



Empirical Methods in Semiconductor Nano-Structures Design and Modelling

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ABSTRACTS

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TALK ABSTRACTS
Day 1 – Wednesday 23 June

Stanko Tomic
(STFC Daresbury Laboratory)

Welcome: Advance in Empirical Electronic Structure Methods for Nanostructures

Theory, modelling, and computational methods for semiconductor materials and nanostructures is a topic of rapid growth and great international interest. A lot of the world-wide effort over the past 50 years in establishing the theoretical foundation of methodologies for calculations of structural, electronic, optical and transport (electrical and thermal) properties of semiconductor nanostructured materials are now coming to fruition.

Modern crystal-growth techniques, such as molecular beam epitaxy or metalorganic chemical-vapour deposition, are capable of producing prescribed crystal structures, sometimes even in defiance of equilibrium bulk thermodynamics.

To correlate desired electronic and optical properties with the structure cannot be efficiently done experimentally solely by trial-and-error methods. Hence computational methods and novel algorithms that combine fast empirical solvers, detailed knowledge of the nanostructure shape and size, chemical composition, and mechanical properties, together with ever increasing computational power available are required to address this fundamental problem.

A variety of modelling implementations [multiband k-p, empirical tight-binding (TB), valence force field (VFF), empirical pseudopotential method (EPM), etc.] are being employed that 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 empirical methods inherently facilitates synergy between experiment and theory. Proper implementations of 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.

Empirical electronic structure methods, have recently seen much improvement in both the methodology, parameterizations and computational speed. The next step will certainly be that of condensing and interfacing all the individual efforts to produce tools that are of more general use to the wider community. We devote two closely coupled CECAM Workshops to the use of empirical methods for semiconductor nanostructure design and modelling, with the first (ACAM) Workshop focused primarily on computational/technical issues, numerical implementations and parametrisation strategies, followed immediately by the second STFC Daresbury Workshop, at the University of Manchester, highlighting the scientific issues and demands related to empirical nanostructure design and modelling.

Frederic Aniel
(University of Paris)

The k.p Theory Beyond Standard 8-Band Theory Parametrization Strategies and its Applicability in Electronics and Optoelectronic Devices Design

The k.p method is known to be very efficient to accurately describe either the conduction band or the valence band or even both of them in the vicinity of a given point of the Brillouin zone. Recently multiband k.p Hamiltonians including up to 30 bands (and above), which allow us to calculate the band diagram of bulk materials for Td or Oh group semiconductors, have been proposed [1]. The strain effect on the electronic structure has been included through the strain Bir-Pikus Hamiltonian. An envelope function formalism based on this 30-band k.p method which allows to calculate the subband structure of both electron and hole quantum wells, even for indirect band gap semiconductors, has been introduced some time after [2,3]. Many physical phenomena such as optical generation or recombination, optical gain realization, Auger effect, impact ionization and more generally hot carriers and hot phonons mechanisms require an accurate Bloch state description for the conduction bands (resp. valence bands) well above (resp. well below) the conduction (resp. the valence) band extremum. Such multiband k.p electronic structures are consequently used in the modelling of optoelectronic and electronic devices. An example is the description of optical gain in an indirect band gap material like germanium under tensile strain [4] corresponding usefully to actual experimental configuration investigated presently [5]. Under a magnetic field perturbation, the k.p method is without rival while for all other cases, in particular nanostructure electronic structure descriptions, the question of the best approach between the k.p method, the empirical pseudo-potential method or the LCAO method can be discussed.

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Wlodek Zawadzki
(Polish Academy of Sciences)

Effects of Spin-Orbit Interaction on Spin Properties of Electrons in III-V Semiconductor Heterostructures

Effects of spin-orbit interaction (SOI) on the spin electron energies and wave functions in III-V semiconductor heterostructures are considered theoretically and compared with experimental data of various authors. The situations in absence of a magnetic field and in the presence of magnetic field are discussed.

SOI influences strongly the energies and wave functions of electrons in semiconductors. In bulk materials, it enhances the electron spin Lande factors which change from the value of $g = +2$ for free electrons to $g = -15$ in InAs, $g = -50$ in InSb, etc. Also, the resulting wave functions represent mixed spin states which gives a possibility to excite spin-flip transitions with the use of different types of electric perturbations: photons, phonons, impurities, etc. These perturbations are also a source of spin relaxation. If, in addition, a crystal exhibits a bulk inversion asymmetry (BIA), the spin-orbit interaction lifts the spin degeneracy so that, for a given direction of the electron wave vector k , the two spin states have different energies (the Dresselhaus splitting).

In semiconductor heterostructures, one can have in addition a structure inversion asymmetry (SIA). Together with SOI this results in a splitting of the two spin energies called the Bychkov-Rashba splitting (or the Rashba splitting) proportional to the value of k . The subject of BR splitting had been quite controversial, as discussed in the review [1]. Different manifestations of BR spin splitting are discussed. The presence of an external magnetic field introduces the Zeeman spin splitting which combines in a nontrivial way with the Dresselhaus and Bychkov-Rashba splittings. Examples of such situations are shown.

Finally, the influence of SOI and band's nonparabolicity on the electron spin g factors in the quantum wells of GaAs/GaAlAs heterostructures is considered for two configurations of an external magnetic field: parallel and transverse to the growth direction. It is shown that the width of a quantum well has a strong effect on the spin g value in both configurations and, in case of GaAs wells, it leads to a change of the sign of g from negative (for large widths) to positive (for small widths) [2].

