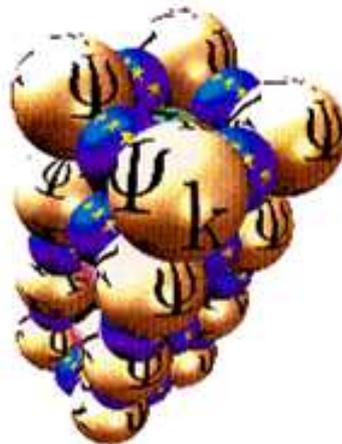

AB INITIO (FROM ELECTRONIC STRUCTURE) CALCULATION OF COMPLEX PROCESSES IN MATERIALS

Number 86

April 2008



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Sponsored by: UK's CCP9
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1 Editorial

This is the first newsletter of a substantially reduced size. We write about it in one of the sections below. Presently, we are in a transition period, trying to switch from treating the Psi-k newsletters as a kind of a systematic database/archive of all the activities that Psi-k as a community is involved with to a shorter publication of mostly an informative content. The database/archive feature is to be taken over by the Psi-k Portal, which is also intended to replace the Psi-k mailing list. So, in addition to all the information already available on the Psi-k Portal, in this Psi-k newsletter we have only one short report, a few meeting and position announcements, several abstracts of newly submitted or recent papers and, most importantly, a scientific highlight by N. Skoulidis and H. M. Polatoglou (*Thessaloniki, Greece*) on ”**Modeling semiconductor QDs**”. We would like to encourage our readers to read below about the Psi-k Portal and how to join it, as well as about changes that we plan for the future newsletters. We would also like to invite everybody to send us their comments and suggestions regarding the Psi-k Portal and the format of the future Psi-k newsletters. In addition, we would like to thank all the people who contribute to the newsletters, helping in making them useful and informative for the whole Psi-k community.

The Psi-k has a home page on World Wide Web (WWW). Its *Uniform Resource Locator* (URL) is:

<http://www.psi-k.org/>

Please submit all material for the next newsletters to the email address below.

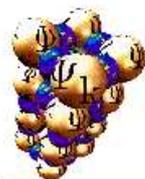
The following email addresses, which remain in operation, are repeated for your convenience, and are the easiest way to contact us.

	function
psik-coord@dl.ac.uk	messages to the coordinators, editor & newsletter
psik-network@dl.ac.uk	messages to the whole Ψ_k community

Dzidka Szotek, Martin Lüders and Walter Temmerman
e-mail: psik-coord@dl.ac.uk

2 General News

2.1 Call for Subscriptions to Psi-k Portal



Psi-k Portal

The Psi-k Portal, as already explained in the Psi-k Newsletters No 83 and 85, is a new interactive facility available on the Psi-k web pages (<http://www.psi-k.org>). From the Psi-k Portal it is possible to send e-mails to all the members of the Portal. The idea is that in the near future the Psi-k Portal replaces the existing Psi-k mailing list, so that no human intervention will be necessary to distribute announcements to the Psi-k community. Recall, that the Psi-k mailing list is moderated, and every e-mail has to be physically approved by the Psi-k coordinator to be distributed. Also, only the members of the Psi-k Portal will be allowed to distribute announcements. Right now, the original Psi-k mailing list is a member of the Portal, and so the announcements uploaded to the Portal are also distributed across the list, although the latter may happen with some delay, due to the need of approval. This unfortunately causes that multiple copies are sent to those who are members of both the Psi-k Portal and Psi-k mailing list. To eliminate these multiple copies, from June 2008, the Psi-k mailing list will be removed from the Portal, and the only announcements distributed will be exclusively those by the Psi-k Portal members to the Portal members. While the Psi-k mailing list will not be destroyed, we will no longer approve any e-mails sent to the list. Thus, it is in the interest of all the members of the Psi-k mailing list to join the Psi-k Portal as soon as possible. At the moment we have about 2100 names on the Psi-k mailing list, but only just over 400 names on the Psi-k Portal.

To join the Psi-k Portal go to the Psi-k web page at

<http://www.psi-k.org>

and choose the option 'Login to Ψ_k Portal', and then 'New Account'. While filling in all the necessary spaces choose your full e-mail address as your 'id', followed by a suitable password. Of course, you need to fill in all the requested fields while joining the Portal. If your account was successfully created, then next time you access Psi-k Portal you just simply login to it with your 'id' and password, which will put you into 'My workspace'. To have access to all the information and functionality, while logged in to your workspace (My Workspace) you need to choose 'PSI-K' option by clicking on it. In the 'PSI-K' you will have the whole menu at your disposal and then you will be able to upload, view, etc., any information. Please be patient when uploading information, like announcements, reports, etc., as it is rather slow, and by pressing on a 'submit' button, you keep on uploading the same information several times. The result being that your information gets send to all the members of the Psi-k Portal as many times as you

have pressed 'submit'. Of course, you have a choice either to distribute your information or just upload it to the Portal, but not distribute it by e-mail. In order not to have the information distributed you need to choose for the 'E-mail Notification' the option 'None'. For example, the workshop/meeting reports should not be distributed by e-mail, but should be uploaded to the Portal for 'keeps' and an easy reference for everybody.

Regarding announcements, at the moment there is only one choice for announcements, but in the nearest future we will have separate choices for the job and meeting announcements for an easier overview. Also, it is advisable to give a time limit for the announcements so that after the job was filled or a meeting happened, they would get automatically removed from the Portal. Another possibility is that people uploading the announcements remove them at the time chosen by them to be appropriate.

A useful calendar tool on the Portal shows the dates of upcoming workshops and conferences. Users of the Psi-k Portal can enter their own workshops directly into the calendar.

In case of any problems with the uploads of reports, job/workshop announcements, etc., please do not hesitate to contact us and ask for help.

Note that the existence of the Psi-k Portal facility will also lead to changes in the format of the forthcoming Psi-k newsletters, as elaborated upon in the section below.

2.2 Changes to the Psi-k Newsletters

We envisage the Psi-k Portal not only as a replacement for the Psi-k mailing list and a means of distributing announcements to the Psi-k community, but most importantly also as a kind of an easy-access database where announcements and reports can be stored. Until now, all the announcements and reports have always been included into the Psi-k newsletters, sometimes making them prohibitively large. In future, however, we shall keep full meeting/workshop reports, including abstracts of presented papers and lists of participants, only on the Psi-k Portal, while in the newsletters only short summary reports, including programmes, will be published. Therefore, we ask the meeting organizers to upload to the Psi-k Portal their complete workshop/meeting reports, i. e., containing also a programme of the meeting, list of participants, and abstracts of presented papers, in addition to a one page summarizing report. The latter, namely the short report, plus the workshop programme, should also be sent, as a LaTeX file, to `psik-coord@dl.ac.uk` to be included in the Psi-k newsletters.

Regarding the position and meeting announcements, in the newsletters we shall only include the ones that are submitted to the `psik-coord@dl.ac.uk` in the LaTeX format files. In fact, any information that anybody wants to have published in the newsletters will have to be submitted to us exclusively in the LaTeX format. All the relevant templates for the newsletter submissions are available on the web at

<http://www.psi-k.org>

in the Psi-k Newsletter No 67.

We plan that, in addition to a short editorial, the future newsletters will most of all contain scientific highlights, abstracts of newly submitted or recent papers, short meeting reports, position/meeting/book and other announcements that might be of interest to the whole Psi-k community. Also, we would like to invite our readers to contribute short comments and reports on some interesting events, happenings, etc., anything that you think might be of interest to the whole community. In addition, we would welcome any further suggestions from the community, regarding the future format of the Psi-k newsletters.

3 News from UK's CCP9 Programme

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

3.1 2008 CCP9 Conference Announcement

"New Developments in Electronic Structure"

4-5 September, 2008



Robinson College, Cambridge, U. K.

Organisers

Prof James Annett (University of Bristol, U. K.)

Prof Mike Payne (University of Cambridge, U. K.)

Prof Walter Temmerman (Daresbury Laboratory, U. K.)

General Information

The scope of the conference is all ab-initio and materials specific calculations of the electronic properties of condensed matter systems such as metals, semiconductors, magnets, superconductors, biological systems, minerals, surfaces. etc. Topical areas incorporated in the conference are magneto-electronics, catalysis, nanotechnology, high temperature superconductors, novel wide band gap semiconductors, etc. Techniques covered by the conference include QMC, DFT, GW, TDDFT, DMFT, SIC-LSDA, LSDA+U. We welcome all contributions dealing with the solution of the Schrodinger/Dirac equation in condensed matter systems.

Tentative list of speakers includes:

Hardy Gross (Berlin, Germany) (tbc)

Steve Louie (Berkeley, USA) (tbc)

Nicola Marzari (MIT, USA)

David Ceperley (Chicago, USA) (tbc)
Gustavo Scuseria (Houston, USA)
Hubert Ebert (Munich, Germany)
Leon Petit (Aarhus, Denmark)
Dario Alfe (London, U. K.)
Neil Drummond (Cambridge, U. K.)
Jonathan Yates (Cambridge, U. K.)
Massimiliano Stengel (Santa Barbara, USA) (tbc)

Important Dates

Deadline for submission of abstracts: by 1st of July, 2008

Registration and fees paid: by 15th of July 2008

Talks and Posters

We welcome all your contributions. Please submit an abstract by 1 July 2008.

Registration & Fees

We will soon open an online registration on the CCP9 web pages

(<http://www.ccp9.ac.uk>). Fees are £200 and include two nights accommodation (Thursday and Friday night), all meals and refreshments.

