13h00 Optimization - Part 2 -

13h00-14h00 *Lunch*

14h00-15h00 Introduction practicals: input, output, analysis tools vmd, cube-files (Elske Leenders)

15h00-16h00 Computer Classes

16h00-16h30 *Coffee*

16h30-18h00 Computer Classes

Tuesday 15th

09h00-09h45 ab initio Molecular Dynamics - Part 1 - (EJM)

10h00-10h45 ab initio Molecular Dynamics - Part 2 -

10h45-11h15 *Coffee*

11h15-12h00 Atoms and Molecules - Part 1 - (RV)

12h15-13h00 Atoms and Molecules - Part 2 -

13h00-14h00 *Lunch*

14h00-16h00 Computer Classes: Generating PPs & Atoms & Molecules: optimization (EL)

16h00-16h30 *Coffee*

16h30-18h00 Computer Classes: Generating PPs & Atoms & Molecules: optimization

Wednesday 16th

09h00-09h45 Properties calculation(RV)

10h00-10h45 Linear Response (RV)

10h45-11h15 *Coffee*

11h15-12h00 Infrared and Raman Spectroscopy (RV)

12h15-13h00 Time-dependent density functional theory (RV)

13h00-14h00 *Lunch*

14h00-16h00 Computer Classes: Liquid Simulation: proper md, wannier centers, liquid structure, reactivity (EL)

16h00-16h30 *Coffee*

16h30-18h00 Computer Classes: Liquid Simulation: proper md, wannier centers, liquid structure, reactivity

Thursday 17th

09h00-09h45 QM/MM techniques - Part 1 - (Ivano Tavernelli)

10h00-10h45 QM/MM techniques - Part 2 -

10h45-11h15 *Coffee*

11h15-12h00 Reactivity - Part 1 - (EJM)

12h15-13h00 Reactivity - Part 2 -

13h00-14h00 *Lunch*

14h00-16h00 Computer Classes: Analysis electronic structure (EL)

16h00-16h30 *Coffee*

16h30-18h00 Computer Classes: Analysis electronic structure

Friday 18th

09h00-09h45 Quickstep - Part 1 - (Matthias Krack)

10h00-10h45 Quickstep - Part 2 -

10h45-11h15 *Coffee*

11h15-12h00 Advanced topics - Part 1 - (RV)

12h15-13h00 Advanced topics - Part 2 -

13h00-14h00 *Lunch*

14h00-16h00 Computer Classes: Introduction to CP2K (EL+MK)

16h00-16h30 *Coffee*

16h30-18h00 Computer Classes: Introduction to CP2K

Miniworkshop: presentations from participants.

POSSIBLE TRANSFORMATION PATHS CONNECTING THE $C11_b$, C40 AND C54 STRUCTURES IN $MoSi_2$

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Abstract

We suggest three transformation paths between the ideal $C11_b$, C40 and C54 structures of transition-metal disilicides. These three structures can be regarded as different stackings of identical planes of atoms. Each suggested transformation path consists in shifting these atomic planes in three directions. The shift of planes is described by one parameter *p, p* lies in the interval *<0;1>*. Along each path, we calculate the total energy of $MoSi_2$ as a function of *p*. Our results confirm the structural order $C11_b$ -C40-C54 in $MoSi_2$. The $C11_b$–C54 path exhibits the largest energy barrier, 2.5 eV/f.u (f.u. means the formula unit). The energy barrier of the $C11_b$–C40 path is lower, 1.7 eV/f.u. and finally the energy barrier of the C40–C54 path is the lowest one, 1.4 eV/f.u.

Magnetism of AlPdMn quasicrystal from first principles.

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Electron and magnetic properties of 1/1 approximant of quasicrystalline AlPdMn are studied by means of density functional theory and all-electron PAW potentials. Magnetic moments of Mn atoms are analyzed in dependence on Mn concentration and its chemical environment. We have found that large local magnetic moment of Mn atoms is appeared at 8 at.% of Mn though the local Stoner criteria was not fullfiled. Boron and lithium substitution of Al atoms in AlPdMn is

resulted in enhanced local magnetic moment for Mn atoms. The (Al)s-p-(Mn)d hybridization of atomic orbitals is important for the onset of magnetic moment of Mn atoms. The total energy calculations were carried out for a number of magnetic configurations in order to determine energetically more preferable magnetic ordering of Mn atoms in the system.

Ab initio studies of Mn-impurity in wurtzite-type GaN

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Investigation of electron and magnetic properties of transition metal impurities in semiconductors is of great interest due to ferromagnetic ordering of these impurities with the Curie temperature around 110K and even higher.
In this work the electron structure and magnetic properties of Mn impurities in wurtzite-type GaN are studied by means of density functional theory and first principles pseudopotentiales and in dependence on concentration and chemical environment of Mn atom. We have shown that magnetic moment of Mn atom in the GaN strongly depends on whether the impurity atom is substitutional or interstitial. The magnetic moment of Mn atom on the Ga-site of GaN is 4μ_B. Analysis of partial density of states (DOS) has shown that there is 100\% spin polarization of carriers in (Ga, Mn)N and the main contribution to the DOS at the Fermi level originates from Mn impurity.

Discontinuously Reinforced Aluminum Made by Novel Ion Exchange Process

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Scientists around the world have already assigned an important role to Nanotechnology and Materials recognising them as the driving forces for the future of the world economy. This results from the simple premise that using building blocks with dimensions in nanosize makes it possible to design and create new materials with unprecedented flexibility and improvements in their physical properties. We focused on the special case of Discontinuously Reinforced Aluminium (DRA) metal matrix made by a novel solid state exchange process of magnesium ions in magnesium aluminate spinel with aluminium. This process leads to DRA composites consisting of a nanosized, highly stable and nearly insoluble aluminium oxide phase into an aluminium matrix, with greatly enhanced elastic stiffness, yield strength, ductility and resistance to high temperature deformations. Surface to volume ratio of the spinel particles strongly influences reaction kinetics in the initial composite. Reaction rate appears to increase remarkably when the particle size is decreased. To achieve better properties, a good interface between the two phases of the composite is

of paramount importance. Unfortunately, nowadays the nature of the interactions involved in metal-ceramics adhesion is still far from being understood in detail. While the cohesion of metals originates from the delocalization of electrons, oxides predominantly exhibit localized ionic bonding. An interface between a metal and an oxide, therefore, requires some sort of transition between these fundamentally different type of interatomic interaction. We investigated the hypothesis that the reinforcement efficiency is very high due to chemical processes taking place at the coherent matrix/reinforcement interface. Our aim is to reveal, from a theoretical point of view, whether and how the ion exchange process can yield enhanced interface adhesion and therefore represent a viable strengthening and toughening mechanism.

Molecular Dynamics with Quantum Transitions Using Time-Dependent Density Functional Theory

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