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Guido Goldoni

(University of Modena and Reggio Emilia and Centro S3, CNR-Istituto di Nanoscienze)

Few-Body Physics in Semiconductor Quantum Dots with the Configuration Interaction Approach

Quantum dot based devices often rest on the collective properties of few confined electrons in the nanostructure in the meV energy scale. This is a regime of kinetic-to-Coulomb energy ratio where a single-particle description is completely inadequate, and the mean-field approach can fall short of accuracy when quantitative comparison with experimental evidence is possible, particularly if the collective properties of excited states are involved [1].

In this context the configuration interaction (CI) approach is the method of choice, as both ground and excited states are provided with comparable accuracy, which can be systematically improved. Nanostructures with confinement energies of a few meV require macroscopic description of the electronic states, where only free electrons in the conduction and valence band are described within a k.p approach, interacting through electrostatic forces screened by the macroscopic, possibly space dependent, dielectric constant of the host materials.

We have implemented such a CI approach [2] which diagonalizes exactly the few interacting Hamiltonian of N confined electrons. Assuming no truncation of the Fock space of Slater determinants generated from a chosen set of spin-orbitals, the method may tackle regimes where Coulomb interaction is the dominant energy scale. Exploitation of all possible symmetries and excellent code scalability in parallel environments allows to treat highly correlated systems deep into the Wigner regime [1,2]. Inclusion of spin-orbit coupling, which is needed when spin dynamics is involved, is implemented without increasing memory requirements, which is the limiting factor in this type of numerical calculation [3].

The predictive quality of this approach will be discussed with reference to recent experimental investigations of inter-band and intra-band spin and charge excitations.

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Vladimir Falko
(Lancaster University)

Electrons in Bilayer Graphene: Lifshitz Transition and Spontaneous Symmetry Breaking

Bilayer graphene is a gapless semiconductor with parabolic spectrum in the conduction and valence bands at intermediate energies and quasiparticles characterised by the Berry phase 2π . Since the Berry phase 2π is not topologically stable, two scenarios are possible for the low-energy properties of electrons:

(i) At some energy topology of isoenergetic lines undergoes Lifshitz transition, from single-connected at higher energy to four pieces at lower energy, surrounding four Dirac points (one in the middle with Berry phase $-\pi$ and three off-side, each carrying Berry phase π).

(ii) The hexagonal symmetry of bilayer is unstable, and electronic system undergo phase transition into state with a deformed spectrum.

We derived the renormalization group equations describing all the short-range interactions in bilayer graphene allowed by symmetry, the long range Coulomb interaction, and the band parameters.

We find that the system is likely to undergo the first order phase transition into the uniaxially deformed gapless state. This transition is accompanied by the change of the topology of the electron spectrum, such that the asymmetric spectrum at low energies features two Dirac points, each carrying Berry phase π .

The difference between two phases can manifest itself through the persistence of different filling factors in low-field Shubnikov - de Haas oscillations.

Bart Partoens
(University of Antwerp)

Tight-Binding Description of Graphene, Graphene Multilayers and Graphite

A simple tight-binding model is used to study the electronic structure of different graphene multilayer systems. The evolution of the electronic structure from graphene to graphite for different stackings is discussed. It is well known that a single graphene layer is a zero-gap semiconductor with a linear Dirac-like spectrum around the Fermi energy, while graphite shows a semimetallic behavior with a band overlap of about 41 meV. In contrast to a single graphene layer, we show that two graphene layers have a parabolic spectrum around the Fermi energy and are a semimetal like graphite; however, the band overlap of 0.16 meV is extremely small. Three and more graphene layers show a clear semimetallic behavior. For 11 and more layers the difference in band overlap with graphite is smaller than 10%. From the tight-binding model it can also easily be shown that Dirac fermions are only present in AB stacked graphene multilayers if they have mirror plane symmetry. In other words, Dirac fermions are present in graphene stacks with an odd number of layers.

We also considered the recently experimentally realized AA stacked form of graphite and show that in essence two types of massless relativistic Dirac particles are present with a different effective speed of light. In contrast to AB stacked graphene layers, the spectrum of AA stacked graphene layers can be considered as a superposition of single layer spectra and only particles with a linear spectrum at the Fermi energy around the K point are present. From the evolution of the band overlap we show that 6 multilayers of AA stacked graphene already behave as AA stacked graphite. The evolution of the effective speeds of light of the Dirac particles to their bulk values shows exactly the same behavior.

Michael Flatté
(University of Iowa)

Empirical Tight-Binding and Real-Space Envelope-Function Calculations of Single-Donor Spin Dynamics

In systems with sizable spin-orbit interaction an electric field can generate a "pseudomagnetic field" which replaces a true applied magnetic field for the efficient and rapid manipulation of spins. These electric fields can be controlled locally and used to address individual dopant spins in a scalable architecture.

Here two examples of the electrical control of spin dynamics will be compared, one relying on envelope-function calculations of the g tensor of a silicon donor in gallium arsenide and the other on tight-binding calculations of the electronic properties of a manganese acceptor in gallium arsenide. For the silicon donor a nonlinear anisotropy of the g tensor is introduced by the electric field, which provides a handle to control the spin of donor-bound electrons[1]. For dopants with integer spin ground states, such as manganese embedded in gallium arsenide (which has a $J=1$ ground state), the spin can be manipulated entirely with electric fields without even the requirement of a static magnetic field[2]. The local symmetry of the manganese hybridization with neighboring arsenic atoms in the zincblende lattice (tetrahedral symmetry), which arises naturally in the tight-binding calculations, also provides a constraint on envelope-function theories of the manganese dopant which permit accurate envelope-function calculation of the shape of the wave function of the hole bound to the dopant[3].