3.2 Report on CASTEP Training Workshop



September 17-21, 2007

Sponsored by STFC Centre for Molecular Structure and Dynamics and
CCP9

Organised by CASTEP developer's Group

<http://www.tcm.phy.cam.ac.uk/castep/workshops.html>

The CASTEP 2007 training workshop was held at the University of York from September 17 to 21, 2007. The aim was to provide an introduction at the postgraduate student level to plane-wave DFT simulation using the CASTEP code. Thirty-one students attended. Thanks to a contribution of £4500 from CCP9 we were able to fully refund the half-board accommodation and attendance costs (£500) of 8 residential students and the attendance charges for a further 2 non-residential (£220). The Centre for Molecular Structure and Dynamics at STFC contributed £5000, and a further contribution of £1400 from the Institute of Physics.

The organisers and lecturers were

Dr Stewart Clark	(Durham University)
Dr Matt Probert	(York University)
Dr Matt Segall	(BioFocus DPI/Cambridge University)
Dr Phil Hasnip	(York University)
Dr Jonathan Yates	(Cambridge University)
Dr Keith Refson	(STFC Rutherford Appleton Laboratory)
Professor Mike Payne	(Cambridge University)
Dr Johan Carlsson	(Fritz-Haber Institute, Berlin)
Alexander Perlov	(Accelrys Inc)

and the topics covered included

- Fundamentals of density functional theory
- DFT in the solid state, kpoints, Brillouin zones
- Plane-wave basis sets
- Pseudopotentials, ultrasoft, norm-conserving and self-consistent

- Simulations using plane-wave DFT
 1. Geometry optimisation
 2. Molecular dynamics in various ensembles
 3. Quantum path-integral molecular dynamics
 4. Ab-initio lattice dynamics and spectroscopy
 5. Dielectric properties
 6. Electric fields, Berry phase and Wannier functions
 7. NMR properties and chemical shifts
- Ab-initio beyond the LDA and GGA, EXX, hybrid functionals
- Practical aspects of ab-initio calculations
- Application to structural and surface calculations
- Convergence - how to get accurate results

A full programme and downloadable lecture notes are available on the WWW at <http://www.tcm.phy.cam.ac.uk/castep/workshops.html>.

This was a “hands-on” workshop divided into roughly 50% lectures in the morning and 50% practical sessions with exercises to demonstrate the lecture material in the afternoon. Parallel computing power was provided on an Opteron cluster at Durham University, which enabled the students to complete some reasonably challenging computations in the afternoon sessions. One afternoon session was devoted to a demonstration of the Materials Studio GUI by Alexander Perlov of Accelrys Inc., and exercises using this. Other afternoon sessions were devoted to exercises on molecular dynamics, pseudopotentials, NMR chemical shift and other topics.

During the workshop many students took the opportunity to discuss their own research with the lecturers, and the informal impression was that almost all students enjoyed the course and were able to derive considerable benefit from the lectures and practical exercises. Despite the lower than anticipated attendance, this was a successful and productive event.

4 Workshop/Conference Announcements

4.1 Summer School on Nanomagnetism and Spintronics

Prague, Czech Republic

September 5–13, 2008

Sponsors

Psi-k Training in Computational Nanoscience
Towards Atomistic Materials Design (Psi-k)

Organizing committee

I. Turek – Charles University, Prague
J. Kudrnovský – Academy of Sciences of the Czech Republic, Prague
P. Bruno – European Synchrotron Radiation Facility, Grenoble

<http://cmd.karlov.mff.cuni.cz/Spintronics-2008/>

Purpose

The purpose of the Summer School is to provide a qualified overview on the rapidly developing areas of spintronics, magnetoelectronics and nanomagnetism. The lectures will be oriented on last year PhD students and postdoctoral researchers in the field of *ab initio* electronic structure theory. The scientific scope will include important topics, such as diluted magnetic semiconductors, hybrid systems, spin-dependent transport properties, effects of finite temperatures, spin dynamics, magnetism of nanostructures, relativistic effects, and electron correlations.

Most of these topics will be covered by theorists, mainly by experts in the community of first-principles electronic structure calculations, to which majority of the participants will probably belong. However, theoretical lectures will be followed by experimental ones wherever possible.

Program

The school program will last eight days (September 6–13) with six hours of lectures each day. There will be no parallel lectures. Sufficient time for discussion will be planned at the end of all lectures as well as during coffee breaks. Poster sessions will be organized in order to give the participants an opportunity to present results of their own research.

Registration

Applicants should follow instructions on the school website. The pre-registration form has already been opened, the registration form will be available in the beginning of April. The deadline for registration is June 15. The registration fee will be around 350 euro, which covers lectures, accommodation and meals during the days with lectures. The number of students is

limited to 100. Partial financial support (subject to nationality restrictions for the participants) is available.

Lecturers

A. Fert	Unité Mixte de Physique, CNRS/Thales, Palaiseau, France
P. Grünberg	Forschungszentrum Jülich, Germany
G. E. W. Bauer	Delft University of Technology, The Netherlands
H. Ebert	Ludwig-Maximilian-University Munich, Germany
B. Velický	Charles University, Prague, Czech Rep.
G. Bihlmayer	Forschungszentrum Jülich, Germany
C. Carbone	Instituto di Struttura della Materia, Trieste, Italy
T. Jungwirth	Institute of Physics, Acad. Sci. Czech Rep., Prague
B. Gallagher	University of Nottingham, England
G. Bouzerar	Institut Néel, Grenoble, France
C. Ederer	Trinity College, Dublin, Ireland
D. Wortmann	Forschungszentrum Jülich, Germany
I. Mertig	Martin-Luther-University, Halle, Germany
J. Mašek	Institute of Physics, Acad. Sci. Czech Rep., Prague
J. Fabian	University Regensburg, Germany
K. Výborný	Institute of Physics, Acad. Sci. Czech Rep., Prague
J. Sinova	Texas A&M University, USA
P. Weinberger	Computational Nanoscience Vienna, Austria
S. Biermann	CPHT, École Polytechnique, Paris, France
P. J. Kelly	University of Twente, The Netherlands
O. Eriksson	Uppsala University, Sweden
S. Sanvito	Trinity College, Dublin, Ireland
L. Sandratskii	MPI for Microstructure Physics, Halle, Germany
P. Bruno	European Synchrotron Radiation Facility, Grenoble, France
B. Barbara	CNRS Grenoble, France
J. Wunderlich	University of Cambridge, England
S. Blügel	Forschungszentrum Jülich, Germany
W. Wulfhekel	University of Karlsruhe, Germany
P. Jelínek	Institute of Physics, Acad. Sci. Czech Rep., Prague

Contact

Ilja Turek – turek@ipm.cz

Josef Kudrnovský – kudrnov@fzu.cz

School leaflet (in A4/A3 format) is available at the school website.

4.2 CECAM/Psi-k Workshop on Quantum Wires

CECAM, Lyon, 9-12 June, 2008



Lyon, France

We would like to draw your attention to the joint CECAM/Psi-k Workshop on "Structural, electronic and transport properties of quantum wires" that will be held at CECAM, in Lyon (France) from 9th to 12th of June 2008.

The workshop attendance is open to everybody. No fee is required. Besides 20-25 invited talks we will have a poster session which we encourage you to join.

Further details (including the provisional list of invited speakers) can be found at:

<http://www.cecarn.org/workshop-189.html>.

Interested participants should send an e-mail to any of the organizers, including a brief abstract in case of applying for a poster presentation.

We think this is going to be an excellent chance for people working with quantum and nanowires to gather for a few days and we look forward to meeting you in Lyon.

Organizers

Riccardo Rurali (Riccardo.Rurali@uab.cat)

Mads Brandbyge (MBr@mic.dtu.dk)

Xavier Blase (xavier.blase@grenoble.cnrs.fr)

5 Job Announcements

Ph. D. Position: “Multi-scale study of the charge effect on the diffusion in silicon”

Commissariat à l'Énergie Atomique (CEA), Grenoble, France

Recent and future electronic devices are of nanometric dimensions and it raises new challenges, that deal with the understanding of the thermodynamic of silicon-germanium alloys. It is also related to the diffusion of impurities, dopants or points defects in these alloys. Numerical studies can bring information [1] on these phenomena, especially through a multi-scale approach, using precise computations at atomic level and statistical simulations at bigger scales. Possible applications would be atomistic simulations of realistic transistor channels, made of silicon, or silicon-germanium, doped, under elastic constraints and electric field.

Up to now, only model behaviours have been investigated, without electric field or non-homogeneous constraints. The attendee will investigate such aspects at atomistic levels. The study will be made at two scales. The first is about the effect of the electric field on dopants using *ab initio* methods. The second deals with Monte Carlo simulations of dopant diffusion under electric and elastic fields.

This work will start on methods already developed in the laboratory, and presents also challenging theoretical and programming aspects. These questions concern the capability of *ab initio* calculations to treat charged defects. It implies the investigation of a new methodology that circumvents the issue of charged replica in periodic calculations, using results obtained by the BigDFT European project [2]. On the bigger scale, developments will be done to include the elastic and electric fields in the Monte Carlo program of the lab. Simulations should also take into account charge transfers during migration. Finally a mathematical treatment of rare events should be investigated to obtain long physical times for the diffusion study in Monte Carlo.

Attendee should have a strong background in solid physics, quantum mechanics, statistical physics and a keen interest in programming.