This work was supported by an ARO MURI and an NSF NIRT.

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TALK ABSTRACTS
Day 2 – Thursday 24 June

Aldo Di Carlo
(University of Rome "Tor Vergata")

Multiscale Simulations of Nanostructured Devices with TiberCAD

The need for high performance devices and high integration together with technological progress has led to a downscaling trend of the dimensions of conventional electronic devices. At the same time, new devices are emerging where the functionality is based on quantum dots, nanowires or carbon nanotubes. The semi-classical models used to describe conventional devices are not satisfactory or not applicable for such structures.

Therefore a fully quantum mechanical treatment is needed. In very small structures, methods based on the envelope function approximation (EFA) – widely used for the description of heterostructures – can break down and atomistic approaches become inevitable. The computational cost of such methods, however, limits their application to rather small structures consisting of up to tenthousand of atoms. A reliable simulation of a device including not only the nanometric active regions, but also the substrate and contact regions has therefore to be done by coupling quantum mechanical and atomistic approaches to semi-classical models in the framework of a multiscale simulation.

The TIBERCAD project [1-2] is aimed at the implementation of a device simulator which on the one hand meets the need for a multiscale simulation environment and on the other hand captures the most important physical concepts encountered in present and emerging electronic and optoelectronic devices such as strain and strain-induced effects, self-heating / thermal transport, transport of electrons, holes and of other quasiparticles as excitons/polaritons, quantum mechanical effects such as confinement and tunneling and quantum mechanical transport. Atomistic details, described with empirical or density functional tight-binding hamiltonians, are connected to continuous models (k.p, drift-diffusion etc.) by using bridge or overlap methods.

In the present talk I will present the multiscale methodologies of TiberCAD and I will show some applications including the simulation of hybrid organic/inorganic solar cells. The simulation takes in count the photo-generation of electrons, the loss at the semiconductor and electrolyte interface and the distribution of charge densities (electrons, redox pair and cations) inside the cell.[3]

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Pawel Hawrylak

(Institute for Microstructural Sciences, National Research Council)

QNANO: Computational Platform for Semiconductor Nanostructures

The size of semiconductor nanostructures such as self-assembled quantum dots, nanowires, and nanocrystals involving millions of atoms precludes calculation of their electronic properties using ab-initio methods, such as, e.g., GW-BSE approach [1]. We discuss here one of the approximate methods, VFF-tb-CI, implemented in QNANO computational platform. QNANO combines three steps [2]: (a) calculation of equilibrium position of constituent atoms using valence force field model (VFF)[2,3], (b) calculation of quasi-electron and quasi-hole states (equivalent to the GW step) using a linear combination of $sp^3d^5s^*$ atomic orbitals approach in a tight binding approximation (tb)[2,3], and (c) inclusion of the effect of final state interactions by defining an effective Hamiltonian of interacting excited quasi-particles, solved using the configuration interaction method (CI).

In the VFF calculation for 109 atoms we use the Keating model with material parameters derived from bulk elastic constants c_{ij} [4]. The tb parameters for unstrained InAs and GaAs are obtained by fitting of the tb bulk band edges and effective masses to those obtained in experiment or by ab-initio calculations, with the valence band offset (VBO) built into the parameter set [3]. The dependence of band edges on lattice deformation computed using DFT [5,6] is used to find strain corrections to tb parameters. The Coulomb matrix elements for CI are obtained with tb wave functions involving ~ 108 orbitals, with onsite and nearest-neighbor terms computed by approximating the tb basis with Slater orbitals. The interactions are screened by a distance-dependent dielectric function and, typically ~ 104 configurations are used as a basis for multiexciton complexes.

We illustrate the method by computing and analysing the electronic and optical properties of a lens-shaped and disk-shaped InAs/GaAs SAs and CdSe nanocrystals.

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Lin-Wang Wang
(Lawrence Berkeley National Laboratory)

LCBB Method for CMOS Device Simulations

Linear combination of bulk band (LCBB) method has been used for many nanostructure calculations in recent years. It can be used as an alternative to the traditional k.p calculations. I will first discuss some basic computational steps in a LCBB calculation. I will then present our recent work in using LCBB method for CMOS device simulations. In such a simulation, selfconsistent calculations are carried out for the carrier states. An important issue is how to use an eigen state solver like LCBB to calculate the transport in a nonequilibrium device. Various approximations will be discussed to calculate the current and the occupied charge density.

Elisa Antolin
(Universidad Politécnica de Madrid)

Empirical Methods in Quantum Dot Intermediate Band Solar Cell Research

Intermediate band solar cells (IBSCs) aim to improve the efficiency of solar cells by absorbing below bandgap energy photons. These photons are absorbed thanks to the existence inside the bandgap of a collection of energy levels, named "intermediate band (IB)", with the appropriate properties. Quantum dots (QDs) have been proposed as one of the means to take to practice the concept. Under the QD approach, the IB arises from the energy levels associated to the electrons confined in the conduction band (CB). In fact, QD-IBSCs have been manufactured in which the physical principles of the IBSC have been empirically tested. These work reviews these empirical methods which cover mainly: the analysis of the IB to CB transition, the voltage loss and the quasi-Fermi level split between the IB and CB.

David Binks
(University of Manchester)

Experimental Aspects of Multiple Exciton Generation

In bulk semiconductors, the energy of an absorbed photon in excess of the band gap is largely dissipated as heat. This process accounts for most of the energy lost in a conventional solar cell and places a theoretical limit of ~31% on their efficiency[1]. Multiple exciton generation (MEG), also known as carrier multiplication, is a competing process by which the excess photon energy is used instead to generate one or more additional excitons. MEG has been observed in bulk materials for many years but is too weak to have an impact on solar cell efficiency[2]. However, in recent years several groups have reported MEG efficiencies in colloidal nanoparticles (NPs) that are high enough to have a significant impact on solar cell performance[3-5]. However, other groups[6-8] have reported no or significantly weaker MEG in ostensibly similar NPs.

In this talk, I will describe the experimental techniques and the data analysis used to detect MEG and determine its efficiency. I will also discuss the experimental artefacts that complicate the interpretation of data and have probably led to the

recent controversy. Finally, I will outline the current status of this field and some considerations for the design of NP optimised for MEG.

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Guy Allan

(Institut d'Electronique, de Microelectronique et de Nanotechnology)

Carrier Multiplication in Bulk and Nanocrystalline Semiconductors: Mechanism, Efficiency, and Interest for Solar Cells

Carrier multiplication (CM), the possibility to generate more than one exciton in a semiconductor quantum dot (QD) after absorption of a single photon has been intensely debated in recent years. Tight-binding is well suited to calculate the electronic structure of nanomaterials (dots or wires) and can be applied to study CM. While first-principles local density calculations are limited to small size nanocrystals (~100 hundred atoms) and while effective mass approximation is applied to the very large ones, tight-binding fill the range between these two methods (~100 atoms to 100 000 or more depending on the symmetry). Thanks to the sparse tight-binding hamiltonian, we use the conjugate gradient method to calculate a few thousands of eigenstates close to the gap. Due to quantum confinement, the blue shift of the electronic levels close to the gap of a semiconductor is well known. This does not seem to affect the dielectric screening of these materials although one must take into account the « image charges » due to the zero-, one- or two dimensional geometry of the sample. This is an important effect and classical electrostatic well describes this phenomena.

Coming back to CM, we show that the impact ionization process is efficient at high energy, with lifetimes as small as 10 fs. The behavior of the impact ionization rate versus the energy is basically the same in all materials in spite of large differences in their electronic structure. This effect could not explain the experimental high yield (until 7 excitons per absorbed photon). Following another model developed in the literature, we have also calculated the spectral densities of multiexciton states and we have evaluated the possibility of direct and instantaneous photogeneration of multiexcitons. We confirm the importance of the multiexciton spectral densities in the MEG problem because of their rapid variation over several orders of magnitude as a function of the energy. However, we show that the high MEG efficiencies in PbSe and Si nanocrystals would imply a very efficient relaxation in multiexciton states.

Recent new measurements show that the effect is much smaller than the initial results and we have revisited our CM model. We show that our results are now in

good agreement with the experimental ones for bulk and nanocrystals semiconductors. We show that the density of one-electron states near the gap of the nanocrystal is one important parameter. Unfortunately, the relaxation energy of a carrier (electron or hole) is much larger than the gap such as it is difficult to reach the maximum value equal to the integer ratio of the photon energy divided by the nanocrystal gap energy.

We show that: (1) although the CM factor (i.e., number of generated photons per absorbed photon) at a given photon energy is higher in bulk than in QDs of the same material [Pijpers et al., Nature Phys. 5, 811 (2009)], the energy efficiency (the relative fraction of the photon energy that is transformed into excitons rather than heat) is higher in QDs; (2) for the same 1.2eV band gap, CM is more efficient in PbSe QDs than in bulk silicon; (3) nonetheless, the efficiency of solar cells based on PbSe QDs is not significantly enhanced by CM compared to a bulk silicon-based device.

Marco Califano
(University of Leeds)

An Atomistic Semiempirical Pseudopotential Guide to Excitation and De-Excitation Processes in Semiconductor Nanocrystals

Modern spectroscopic methods are becoming increasingly sophisticated and allow experimentalists to measure a wide range of optical properties with extremely high accuracy, enabling them to routinely resolve multiple features in the optical spectra of semiconductor nanocrystals and to investigate their carrier dynamics on the femtosecond time scale. This places unprecedented pressure on the theoretical models that are expected not only to produce a comparatively good level of agreement with experiment but also to correctly identify the different spectroscopic features assigning them to transitions between specific excitonic states, and to calculate decay rates for highly complex processes, such as Carrier Multiplication or Auger multiexciton recombination, where multiple electron-hole pairs are involved. In this talk I will give some examples of the degree of accuracy achievable by the semiempirical pseudopotential method [1] in reproducing many of the observed electronic and optical properties (from the extinction coefficients to the inter- and intra-band absorption spectra, from the Stokes' shifts to the Auger lifetimes) in nanocrystals made of different materials, ranging from rocksalt PbSe to wurtzite CdSe and zincblende InAs, highlighting the importance of the atomistic detail to build the correct picture at the single-particle level.