For further information or submission of application, please contact:

Damien Caliste or Thierry Deutsch
Laboratoire L_Sim - CEA Grenoble / INAC / SP2M
17, avenue des Martyrs
38054 Grenoble Cedex 9 FRANCE
Tel.: +33 4 38 78 01 72 Fax: +33 4 38 78 51 97
e-mail: damien.caliste@cea.fr or thierry.deutsch@cea.fr
Internet: http://inac.cea.fr/L_Sim

References

- [1] D.Caliste and P.Pochet, “Vacancy-assisted diffusion in silicon: a three temperatures model”, Phys. Rev. Lett. 97, 135901 (2006).
- [2] BigDFT: http://inac.cea.fr/L_Sim/BigDFT and L.Genovese, T.Deutsch, A.Neelov, S.Goedecker and G.Belkin, “Efficient solution of Poisson’s equation with free boundary conditions”, J. Chem. Phys. 125, 074105 (2006).

Ph.D Position in spin transport/spin-injection in semiconductors

Department of Physics, University of York, York, UK

Public demand for increasingly faster and smaller electronic devices, such as computers, requires that more and even smaller transistors are packed on every chip. This has led to the birth of nanotechnology and, more recently of the nanotechnology field called ‘spintronics’. Here not only the charge, but also the spin – another fundamental property of electrons and holes – is used to design device functionalities. Among the potential benefits of spintronics devices is the possibility of computers in which the same unit is used for computation and storage, of lower power consumption, of miniaturisation, and more generally the possibility of designing conceptually new devices which mix old functionalities with completely new ones.

The basis of spintronics is understanding the spin dynamics. Unfortunately key issues such as how to inject a current of spins in a semiconductor, how to sustain it across the interfaces of the different materials forming the devices, which materials/nanostructures are best and what lengths a current of spin can travel in a specific material are still open questions.

This project aims to master the principles underlying the spin dynamics, with particular attention to applications such as nanocircuits and their components. Objectives are to fully understand spin transport, diffusion and injection into semiconductors. These properties are fundamental for developing semiconductor and hybrid (metal/semiconductor) spintronics devices.

This is an EPSRC-funded studentship, with a stipend in line with EPSRC directions.

We are looking for highly motivated students, possibly with a background in solid state physics and good computational skills.

For more details please contact Dr Irene D’Amico, ida500@york.ac.uk,

<http://www-users.york.ac.uk/~ida500/>

Applications will be accepted until the position is filled.

To apply please go to our Application Procedure at

http://www.york.ac.uk/depts/phys/gsp/app_proc.htm

or email phys-grad-admin@york.ac.uk for an application pack. If applying please inform Dr D’Amico (ida500@york.ac.uk).

Ph. D Position in Theoretical Physical Chemistry

LAMBE UMR CNRS 8587

Laboratoire Analyse et Modélisation pour la Biologie et l'Environnement
Université d'Evry val d'Essonne - Paris - FRANCE

Direct Molecular Modelling of ElectroSpray Processes in Mass Spectrometry

This thesis is aimed at modelling and understanding the electrospray technique at an atomistic level. This work is part of a global laboratory project devoted to theoretically describe electrospray/mass spectrometry experiments (ESI/MS). Electrospray - daily used in experiments performed in our laboratory to produce ions in the gas phase which are subsequently analysed by mass spectrometry - is supposed to produce ions in a "soft way". This technique is thought to preserve the ion liquid phase structure, after evaporation of all the water molecules. Many experiments show that this is not true, though. The thesis proposed here will try to answer the following question: during the electrospray process, are liquid phase structures preserved in the gas phase (where they are characterised by mass spectrometry) ?

To understand the mechanism producing ions in the gas phase from a system initiated in an aqueous medium, we will set up molecular dynamics simulations using a classical description of interactions between the different particles (quantum chemistry calculations will help in the parameterisation procedure) and Newton dynamics (including dissipation). The laboratory has a home made molecular dynamics code (MDVRY). In the dynamics algorithm, electric field and pressure gradient effects will be added. Also ab initio molecular dynamics will be performed as reference for classical simulations.

During the thesis, the PhD student will gain skills in different domains of molecular modelling: quantum chemistry, ab initio and classical molecular dynamics simulations and force field development. Furthermore, he/she will be involved in developing our MDVRY molecular dynamics code, such that he/she will also gain skills in scientific programming. The supervisors are specialists in atomistic modelling and theoretical physical-chemistry.

The thesis will be held in France near Paris (about 40' from downtown by city train) in a laboratory with researchers from CEA (Saclay), CNRS and University (Evry). A master in chemistry or physics is required.

The thesis is founded by CEA and the gross monthly salary will be around 1990 euro during the first two years and 2050 euro the third year. Applications should be done as quickly as possible and the thesis will begin in september/october 2008.

Contacts: Dr. Riccardo Spezia & Prof. Marie-Pierre Gaigeot

Emails : riccardo.spezia@univ-evry.fr & mgaigeot@univ-evry.fr

Web sites : www.lambe.univ-evry.fr/rspezia & www.lambe.univ-evry.fr/mpgaigeot

Post-Doctoral position in Theoretical Physical Chemistry

LAMBE UMR CNRS 8587

Laboratoire Analyse et Modélisation pour la Biologie et l'Environnement
Université d'Evry val d'Essonne - Paris - FRANCE

Development of a Valence Bond force field for molecular dynamics investigations of environmental effects on the peptide bond

One-year Post-Doctoral position funded by PRES-UniverSud-France : joint project between LCP-Laboratoire de Chimie Physique (Orsay) and LAMBE-Laboratoire Analyse et Modlisation pour la Biologie et l'Environnement (Evry). Both labs are located south of Paris, 40 minutes train from Paris downtown. The candidate will work in both labs. Salary will be around 2000 Euros/month.

The candidate should have a PhD in Chemistry or Physics, with experience in Quantum Chemistry and/or Molecular Dynamics. Experience in scientific programming is also required. Position opened, to be fulfilled ASAP & preferentially no later than october 2008.

We are looking for a Post-Docotoral candidate who will be in charge of the development of a Valence Bond-type (VB) or 'matrix' force field in order to characterise solvent induced vibrational effects in the O=C-N-H peptide bond.

In such a force field, the elements of the matrix representation of the system Hamiltonian are approximated by simple analytical expressions similar to the one used in usual or 'scalar' force fields. A simple analytical form is needed in order to investigate peptides of increasing size and complexity (up to proteins) in solution. In addition, a matrix form with coupling between states of different charge distributions is needed particularly to study environmental effects on hydrogen bonded systems, proton transfers, chemical reactions, chromophore/solvent dynamics and vibrational dynamics in relation with IR/Raman spectroscopy. These applications are generally beyond capabilities of typical classical force fields.

The developped VB force field will be implemented in a molecular dynamics (MD) code developed at the University of Evry (MDVRY). This code is particularly well suited for classical MD of biomolecules.

Contacts: Prof. Isabelle Demachy & Prof. Marie-Pierre Gaigeot

Emails : isabelle.demachy@lcp.u-psud.fr & mgaigeot@univ-evry.fr

Web sites : pagesperso.lcp.u-psud.fr/demachy & www.lambe.univ-evry.fr/mpgaigeot

Postdoctoral Position in Materials Modelling in Paris

A post-doc position is available at LEM (ONERA-CNRS) : "Transport properties modeling of MAX phases". The position is available immediately for one or two years.

Further information can be found at:

<http://www.onera.fr/formationparlarecherche/propositions/pdoc-mas2008-01.pdf>

Applications with resumes, list of publications, and name (address) of referees should be sent to (preferable by email):

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6 Abstracts

Self-trapped interstitial-type defects in iron

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(4) *Service de Recherches de Métallurgie Physique,
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Abstract

Small interstitial-type defects in iron with complex structures and very low mobilities are revealed by molecular dynamics simulations. The stability of these defect clusters formed by non-parallel '110' dumbbells is confirmed by density functional theory calculations and it is shown to increase with increasing temperature due to large vibrational formation entropies. This new family of defects provides an explanation for the low mobility of clusters needed to account for experimental observations of microstructure evolution under irradiation at variance with the fast migration obtained from previous atomistic simulations for conventional self-interstitial clusters.

(Approved for publication in *Phy. Rev. Lett.*)

Contact person: lmalerba@sckcen.be | <mailto:lmalerba@sckcen.be>

Platinum-group and noble metals under oxidizing conditions

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*Fakultät Physik, Universität Wien,
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Abstract

Platinum-group and noble metals play an important role in catalysis, for total oxidation as well as for partial oxidation reactions. Only in recent years advances in microscopic, spectroscopic and computer simulation techniques have made it possible to investigate the interaction of oxygen with the metallic substrates at an atomistic level. We present an overview on the formation of adsorption structures and surface oxides on Rh, Pd, Ag, Cu and Pt surfaces, with particular focus on the phase diagrams calculated from first-principles thermodynamics. The low-index (111), (100) and (110) surfaces as well as selected high-index surfaces have been considered. We predict the stability of novel structures such as the $c(4\times 6)$ on Cu(100) and the α -PtO₂ trilayer on Pt(100). The knowledge of the Gibbs free surface energies allows to predict the adsorbate-induced changes in the thermodynamic equilibrium shape of metal nanoparticles. At low oxygen chemical potential, corresponding to clean surfaces, the (111) facets dominate the particle shape, with a significant contribution from (100) facets. But even under these conditions a small fraction of the overall surface corresponds to more open facets. As oxygen adsorption sets in, their contribution becomes larger. At high oxygen partial pressures, surface oxides form on the platinum-group metals. They do not only display different chemical properties than the metal, but also determine the exposed surface orientations of the particles. The latter effect might play an important role for the catalytic activity of transition metal nanoparticles.