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TALK ABSTRACTS
Day 3 – Friday 25 June

Bernd Witzigmann
(University of Kassel)

*The Non-Equilibrium Green's Function Formalism for
Optoelectronic Devices*

The Green's function method is a powerful technique for analyzing many body quantum systems. For the description of non-equilibrium carrier dynamics in nanostructures, this technique allows the study of coherence in the presence of scattering in a natural way. In this contribution, the application of the Non-equilibrium Green's function (NEGF) technique to optoelectronics is reviewed. Electron and hole dynamics need to be studied, as well as the radiative recombination as non-local scattering process. The focus is set on the inclusion of radiative recombination and the applicability of the method to light emitting diodes.

INTRODUCTION

With the constant advances in nanotechnology, the performance of electronic devices routinely relies on electronic quantum effects. The underlying physics constitute a complex many-particle non-equilibrium quantum system, which makes a detailed theoretical description a challenging task. The NEGF formalism introduced by Kadano, Baym[1], and Schwinger, is a formidable method to study the time evolution of a many-particle quantum system.

This contribution gives an overview of the NEGF method applied to optoelectronic devices. Nanostructures such as quantum wells were used from the early days of semiconductor lasers on in order to engineer the electronic density of states in order to achieve high optical gain. Recently, the use of nanostructures for light emitting diodes and solar cells have gained much attraction. In semiconductor quantum wells, wires or dots, hetero structures form a nanoscale conning potential. Carriers populating the conned states have several channels for entering/leaving this system: they can surpass the energy barrier by thermionic emission type process, or tunnel through potential spikes formed by any electric field. Moreover, they can recombine via radiative or non-radiative channels. Fig. 1 illustrates these processes. In essence, the nanostructure forms an open quantum system where carriers possess partial coherence. The NEGF method has been applied to optoelectronic devices in[2] for quantum-well solar cells, in[3] for carbon nanotube photodetectors, and in[4] for light emitting diodes.

SIMULATION MODEL AND EXAMPLE

In our model, we employ an orthogonal finite element real-space basis and the equation of motion for electrons is given by the Dyson equation for the retarded Green function.

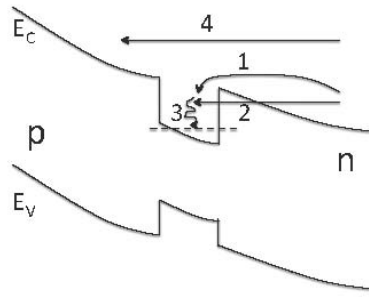


FIG. 1: Carrier dynamics in a quantum-well p-n junction as used in light emitting diodes. The different processes are: 1. Capture by thermionic emission 2. Capture by tunneling 3. relaxation scattering 4. carrier overpass.

The two-band effective mass Hamiltonian H contains the energy of the electrons, photons, phonons and their respective coupling terms. Inclusion of other band structure models is under way. Scattering involves polar optical phonon scattering and acoustic phonon scattering. Spontaneous emission of photons is described via a non-local scattering process and a coupling to an empty modal light field (i.e. no re-absorption of the photons occurs). Electron and hole densities are extracted from the lesser and greater Green's functions. In the presentation, electroluminescence and current voltage characteristics of a GaAs-based quantum-well LED is analyzed. The validity of current NEGF models for optoelectronics will be discussed and for the LED case, the NEGF results will be compared to other simulation approaches.

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Urs Aeberhard

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Non-Equilibrium Green's Function Theory of Quantum Photovoltaic Devices

Many high-efficiency photovoltaics concepts require an advanced control and manipulation of the optoelectronic properties of the active device structure, leading to a prominent role of low dimensional absorbers such as quantum wells, wires and dots in the implementation of these concepts. However, the quantum effects governing the optoelectronic characteristics of the nanostructures not only provide the desired design degrees of freedom, but also request new models for the description of the photovoltaic operation, since conventional macroscopic theories of generation, transport and recombination do not allow for a consistent consideration of such effects and the related device behaviour.

One of the common features of quantum photovoltaic devices is the dominant contribution from the strongly localized states of the low dimensional absorbers to

generation and recombination, while transport is mediated mainly via extended states. This means that one either has to find the ideal degree of localization which provides the best compromise between efficient transport and strong absorption, as indicated e.g. in the case of quantum well or quantum dot superlattices used in multi-junction solar cells, where miniband transport is required, or to optimize the processes that couple maximally localized absorbing states with maximally extended current carrying states, which corresponds to the situation encountered in quantum well solar cells.

The conventional approach to the problem described above is to combine a microscopic model for the physical processes involving confined states with a macroscopic, semiclassical theory for charge transport via the use of detailed balance rates determined within the microscopic theory. The resulting hybrid approach often provides effective fitting models able to quantitatively reproduce experimental device characteristics. However, at the same time, the large number of required ad-hoc assumptions tends to obscure the underlying mechanisms of quantum photovoltaic device operation, especially concerning the crucial processes of carrier escape and capture which couple localized and extended states. To go beyond the existing approaches in capturing the essential physics of quantum photovoltaic devices, a microscopic theory based on the non-equilibrium Green's function formalism (NEGF) for the electronic, optical and vibrational degrees of freedom was developed and applied to the simulation of quantum well solar cells [1,2]. The theory is capable to describe both optical and transport properties including quantum effects such as confinement and tunneling in an open non-equilibrium system under consideration of elastic and inelastic scattering effects leading to incoherence and relaxation.

In this talk, after an introduction to the theoretical framework of the NEGF for quantum photovoltaics, the approach is illustrated on the example of generation, escape and capture of charge carriers in quantum well solar cells.

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Ned Ekins-Daukes
(Imperial College London)

High Efficiency Quantum Well Solar Cells

The absorption of a p-i-n solar cell can be extended to lower photon energies by placing quantum wells into the intrinsic region. Photogenerated carriers escape the quantum well via a thermally assisted tunnelling process and contribute to the photocurrent of the solar cell. By using alternating compressive and tensile materials, a strain-balanced stack of quantum well and barrier layers can be grown, defect free, providing absorption-edge / lattice parameter combinations that are inaccessible using bulk materials. The high purity of the semiconductor material leads to radiatively dominated recombination enabling further efficiency gain by controlling the optical losses. When using compressively strained quantum well material, a small but fundamental efficiency advantage is realised over conventional bulk semiconductor solar cells on account of suppressed radiative emission from the light hole band. As a result, a strain-balanced GaAsP/InGaAs quantum well solar cell recently set a new record power conversion efficiency for a single semiconductor junction of 28.3%.

Andrei Schliwa

(Konrad-Zuse-Zentrum für Informationstechnik Berlin)

Application of Eighth-Band $k.p$ Theory to the Electronic Structure of Quantum Dots

Envelope function based eight-band $k.p$ theory in conjunction with the configuration interaction method developed into a workhorse for electronic structure calculations in nano-technology.

In this talk, we first outline the method of calculation with emphasis on the role of strain, piezoelectricity and the morphological properties of quantum dots.

In the second part, we focus on the application side and address three main topics:

(a) The bandstructure inversion problem, that is the possibility to gain information on the quantum dot (QD) morphology from its spectroscopic signature alone.

(b) The creation of entangled photon pairs by using InGaAs QDs grown on the (111)-substrate orientation.

(c) Nonvolatile flash memories based on GaAsSb/GaAs QDs. We address the dependence of the hole localization energy on QD size and composition.

Jose Manuel Llorens Montolio

(Insitute of Microelectronics of Madrid, CSIC)

Towards the Understanding of the Optical Properties of GaInAsSb/GaAs Self-Assembled Quantum Dots

The quest for laser diodes operating at $1.55 \mu\text{m}$ is currently leaded by InGaAsP/InP multi-quantum well (MQW) devices. It would be however desirable to achieve such operation wavelength in devices manufactured on inexpensive GaAs substrates. InAs/GaAs self-assembled quantum dots (SAQDs) are a feasible technology for developing laser diodes working at $1.3 \mu\text{m}$. However, shifting further the central emission towards longer wavelengths is still a challenge. Strain, confinement and intermixing effects

are mostly responsible of preventing InAs/GaAs QDs to emit at such longer wavelengths. Antimony can help in shifting the emission towards the spectral range of interest. On the one hand, the inclusion of Sb in the capping process reduces the elastic strain in the nanostructures, technique known as strainreducing-layer (SRL). On the other hand, the incorporation of Sb inside the QDs reduced the band-gap of the constituent material.[1, 2]

In this work, we present a theoretical study to understand the impact that Sb has on the electronic structure of InAs/GaAs QDs. We show that depending on the Sb concentration in the QD, the transition energy exhibits either a redshift or a blueshift. Such behaviour results of the trade-off between the bandgap reduction of the QD material and the increase of the strain due to the larger lattice constant of Sb based compounds with respect to As based ones.[3] At higher Sb concentrations, a type-II conduction band alignment takes place associated with a larger redshift. In addition, QDs exposed to Sb experience a change in their size. We discuss to which

extend the experimentally observed red shift should be attributed to changes in QD's composition or size. All calculation have been perform with the Nextnano software package.[4]

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POSTER ABSTRACTS

Soline Boyer-Richard
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Superlattice Band Diagram Calculation Using 30 Band k.p Method

The 8 band k.p method is efficient to obtain accurate semiconductor band structure at the center of the Brillouin zone (BZ) [Even, PRB 2008]. Extended to 30 bands, it allows obtaining the full BZ structure over 10 eV around the bandgap for bulk and strained semiconductors [Richard, PRB 2004],[Rideau, PRB 2006]. Quantum well band structures are also available in the valence and conduction bands even for indirect bandgap semiconductors [Richard, PRB 2005].

To describe superlattices along [001], the full band structure is necessary because X states are folded and mixed with Γ states. The k.p method develops wave functions on Γ periodic part of Bloch functions ψ_0 . For bulk band structure calculation, the Bloch function expressions are unnecessary to obtain energy levels. For heterostructures, Bloch functions are different in each material but they are usually taken equal in both materials. However, when considering folded X states, this approximation is too strong [Wang, PRB 1996].

To perform superlattice band structure calculation, an empirical pseudo-potential method has then been used to obtain Bloch functions ψ_0 in each material. Structure factors are introduced to obtain unitary transforms between the Bloch functions in each bulk material.

This calculation has been performed on the benchmark AlAs/GaAs superlattice and results are similar to those presented by Scholz et al. using tight binding calculations [Scholz, MRS 1998] and by Wang and Zunger [Wang, PRB 1998].