J. Phys.: Condensed Matter, in press

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Surface Metal-Insulator Transition on a Vanadium Pentoxide (001) Single Crystal

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Abstract

In situ band gap mapping of the $V_2O_5(001)$ crystal surface revealed a reversible metal-to-insulator transition at 350–400 K, which occurs inhomogeneously across the surface and expands preferentially in the direction of the vanadyl (V=O) double rows. Supported by density functional theory and Monte Carlo simulations, the results are rationalized on the basis of the anisotropic growth of vanadyl-oxygen vacancies and a concomitant oxygen loss driven metal-to-insulator transition at the surface. At elevated temperatures irreversible surface reduction proceeds sequentially as $V_2O_5(001) \rightarrow V_6O_{13}(001) \rightarrow V_2O_3(0001)$.

(Phys. Rev. Lett.: <http://link.aps.org/abstract/PRL/v99/e226103>)

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Counting Electrons Transferred through a Thin Alumina Film into Au Chains

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Abstract

Low-temperature STM measurements combined with density functional theory calculations are employed to study the adsorption of gold on alumina/NiAl(110). The binding of Au monomers involves breaking of an oxide Al-O bond below the adatom and stabilizing the hence undercoordinated O ion by forming a new bond to an Al atom in the NiAl. The adsorption implies negative charging of the adatom. The linear arrangement of favorable binding sites induces the self-organization of Au atoms into chains. For every ad-chain, the number of transfer electrons from the support is determined by analyzing the node structure of the corresponding highest occupied molecular orbital.

(Phys. Rev. Lett.: <http://link.aps.org/abstract/PRL/v100/e096802>)

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First principles calculation of spin-interactions and the magnetic ground states of Cr trimers on Au(111)

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Abstract

We present calculations of the magnetic ground states of Cr trimers in different geometries on top of a Au(111) surface. By using a least square fit method based on results obtained by means of a fully relativistic embedded-cluster Green's function method first we determined the parameters of a classical spin vector model containing second and fourth order interactions. The newly developed method requires no a priori assumed symmetry constraints, therefore, it is throughout applicable for small nanoparticles of arbitrary geometry. The magnetic ground states were then found by solving the Landau-Lifshitz-Gilbert equations. In all cases considered the configurational energy of the Cr trimers is dominated by large antiferromagnetic nearest neighbor interactions, while the biquadratic spin-interactions provide the second largest contributions to the energy. We find that an equilateral Cr trimer exhibits a frustrated 120° Néel type of ground state with a small out-of-plane component of the magnetization. Furthermore we show that the Dzyaloshinsky-Moriya interactions determine the chirality of the magnetic ground state. In cases of a linear chain and an isosceles trimer collinear antiferromagnetic ground states are obtained with the magnetization lying parallel to the surface.

(Close to final) manuscript available at [arXiv:0802.3113](https://arxiv.org/abs/0802.3113)

Onset of Magnetic Order in Strongly-Correlated Systems from *ab initio* Electronic Structure Calculations: Application to Transition Metal Oxides

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Abstract

We describe an *ab initio* theory of finite temperature magnetism in strongly-correlated electron systems. The formalism is based on spin density functional theory, with a self-interaction corrected local spin density approximation (SIC-LSDA). The self-interaction correction is implemented locally, within the KKR multiple-scattering method. Thermally induced magnetic fluctuations are treated using a mean-field ‘disordered local moment’ (DLM) approach and at no stage is there a fitting to an effective Heisenberg model. We apply the theory to the 3d transition metal oxides, where our calculations reproduce the experimental ordering tendencies, as well as the qualitative trend in ordering temperatures. We find a large insulating gap in the paramagnetic state which hardly changes by the onset of magnetic order.

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Improving the charge density normalization in Korringa-Kohn-Rostoker Green-function calculations

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Abstract

The truncation of angular momentum expansions in the Korringa-Kohn-Rostoker Green-function method introduces a charge normalisation error and disallows calculation of the Fermi level and the charge density in a consistent manner. It is shown how this error can be compensated by Lloyd's formula, in particular if this formula is applied to normalize the Green function everywhere along the complex energy contour used for the integration of the charge density. The advantages of the improved normalization over the conventional one are illustrated by density-functional calculations for CrAs, the dilute magnetic semiconductor $\text{Ga}_{1-x}\text{Mn}_x\text{N}$ and a $\text{Si}_{12}\text{Fe}_8$ multilayer. It is shown that only the improved normalization leads to correct integer values of the magnetic moments in the half-metallic state of CrAs and $\text{Ga}_{1-x}\text{Mn}_x\text{N}$ and to a correct band alignment of Fe and Si states in the multilayer.

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7 SCIENTIFIC HIGHLIGHT OF THE MONTH: "Modeling semiconductor QDs"

Modeling semiconductor QDs

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Abstract

A method to model semiconductor QDs and their properties is presented and various QDs and their properties are investigated in detail. The method consists of a suite of programs for building atomistic models, relaxing them and obtaining their electronic properties such as electronic states, wavefunctions of selected states, and optical properties. A powerful visualization tool is included to present the various properties and to perform additional analysis concerning the structure of QDs. Two systems of high current interest are studied: Ge QDs embedded in Si, and GaN QDs embedded in AlN. Special interest is placed in the study of strains as they are naturally present and their distribution can be altered through the choice of the various structural parameters. We show that strains are important in the determination of the electronic properties and consequently can be used to produce QDs with tailored properties.

1 Introduction

Control of matter at the atomic level has opened whole new ways of producing structures and devices at a smaller scale than previously. This has many consequences both scientific and technological [1]. In addition the properties of these structures include new functionalities and depend on the details. Therefore there is a great need to produce models that will describe realistically these structures and consequently to study their properties.

One of the challenges is that these structures contain a great number of atoms and also the ubiquitous strains are not homogeneous. Two problems should be addressed, that of the equilibrium structure and that of the solution of the quantum mechanical problem. The most appropriate method for this type of problems is the Density Functional Theory in its various manifestations. Unfortunately it cannot be utilized at present due to the necessary computational resources. The next choice is the tight-binding molecular dynamics method which is also very demanding on computer time. A procedure which has acquired a certain degree of popularity is the separation of the problem of finding the equilibrium structure from the calculation of the electronic

properties. The first problem is treated using one of the many and tested semiempirical interatomic potentials [2,3], while the second can be dealt with the tight-binding method [4,5]. From experience gained by applying the above procedure in various circumstances one can ascribe a good degree of reliability.

Another challenge is that the strains are not uniform, the structures do not have simple electronic states, and there is, an interplay between the strains and the electronic states. Therefore there is need to add one important component which will help to visualize and interpret the various properties of the structures. While visualization tools are available and can be utilized, one should integrate the visualization into the design of the software package.

The systems we study are semiconductor QD embedded in another semiconductor. These structures are quite interesting since it is possible to grow 3D periodic structures of QDs and also the QDs are protected from the environment. Many useful combinations of semiconductors have been explored and their properties have studied both experimentally and theoretically. One very important system is Ge QDs embedded in Si. It has been observed that the structure of QDs grown using Molecular Beam Epitaxy (MBE) depends strongly on the growth conditions [6]. Thus when the temperature of the substrate is very high (600 °C), small density ($3 \cdot 10^9 \text{ cm}^{-2}$) large domes are formed (12 nm height with a 80 nm base diameter, with the ratio of height to base being between 5.5 and 7.5) and pyramids (with similar base width but with a ratio of base to height between 11 to 13), i.e. much lower in height than the domes and with a slightly smaller density ($1.1 \cdot 10^9 \text{ cm}^{-2}$) while the sides of the base are aligned along the (100) direction. The domes are multifaceted [7]. At a lower temperature (580 °C) besides pyramids and domes with a smaller size also QDs with the shape of hut appear and the overall density increases a lot ($1.1 \cdot 10^{10} \text{ cm}^{-2}$). The pyramids and the domes that remain have a relative density which depends strongly on the quantity of Ge and on the substrate temperature [8,9]. For still lower substrate temperatures (500 °C) no pyramids or domes are formed but only huts with base size of 20 nm and density of $1.1 \cdot 10^{11} \text{ cm}^{-2}$.

With the Chemical Vapor Deposition (CVD) method and with 5.5 Monolayers (ML) of deposited Ge, QDs with density of $3 \cdot 10^9 \text{ cm}^{-2}$ and sizes between 1-4 nm for 60% of the QDs and 11-16 nm for the rest 40%. With the deposition of 8.5 ML the density of the QDs doubles and the ratio of the low height QDs to the high ones becomes 1 to 4. For a larger number of deposited ML all the QDs have the same height of 15 nm with only 1 nm dispersion [10]. In all the cases the ratio of the base to the height is 11 with the maximum base being 80 nm therefore for a higher deposition of Ge only the height of the QDs increases. With different deposition conditions (pressure, temperature, and deposition rate) it is possible to control the ratio of the base to the height in the range from 5 to 11.

By growing the Ge QDs with Si and repeating the process one can produce a 3D correlated stacking of QDs which in some cases can be periodic [11–13]. Annealing of these structures progressively change the shape of the QDs from pyramids and huts to domes [7, 8]. As the growth techniques are tuned for this system it is possible to form Ge QDs prior to the formation of a typical Ge wetting layer [14, 15].