Miguel Caro
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Co-authors: S. Schulz, S.B. Healy, E.P. O'Reilly

An Interatomic Potential Model for the Study of the Elastic and Structural Properties of Nitride Alloys

In recent years, the use of group III nitrides has gained importance for novel optoelectronic applications. To engineer the electronic and optical properties of these devices, systems made of ternary and quaternary nitride alloys are of major interest. In contrast to conventional III-V materials the wurtzite group-III nitrides exhibit very strong electrostatic built-in fields. However, a direct way to measure and decouple the intrinsic polarization properties of nitride alloys is not easily possible. As a result theoretical studies of these systems are vital.

We present an interatomic potential model for group III nitrides, based on the idea initially presented by Martin[1] of assuming point ions and including the electrostatic interaction as well as Keating's valence force field (VFF), into the total energy of the system.[2] The calculated elastic and structural properties of the

binaries are in good agreement with the values reported by Vurgaftman.[3] A generalized model for nitride alloys may be obtained by an interpolation of the atomic interaction parameters of the binaries.

With our model, we study the elastic and structural properties of nitride alloys. Moreover, using a simple approach that relates the internal parameter u to the built-in polarization, nonlinearities for the alloys under consideration are reproduced.[4] Our preliminary results also show that clustering might be an important source of polarization nonlinearities in III-N alloys.

Given the low computational requirements of an interatomic potential model compared to density functional theory (DFT), our model represents an affordable way to perform calculations of strain and polarization in large supercells or even real size nanostructures, unachievable otherwise.

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Co-authors: B. Gallinet, J. Kupec and B. Witzigmann

Analysis of Photonic Crystal Defect Modes by Maximal Symmetrization and Reduction

Efficient light trapping with high quality factors and small modal volumes can be performed in photonic band-gap microcavities. They offer numerous applications in quantum photonics and information processing, such as low-threshold optically or electrically pumped lasers, all-optical devices based on non-linear photonic crystals and control of spontaneous emission for single photon sources. For this type of applications where discrete geometries govern light trapping and propagation, a symmetry analysis of the defect modes in photonic waveguides and cavities is an extremely relevant investigation and can offer a deep understanding of their structure. The symmetry of defect modes can also be an important aspect of the design in integrated optics, and plays a central role in optical devices such as add/drop filters, quantum entanglement and more recently in cavity optomechanics. Empirical methods based on symmetry considerations have been introduced to describe the structure of defect modes in photonic crystal cavities (PCCs), in order to predict their emission pattern or polarization. It is also well known that they can be classified with the irreducible representations (irreps) of the relevant symmetry group. Symmetry can however be exploited much further, and it is the purpose of the present paper to show that one finds optimal decompositions of vectorial modes, which indeed have intricate internal symmetries due to their vectorial 3D nature. The proposed maximal symmetrization technique (MSR) decomposes the vectorial mode components into completely symmetrized independent scalar functions called Ultimately Reduced Component Functions (URCFs) [1,2]. Coupled to the symmetry analysis of URCFs, drawn from a recently developed technique called Spatial Domain Reduction (SDR), we give analytical predictions about the mode structure with unprecedented detail. In particular all remarkable properties on singular points and along symmetry axes can be

extracted systematically. This is of crucial importance since mode symmetry do impact essential physical characteristics in devices, like radiative coupling. In C_{2v}, C_{3v}, C_{4v} and C_{6v} symmetry (e.g. H1 and L3 cavities) we address both fundamental and excited mode polarizations, degeneracies, as well as some of their most remarkable geometrical properties. To the best of our knowledge, we give the first analytical proofs related to the TE/TM mode electric field at the cavity center for every type of mode in C_{6v} symmetry (e.g. H1 cavities): TE is non-vanishing only for degenerate E₁ dipole-like modes, whilst TM is non-vanishing only for the non-degenerate A₁ monopole-like modes. But many more new features were derived. Another useful outcome is the computation of the fraction of the energy of the mode components in each symmetry (URCF), and the explanation of specific relationships which may occur between them, as a result of symmetry coupling between the eigenmode components. These results will be illustrated by post-symmetrization of full 3D numerical eigenmode calculations, in an L3 and H1 photonic crystal defect, providing a deep test of the heavy numerics in addition to physical insight.

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Daniel Farrell
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Challenges to Realising High-Efficiency Photovoltaics

Conventional solar cells, operating under ideal conditions, perform with an efficiency around 20-28%[1]. This has been reached after many years of research, but still seems relatively low. In fact the opposite is true; conventional solar cells are performing close to their thermodynamic efficiency limit of ~31%[2]. The challenge to realising high-efficiency photovoltaics is to seek materials and devices that have higher fundamental efficiency limits and use these as the basis of the next generation technologies. In this presentation the options for future photovoltaics devices are assessed and grouped into 4 categories: photovoltaic conversion with,

1. multiple junctions,
2. multiple levels [3,4],
3. spectral management [5,6] and,
4. hot-carriers [7,8].

For each category the efficiency limits and the required material properties are discussed.

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Atomistic Description of Large Nanostructures Based on III-Nitride Semiconductors

Semiconductor nanocolumns exhibiting a growth without dislocations and high crystalline quality are of great interest in nanotechnology applications. Specifically, InN-based nanocolumns are good candidates to develop multi-junction solar cells due to their small gap, 0.67 eV, and the possibility of alloying with other nitrides (as GaN and AlN) to cover the entire solar spectrum.