The optical properties of the periodic Ge QDs embedded in Si have been observed through photoluminescence and it is shown to comprise of some peaks which correspond to Si around 1 -

1.1 eV, one broad peak at 0.96 eV, which originates from the strained wetting layer, and another broad peak at 0.8 eV which is due to the QDs [16–19], and is definitely higher than the indirect gap of bulk Ge (0.66 eV) [20,21]. From these studies it is clear that the optical properties of QDs depend on various factors, such as the amount of the deposited Ge, substrate temperature and composition, annealing temperature and processing. Concerning the effect of the size of QDs on the position and the height of the photoluminescence peak, one can notice that as the QDs become smaller the peak shifts to higher energies and its height increases. These shifts are significant and reach 0.03 eV for QDs with height from 12 to 16 nm [22]. The number of stacks of QD layers in the growth direction shift the peak to lower energies up to 0.05 eV for 1 to 10 stacked QD layers, while for a bigger number of stacked layers the shift changes sign and the peak shifts to higher energies by 0.05 eV. The explanation for this reversal of shift is that for less than 10 layers of QDs, the successive layers have QDs with larger size, while for a larger number of stacked QDs layers the size stays the same and also they are more relaxed.

Another interesting system is that of GaN QDs embedded in AlN, due its large band gap which is appropriate for optoelectronic applications in near ultraviolet while GaN nanoparticles show emission in the blue range of the visible spectrum [23]. Although the equilibrium structure of the nitrides is hexagonal it is possible to grow them in the cubic Zinc-Blende structure [24–26]. The advantage of the cubic phase is that it does not show the piezoelectric effect due to its symmetry and therefore the inevitable strains do not produce unwanted internal electric fields [27–29]. The basic difference from the Ge/Si case is that the QDs are smaller, there is no interdiffusion between the comprising compounds [30], the pyramids are strongly truncated with tetragonal base and they are faceted in the (111) direction. The observed pyramids have average height a few nanometers and average base of 13 nm. The ratio of height to base is 1 to 8. If they were complete pyramids that ratio should have been 1 to square root of 2, which indicates a strongly truncated shape [31].

The optical properties of the Wurtzite and Zinc-Blende GaN QDs embedded in AlN differ markedly concerning the dependence of the energy of electronic transitions on the height of the QD, and the radiative time [32]. These differences have been attributed to the presence of the piezoelectric field for the Wurtzite structure, which is absent in the Zinc-Blende case. A serious implication is that the radiative time is much larger for the case of Wurtzite and strongly dependant on the height of the QDs [33,34], thus making the Zinc-Blende GaN QDs more appropriate for applications. The photoluminescence emission peak for Zinc-Blende GaN QDs of height 1.6 nm has been observed experimentally to occur at 3.8 eV [32].

The purpose of the present highlight is to present a software package for the modeling of semiconductor QDs, which includes modules for building atomistic models, finding the equilibrium structure, calculating various structural and energetic properties, and computing the electronic states close to the fundamental gap, the electronic transitions and the optical properties. This package, has a windows front-end, an integrated visualization component and is named STREL from STRuctural and ELectronic properties [35,36].

2 Methods and Tools

2.1 Basic approximations to the quantum mechanical problem

One can easily write the Hamiltonian after the application of the Born-Oppenheimer approximation to the system:

$$H_e = T_e(\mathbf{r}) + V_{eN}(\mathbf{r}, \mathbf{R}) + V_{ee}(\mathbf{r}) \quad (1)$$

where

$$T_e(\mathbf{r}) = -\frac{1}{2m} \sum_i \mathbf{p}_i^2 \quad (2)$$

is the kinetic energy of the electrons,

$$V_{eN}(\mathbf{r}, \mathbf{R}) = -\sum_I \sum_i \frac{Z_I e^2}{|\mathbf{R}_I - \mathbf{r}_i|} \quad (3)$$

is the electron-nuclei interaction, and

$$V_{ee}(\mathbf{r}) = \frac{1}{2} \sum_i \sum_{j \neq i} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \quad (4)$$

is the electron-electron interaction.

The electronic states can be obtained by solving the Schrödinger

$$H_e |\psi\rangle = E |\psi\rangle \quad (5)$$

This is a many body problem and can be efficiently solved by resorting to the Kohn-Sham theorem.

Starting from the above quantum mechanical problem it has been shown [37] that one can write approximately the energy of an ensemble of atoms as a sum of terms of the form

$$E(\{\mathbf{R}_i\}) = \sum_{i,j} u_2(\mathbf{R}_i, \mathbf{R}_j) + \sum_{i,j,k \neq j} u_3(\mathbf{R}_i, \mathbf{R}_j, \mathbf{R}_k) + \text{higher order terms} \quad (6)$$

Where $E(\{\mathbf{R}_i\})$ is the energy of the system for the given state described by the positions of the atoms \mathbf{R}_i , u_2 is the two body term, and u_3 is the three body one. In the summations the subscripts j and k point to neighboring atoms of the central atom i . Functions u_2 , u_3 , etc can be computed from the Hamiltonian, although it is usually the practice to assume a certain form which contains some undetermined parameters. The parameters are determined by comparing the model to experimental results and/or ab-initio results for different atomic configurations, i.e. bulk crystals, surfaces, defects etc. There is a great variety of such functions adapted to particular systems [2,3], are commonly called interatomic potential models (IPM), and have great utility in the modeling of very large systems. One shortcoming is that while an interatomic potential suffice to compute the equilibrium positions of the atoms not only at absolute zero but also for other temperatures, no information about the electronic states and properties can be extracted.

One way to overcome this shortcoming without solving the complete quantum mechanical problem is to follow the method proposed by Slater and Koster [38], which is based on the parametrization of the Hamiltonian. At first the single electron wavefunction is expanded in a sum of atom centered functions much like the actual atomic orbitals. We will denote these function by $|i, \alpha \rangle$, where i specifies the atomic position where the basis function is centered and α indicates the symmetry of the basis function. For a periodic system the basis functions are Bloch sums of atom centered function as

$$\phi_\alpha(\mathbf{k}) = \frac{1}{\sqrt{N_a}} \sum_i e^{i\mathbf{k}\mathbf{r}_i} |i, \alpha \rangle \quad (7)$$

Then the Schrödinger equation becomes an linear algebra eigenvalue problem of the following Hamiltonian matrix

$$H_{\alpha\beta}(\mathbf{k}) = \langle \phi_\alpha(\mathbf{k}) | H | \phi_\beta(\mathbf{k}) \rangle = \frac{1}{N_\alpha} \sum e^{i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)} \langle j, \alpha | H | i, \beta \rangle \quad (8)$$

The matrix elements between specific basis functions and the Hamiltonian operator, $\langle j, \alpha | H | i, \beta \rangle$, can be treated as parameters, which can be determined by comparing the energies of the electronic states to experimental results and/or ab-initio results. The accuracy in the description of the electronic states through this method depends on certain choices, such as the number of basis functions at each non-equivalent atom in the unit cell, and their spatial extend. The first determines the size of the Hamiltonian matrix, while the second the number of parameters needed to be determined. Depending on the problem at hand one can find a suitable approximation.

Since the parameters $\langle j, \alpha | H | i, \beta \rangle$ are determined from the electronic structure of bulk crystals they do not contain the information of the changes they will undergo in structures with strains. To include this important element we assume a scaling based on the distance between the positions that define the centers of the basis functions. This scaling is of the type $\langle j, \alpha | H | i, \beta \rangle = \langle j, \alpha | H | i, \beta \rangle_0 (d/d_0)^n$, where d is the distance in the strained case and d_0 is the bulk crystal distance, n is determined by applying certain distortions to the bulk crystal. Such procedure has been applied to many cases with very good results [39].

The above suffice to calculate the energies of the electronic states, the density of states and the amplitude of basis functions, but since the basis functions are not explicitly specified one can not obtain properties like the charge density. In addition to obtain the optical properties it is necessary to calculate the matrix elements of the momentum operator between the initial and final states

$$\mathbf{p}_{if} = \langle \psi_i | \mathbf{p} | \psi_f \rangle \quad (9)$$

i, f denote the initial and final state for a particular interband electronic transition. Luckily there is a good approximation to the momentum operator due to the localized nature of the basis functions and is the following

$$\mathbf{p} = \frac{m}{\hbar} \frac{dH(\mathbf{k})}{d\mathbf{k}}, \quad (10)$$

which can be calculated easily from the matrix elements of the Hamiltonian. Thus the imaginary

part of the dielectric function from the equation can be calculated [40].

$$\epsilon_2(\omega) = \frac{4\pi^2 e^2 \hbar^2}{3m^2 \omega^2} \sum_i \sum_f \int_{BZ} \frac{2}{(2\pi)^3} |\mathbf{P}_{if}(\mathbf{k})|^2 \delta[E_i(\mathbf{k}) - E_f(\mathbf{k}) - \hbar\omega] d^3\mathbf{k} \quad (11)$$

The real part of the dielectric function can be obtained from the Kramers - Kronig relation [41,42]

$$\epsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\omega' \epsilon_2(\omega')}{\omega'^2 - \omega^2} d\omega' \quad (12)$$

where the P denotes the Cauchy principal part of the integral. Optical properties such as absorption coefficient, refractive index and reflectivity are computed from the following equations:

$$\alpha(\omega) = \frac{\omega \epsilon_2(\omega)}{cn(\omega)} \quad (13)$$

$$n(\omega) = \sqrt{\frac{1}{2} \sqrt{\epsilon_1^2(\omega) + \epsilon_2^2(\omega)} + \epsilon_1(\omega)} \quad (14)$$

$$r(\omega) = \frac{(n(\omega) - 1)^2 + \left(\frac{\epsilon_2(\omega)}{2n(\omega)}\right)^2}{(n(\omega) + 1)^2 + \left(\frac{\epsilon_2(\omega)}{2n(\omega)}\right)^2} \quad (15)$$

2.2 Description of modeling through STREL

In the following we will describe the functionality of STREL and the steps one takes to study a system. A block diagram of STREL is presented in Fig. 1. The building of the models follows three steps. In the first step the primitive cell of the embedding material is defined. This definition is based on simple crystallographic data and for the case of cubic structures,

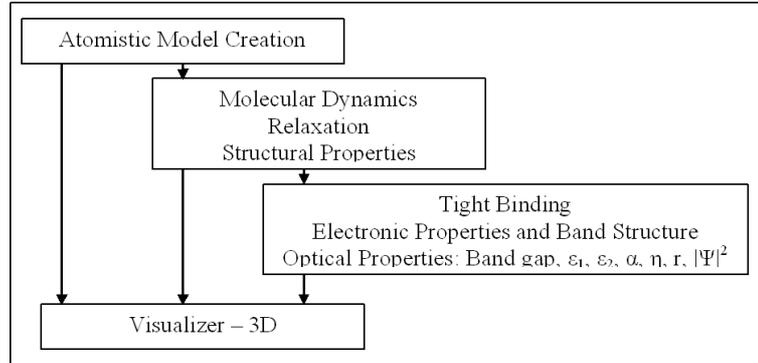


Figure 1: STREL main block structure

the required data are only the Cartesian coordinates of the atoms in the primitive cell, the primitive cell vectors and the lattice constant of the material. In the second step a superlattice by defined by an orthogonal parallelepiped in which the primitive cell is replicated to form the embedding matrix. Finally by replacing atoms within a selected shape the desired embedded QD is formed. The shapes of QDs can be spheres, domes, tetrahedra, pyramids with a tetragonal base, prisms etc. There is also the possibility to define truncated shapes. The size and the exact characteristic of each shape (eg base of the pyramid and height) are also selectable.

A special feature of the software is to create alloys by randomly selecting atoms to be replaced either from the whole superlattice or from within a specified shape. One can define more than one (the maximum number is user defined) replacements with independently selected shapes. For each of the previous steps and each action at each step, 3D visualizations of the structure are generated with full rotational, and zoom capabilities. Also individual or groups of atoms can be viewed along with their properties.

For the visualization of the calculated properties one can select a 3D mode in which specific properties at each atomic site are visualized. The presentation of the values of a particular property at each atomic site are shown through the color, size and opacity or any combination of the above. For a more effective observation of the properties in the various sites of the superlattice, one can select only slices for visualization in all three directions and combinations of such slices or to exclude some atom types from being visible. There is also the possibility for the observation of atoms within a specific range of values of the presented property, which is user selectable.

A very useful observation mode, especially for the visualization of the wave functions, is the automatic selection of atoms with a cumulative value smaller or larger of a user defined percentage of the sum of the selected property. Distributions of the values of specific properties can be calculated and the corresponding bar graphs can be plotted. These distributions can be produced from values of all the atoms in the structure, and/or from selected atom types. 2D graphs are also integrated to present interband transition probabilities and energies, the band structure and optical properties such as imaginary or real part of the dielectric function, absorption, reflectance and refractive index, density of states etc.

3 Application to specific systems

3.1 Periodic Ge QDs embedded in Si

In the infrared part of the spectrum structures containing Si and Ge are very important. The control of the properties is achieved at the beginning by alloying, later by the growth of Si/Ge superlattices and in recent years by preparing QDs. As it is mentioned above the properties of the nanostructures depend on the details. On the other hand there is a great number of possible structures, thus there is a need for a rapid equilibration of the structures, the calculation of the structural and electronic properties, and their visualization.

3.1.1 Structural properties

At first we will examine the structural properties of some relaxed structures and through the study of various visualizations we will try to understand the details of the structures. A property that can be accessed experimentally is the distribution of angles and the distribution of bond lengths. Those distributions are presented in Fig. 2 and Fig. 3 for a different number of spacer Si atomic layers.

The bond lengths distribution can be resolved into three well separated contributions, one that

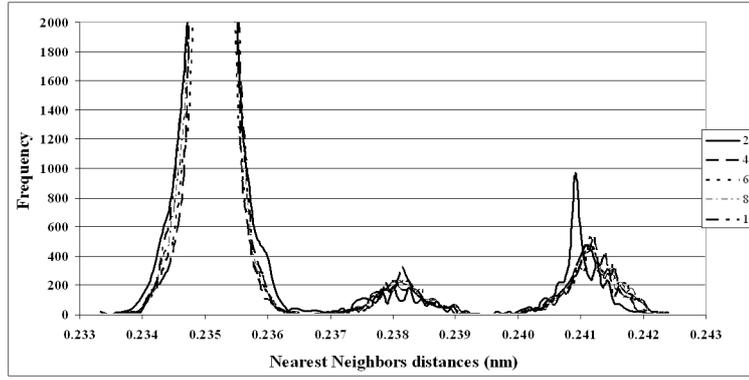


Figure 2: Bond length distribution of embedded Ge QDs.

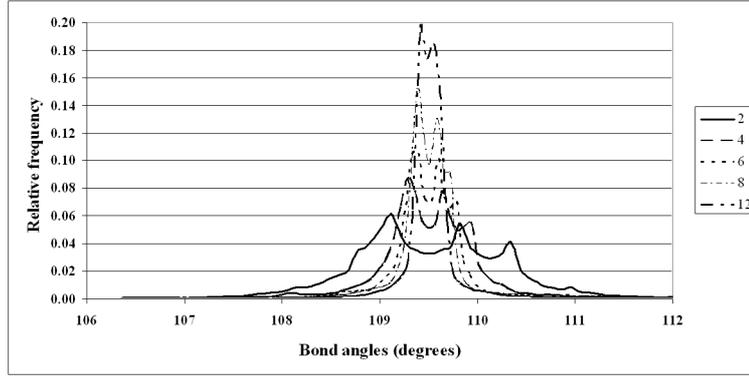


Figure 3: Bond angle relative frequencies distribution of embedded Ge QDs.

comes from Si-Si bonds, one from Ge-Ge bonds and one from Si-Ge bonds. They are similar in shape and share a common width. Also there is no much effect on the number of the spacer Si layers. On the other hand in Fig. 3 it is indicated, that as the Si spacer becomes thicker, the distribution of the bonds angles has smaller variance. This is not case, since the shown distribution, is the distribution of the relative frequencies. Taking into account the last comment we can conclude that the absolute number of distorted bonds and bond angles is constant independent of the thickness of the spacer Si layer.

To access the spatial distribution of the strains we present in Fig 4 for a thin Si spacer layer and Fig 5 for a thick spacer layer. It is a color coded visualization, where the colors vary from blue to red in a particular range of strains. The range of values is the same for both cases to facilitate the comparison.

The red color denotes negative strains and blue the positive ones. As it is expected the majority of Si atoms do not show any significant values of strains, only those close to the interfaces show negative strains, while all the Ge atoms show positive strains as the QD is embedded in Si. The exception occurs for those Si atoms situated just below the QD and adjacent to Ge atoms which exhibit positive strains. Therefore the strains diminish strongly as we distance from the Ge QD. In the case of a thicker Si spacer layer we notice some interesting changes. Now there are two distinct groups of Si atoms close the QD, one at the corners of the cell with negative strains and

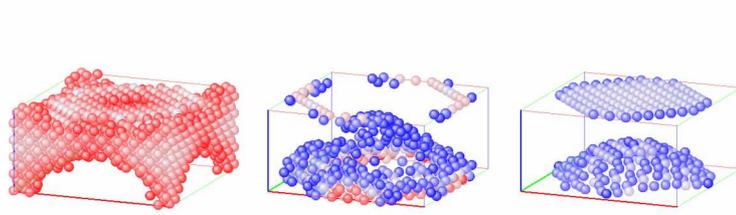


Figure 4: The strain fields for a thin spacer Si layer. Range of values Left: -0.5 to -0.1 %, Middle: 0.05 to 0.5 %, Right: higher than 0.5 %

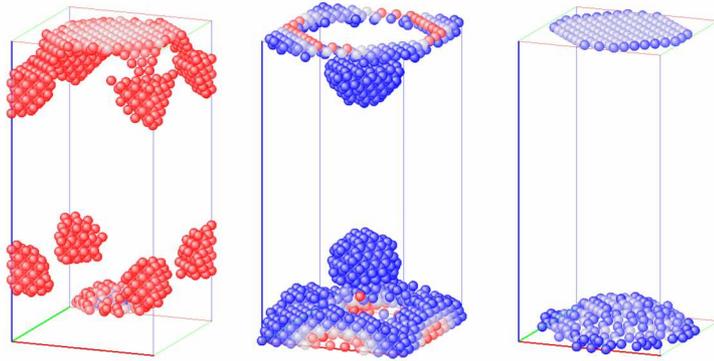


Figure 5: The strain fields for a thick spacer Si layer. Range of values Left: -0.5 to -0.1 %, Middle: 0.05 to 0.5 %, Right: larger than 0.5 %

one a bit above and below the QD with positive strains. We will not go into much detail on the implications of this finding but only state that this can be used to explain why the stacking of QDs on the successive layers is correlated.

Coming back to the point of how fast the strains are diminishing away from the QD, in Fig. 6 we present the percent of the atomic volume change along a line perpendicular to the base and through the center of the unit cell.

In Fig 6, three regions can be noticed, one is the interface between the Si - Ge atoms and the other two inside the Si and Ge part of the structure. We notice the -4% volume change inside the Ge QD, as it is expected because of the lattice mismatch, and also the fast decay of the strains inside the Si region. In addition, the larger strains occur very close to the Si - Ge interface.

3.1.2 Electronic properties

Many of the electronic states of the QDs close to the fundamental gap are localized in the QDs while some others are in the area between the QDs. Predominately the top of the valence states are localized in the QDs. If a transitions occur between a valence state and a conduction state which are both localized in the QD then we expect a high transition probability and this arrangement is called type I. The alternative case where the valence state is localized in the

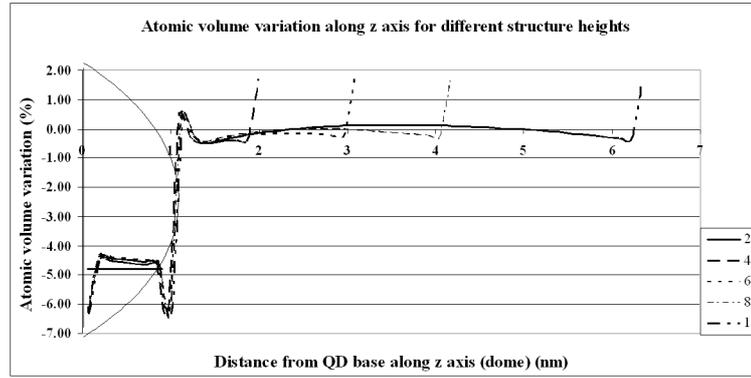


Figure 6: Percentage of atomic volume change along a line starting from the center of the base of the QD and perpendicular to the base

QDs and the conduction state in the area between the QDs, has relatively small transition probability, as there is no much overlap between the two wavefunctions, and is called type II. Ge QDs embedded in Si are of type II for the lowest electronic transitions. Although this is the rule one has to take a close look close at the wavefunctions as the properties of QDs depend on the details.

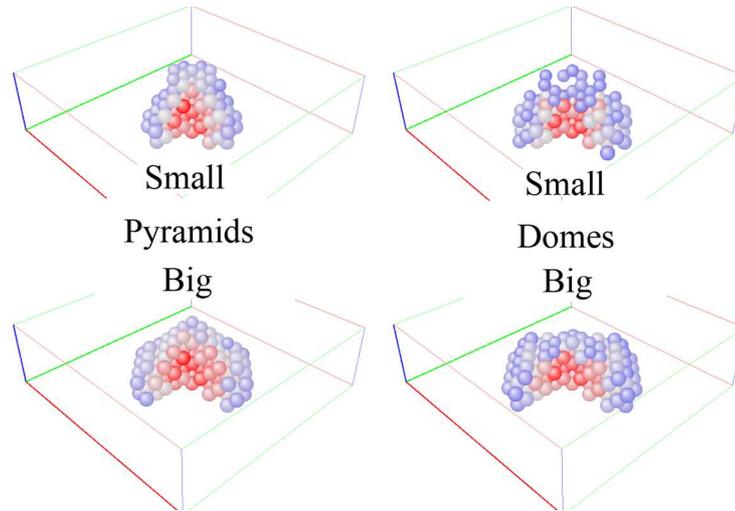


Figure 7: Wavefunction of states at the top of the valence band which are localized in the QD . Left for a pyramid and Right for a dome of similar size.

In Fig. 7 we present the upmost valence wavefunctions of Ge QDs which are clearly localized in the QDs, although the confinement is stronger for the bigger QDs. Also the electronic states have higher amplitude close to the bottom of the QDs. Together with the behavior of the conduction states these details determine the actual probability for each interband transition. In Fig. 8, the energies and the corresponding probabilities are shown for the lowest transition energies for dome shaped QDs. We observe that interband electronic transitions strongly depend on the size of the QDs, both in energy and the probability.

The fundamental gap is smaller for the bigger QDs by as much as 0.12 eV, a manifestation of the size effect.

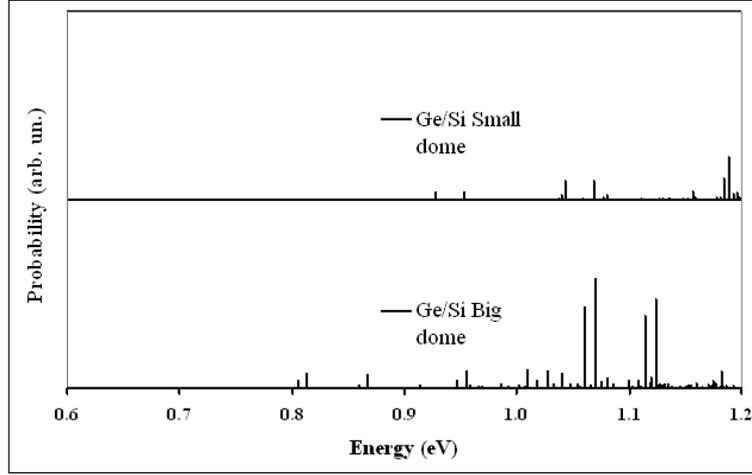


Figure 8: Interband transitions for Ge QDs embedded in Si

3.2 GaN QDs embedded in AlN

The fabrication of device grade nitride semiconductors has resulted a great number of applications in the blue part of the visible spectrum, leading to the realization of white light emitting diodes with great implications to many fields of science, technology and society. Recently it become possible to fabricate GaN QDs embedded in AlN and also GaN QDs embedded in InN. Here we will concentrate on the cubic phases, which have many advantages over the hexagonal phase.

3.2.1 Electronic Properties

A panorama of the upmost valence states of GaN QDs embedded in AlN is presented in Fig. 9. Each row presents one structure, while each column represents a particular valence state. Here the numbering follows the convention for valence states, that the smaller the number the higher is its energy, i.e. number 1 denotes the topmost valence band state. The rows denoted by A are for dome shaped QDs, A2 has more AlN spacer layers compared to the A1 case. Row B is for pyramid shaped QDs with an even thicker AlN layer and QW row is for a GaN Quantum Wire embedded in AlN and included for comparison. For the periodic QD case, the QD is placed in the center of the cell, while for the Quantum Wire is placed in the indicated corner. All the depicted valence states are confined in the GaN QDs. Similar spatial patterns can be observed at each row, but the energy ordering is not the same and also the details are different. One can interpret these spatial patterns in terms of spherical symmetry as it is done for the atom, although this is not very appropriate. The observed differences come from changing the shape of the QDs and/or just a few layers of the spacer AlN layers, while keeping the number of atoms is the QD constant.

The first two lowest conduction states for the structures of Fig. 9 are shown in Fig. 10. We notice that for A1 and QW the C1 state is confined in the QD and QW respectively, while C2 is confined in the intervening AlN region. Therefore the lowest interband transition is of type I for these cases. For A2 none of the conduction are confined in the QDs, therefore all the transition

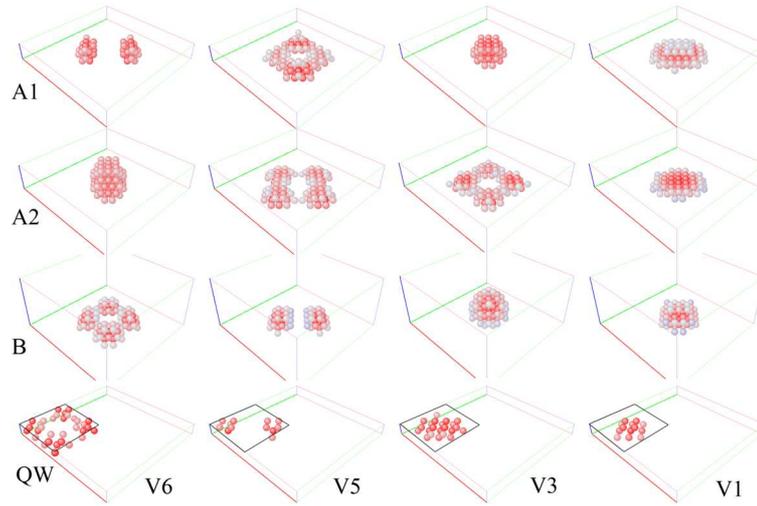


Figure 9: Upmost valence band state V1, V3, V5, and V6 for two dome QDs (A1 and A2, A2 has a thicker spacer layer), pyramid shaped QDs (B) and a Quantum Wire (QW)

are of type II. Case B, has C2 confined in the QDs while C1 is confined in the AlN region, thus the first interband transition is of type II, while the second of type I. We can conclude that the fine details of the structure determine the optical properties and that each case needs to be investigated as a special case.

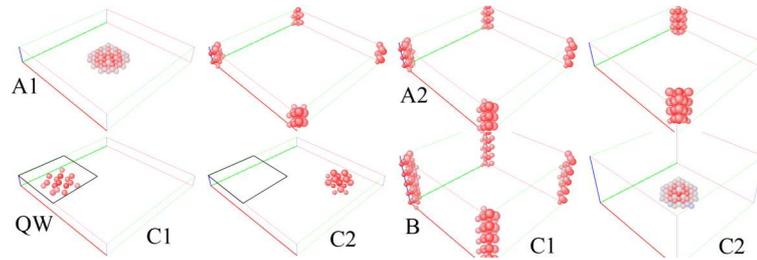


Figure 10: The first two lowest conduction states for structures as described in Fig. 9

Having studied the valence and conduction states for the above structures it is possible to interpret the interband transitions for each structure. These transitions are displayed in Fig. 11. The probabilities for the transitions of the A2 structure are multiplied by 4000. Therefore they are comparatively 4000 times smaller than those of the other structures, and this is a consequence, as analyzed, of the type II interband transitions. Also we observe the larger oscillator strength for the type I transitions which occur for the other structures.

4 Conclusions

A suite of programs under a windows front-end (STREL), specifically designed to facilitate the investigation of the structural and electronic properties of semiconductor nanostructures is presented. Apart for the computational routines, a set of visualization tools is integrated into STREL. The models for the nanostructures can have sizes similar to real fabricated structures comprising of many thousands of atoms. The utility of STREL is demonstrated by studying the

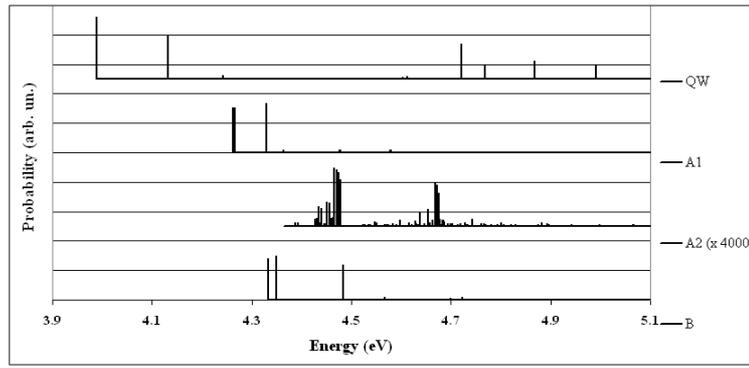


Figure 11: Interband transitions for the structures described in Fig. 9

properties of periodic Ge QDs embedded in Si and GaN QDs embedded in AlN. One important element of STREL is that the study is based on atomistic modeling, which means that it takes into important details of the structures which cannot be considered in the case of models resorting to continuum approximations. A great influence on the optical transitions is found to arise from strains which are naturally included in the present modeling.

References

- [1] K. Brunner, *Rep. Prog. Phys.*, **65**, 27, (2002).
- [2] H. Balamane, T. Halicioglu and W. A. Tiller, *Phys. Rev. B*, **46**, 2250, (1992).
- [3] T. Halicioglu, H. O. Pamuk and S. Erkoç, *Phys. Stat. Sol. B*, **149**, 81, (1988).
- [4] M. Bescond, N. Cavassilas, K. Nehari and M. Lannoo, *J. Comput. Electron.*, **6**, 341, (2007).
- [5] C. Tserbak, H. M. Polatoglou and G. Theodorou, *Phys. Rev. B*, **47**, 7104, (1993).
- [6] O. G. Schmidt, C. Lange and K. Eberl, *Appl. Phys. Lett.*, **75**, 1905, (1999).
- [7] G. Medeiros-Ribeiro, A. M. Bratkovski, T. I. Kamins, D. A. A. Ohlberg and R. S. Williams, *Science*, **279**, 353, (1998).
- [8] J. A. Floro, G. A. Lucadamo, E. Chason, L. B. Freund, M. Sinclair, R. D. Twisten and R. Q. Hwang, *Phys. Rev. Lett.*, **80**, 4717, (1998).
- [9] T. I. Kamins, G. Medeiros-Ribeiro, D. A. A. Ohlberg and R. Stanley Williams, *J. Appl. Phys.*, **85**, 1159, (1999).
- [10] T. I. Kamins, E. C. Carr, R. S. Williams and S. J. Rosner, *J. Appl. Phys.*, **81**, 211, (1997).
- [11] Z. Pei, P. S. Chen, S. W. Lee, L. S. Lai, S. C. Lu, M. -J. Tsai, W. H. Chang, W. Y. Chen, A. T. Chou and T. M. Hsub, *Appl. Surf. Sci.*, **225**, 165, (2004).

- [12] Z. Zhong, G. Katsaros, M. Stoffel, G. Costantini, K. Kern, O. G. Schmidt, N. Y. Jin-Phillipp and G. Bauer, *Appl. Phys. Lett.*, **87**, 263102, (2005).
- [13] P. D. Lacharmoise, A. Bernardi, A. R. Goni, M. I. Alonso, M. Garriga, N. D. Lanzillotti-Kimura and A. Fainstein, *Phys. Rev. B*, **76**, 155311, (2007).
- [14] S. A. Teys, A. B. Talochkin, K. N. Romanyuk and B. Z. Olshanetsky, *Phys. of the Solid States*, **46**, 80, (2004).
- [15] O. P. Pchelyakov, A. I. Nikiforov, B. Z. Olshanetsky, S. A. Teys, A. I. Yakimov and S. I. Chikichev, *J. Phys. Chem. of Solids*, **69**, 669, (2008).
- [16] O. G. Schmidt, C. Lange and K. Eberl, *Phys. Stat. Sol. B*, **215**, 319, (1999).
- [17] G. Bremond, M. Serpentine, A. Souifi, G. Guillot, B. Jacquier, M. Abdallah, I. Berbezier and B. Joyce, *Microelectronics Journal*, **30**, 357, (1999).
- [18] J. Wan, G. L. Jin, Z. M. Jiang, Y. H. Luo, J. L. Liu and Kang L. Wang, *Appl. Phys. Lett.*, **78**, 1763, (2001).
- [19] J. Wan, Y. H. Luo, Z. M. Jiang, G. Jin, J. L. Liu, Kang L. Wang, X. Z. Liao and J. Zou, *Appl. Phys. Lett.*, **79**, 1980, (2001).
- [20] G. G. Macfarlane, T. P. MsLean, J. E. Quarrington and V. Roberts, *Phys. Rev.*, **108**, 1377, (1957).
- [21] J. R. Heath, J. J. Shiang and A. P. Alivisatos, *J. Chem. Phys.*, **101**, 1607, (1994).
- [22] J. L. Liu, S. Tong and K. L. Wang, in *Handbook of Semiconductor Nanostructures and Nanodevices, Chapter 1: Self-Assembled Germanium Quantum Dots on Silicon and Their Optoelectronic Devices*, (American Scientific Publishers 2006)
- [23] M. Benaissa, K. E. Gonsalves and S. P. Rangarajan, *Appl. Phys. Lett.*, **71**, 3685, (1997).
- [24] S. Oktyabrskya, K. Dovidenko, A. K. Sharma, J. Narayan and V. Joshkin, *App. Phys. Lett.*, **74**, 2465, (1999).
- [25] Y. Zhaoa, C. W. Tu, I.-T. Bae and T.-Y. Seong, *Appl. Phys. Lett.*, **74**, 3182, (1999).
- [26] K. Amimer, A. Georgakilas, K. Tsagaraki, M. Androulidaki, D. Cengher, L. Toth, B. Pecz and M. Calamiotou, *Appl. Phys. Lett.*, **74**, 2580, (2000).
- [27] L. S. Dang, G. Fishman, H. Mariette, C. Adelman, E. Martinez, J. Simon, B. Daudin, E. Monroy, N. Pelekanos and J. L. Rouviere, *J. Korean Phys. Soc.*, **42**, S567, (2003).
- [28] N. Gogneau, F. Enjalbert, F. Fossard, Y. Hori, C. Adelman, J. Brault, E. Martinez-Guerrero, J. Simon, E. Bellet-Amalric, D. Jalabert, N. Pelekanos, J.-L. Rouviere, B. Daudin, Le Si Dang, H. Mariette and E. Monroy, *Phys. Stat. Sol. C*, **1**, 1445, (2004).
- [29] J. Simon, N. T. Pelekanos, C. Adelman, E. Martinez-Guerrero, R. Andre, B. Daudin, Le Si Dang and H. Mariette, *Phys. Rev. B*, **68**, 035312, (2003).

- [30] V. Chamard, T. Schulli, M. Sztucki, T. H. Metzger, E. Sarigiannidou, J.-L. Rouviere, M. Tolan, C. Adelman and B. Daudin, *Phys. Rev. B*, **69**, 125327, (2004).
- [31] E. Martinez-Guerrero, C. Adelman, F. Chabuel, J. Simon, N. T. Pelekanos, Guido Mula, B. Daudin, G. Feuillet, and H. Mariette, *Appl. Phys. Lett.*, **77**, 809, (2000).
- [32] V. A. Fonoberov and A. A. Balandin, in *Properties of GaN and ZnO quantum dots. in Handbook of Semiconductor Nanostructures and Nanodevices, Vol. 3* ed. A. A. Balandin and K. L. Wang, (American Scientific Publishers, Los Angeles, 2006).
- [33] I. Vurgaftman and J. R. Meyer, *J. Appl. Phys.*, **94**, 3675, (2003).
- [34] R. Dingle, D. D. Sell, S. E. Stokowski and M. Ilegems, *Absorption, Phys. Rev. B*, **4**, 1211, (1971).
- [35] N. Skoulidis and H. M. Polatoglou, *International Journal of Nanotechnology*, **2**, 271, (2005).
- [36] N. Skoulidis and H. M. Polatoglou, *J. of Materials Education*, **29**, 117, (2007).
- [37] D. G. Pettifor, *Phys. Rev. Lett.*, **63**, 2480, (1989).
- [38] J. C. Slater and G. F. Koster, *Phys. Rev.*, **94**, 1498, (1954).
- [39] W. A. Harrison, *Electronic Structure and the Properties of Solids: The Physics of the Chemical Bond*, (Freeman & Co, San Francisco, 1980)
- [40] H. Ehrenreich and M. H. Cohen, *Phys. Rev.*, **115**, 786, (1959).
- [41] H. A. Kramers, *Atti Cong. Intern. Fisica*, (Transactions of Volta Centenary Congress) Como, **2**, 545, (1927).
- [42] R. de L. Kronig, *J. Opt. Soc. Am.*, **12**, 547, (1926).