A proper description of optical properties of the nanostructures described above can start with an atomistic treatment of the electronic structure in order to keep the essential geometry and symmetry of the objects. Unfortunately, the best description realized with ab initio electronic structure software is strongly limited by the nanocolumn diameter to a few nanometers. By using a combination of ab initio and empirical tight-binding methods, we can connect the quality of the first principles calculations (performed with the Espresso code), with the versatility of an empirical approach.

We propose a methodology to extend the accuracy of ab initio electronic structure calculations to larger nanostructures, significantly reducing the computational time. We study the bulk and small nanostructures with an ab initio method and fit the parameters of the tight-binding model to these results. Once we have an ab initio quality parameter set for the empirical tight-binding code, we can study larger nanostructures with this approach, reducing the computation time in orders of magnitude, without losing the atomistic details, proper symmetry and accuracy of the initial method.

Nikola Prodanovic

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Co-authors: Jelena Radovanovic, Vitomir Milanovic, Stanko Tomic

Optimization of AllnAs/InAs Quantum Well Based up Converter for Si Solar Cells

One of the major obstacles for high efficient power conversion of the sun light with conventional semiconductor materials is that only photons with energies close to that of the semiconductor energy gap (E_g) are effectively converted into electron-hole pairs. Photons with lower energy than E_g are simply lost (the semiconductor is transparent to them); and out of the photons with higher energy ($> E_g$), only a part i.e., those with energy almost equal to E_g are best suited for absorption. The majority of high energy electrons generated by photons with $> E_g$, (hot carriers) decay thermally to the Fermi level of the conduction band before they can contribute to the output current.

The principal aim here must be to make better use of the solar spectrum [1,2]. One of promising concepts is to place another device component, "light converter", attached to the rear of an existing solar cell (SC), to capture sub-energy gap photons and reemitt them at the frequency greated than the energy gap of the SC. If luminescent materials, either bulk or nanostructured, are placed in a layer to

absorb short (long) wavelength light from the sun - a region where many commercially-produced PV modules exhibit a poor spectral response - and re-emit this light at longer (shorter) wavelengths to match the region where SC exhibits a very good spectral response, it is possible to enhance the conversion efficiency of the SC device [1]. Up- or down- conversion occurs in the three- level quantum mechanical systems simultaneously.

In this paper the optimization procedure for up- converter, based on AIAs/AlInAs quantum well structure, for silicon solar cells is proposed. Up- conversion entails the conversion of low frequency photons, whose energy is insufficient for silicon interband transitions, into higher frequency photons which can be absorbed by Si solar cell. Such low frequency photons can be converted by utilizing nonlinear effects in quantum well based structures. To allow for sufficient output photon energy of the converter, we consider the asymmetric step quantum well (AlInAs/InAs) which is deep enough to accommodate two bound states. The continual part of the spectrum is used as the third "state, in particular the state which effectively "selects" the emitting photon frequencies suitable for silicon solar cells. Optimization of up- converter is performed by maximization of the second order susceptibility derived from the density matrix formalism. In our procedure, based on the use of global optimization tools (combined simulated annealing and genetic algorithm) [3], we vary the well structural parameters which affect the nonlinear susceptibility. To minimize overall computational load, starting for 8-band k.p Hamiltonian, we have derived one band model, that takes into consideration effects like strain, band mixing, and band nonparabolicity. This model is used in combination with the optimization algorithm for calculation of electronic states in the quantum well and dipole matrix elements dependent nonlinear susceptibility.

Specifically, for one-step quantum wells we have four input arguments of susceptibility: the widths of step and well layers, the content of AlInAs in the step region and the height of the outer barrier. These input parameters are subject to physical and technological constraints, which enable us to obtain a realistic optimized AlInAs/InAs quantum-well structure which supports three states with suitable energy spacings for up-conversion.

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Theory of Scattering and Impact Ionization in Dilute Nitride Avalanche Photodiodes

It is well established that replacing As by N in GaNAs leads to a strong perturbation of the conduction band structure, generally described using the band-anticrossing (BAC) model [1]. We have solved the supercell zone centre Hamiltonian for a large supercell with 4 million unit cells containing 8000 randomly placed N, to calculate the projected density of states. Our calculations confirm the validity of using the

BAC model (with energy broadening) to describe the evolution of the band dispersion with wavevector k in GaNAs. This strong perturbation also leads to a marked reduction in low-field electron mobility [2], and has been predicted to suppress electron multiplication in avalanche photodiodes [3]. We use the Boltzmann equation [4] to investigate for large electric fields the distribution of electrons and the electron drift velocity in the lowest conduction band of dilute nitride semiconductors. The overall transport behaviour calculated using the Boltzmann approximation is in good agreement with previous calculations using dynamical balance equations [5], but both sets of calculations show a much stronger negative differential velocity at higher fields than is observed experimentally [5].

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The Manchester workshop - which will focus on the scientific applications of the subject - was preceded by a similar workshop hosted by the Tyndall National Institute and held at University College Dublin. The Dublin workshop focussed more on the technical aspects of the subject.

The abstracts from the Dublin workshop are included here for reference.

Gabriel Bester
(Max Planck Institute for Solid State Research)

Empirical and Semi-Empirical Pseudopotential Approaches

In this contribution I will outline the framework, based on empirical pseudopotentials and configuration interaction, to obtain quantitative predictions of the excited state properties of semiconductor nanostructures using their experimental sizes, compositions and shapes. The methodology can be used to describe colloidal nanostructure of few hundred atoms all the way to epitaxial structures requiring millions of atoms. The aim is to fill the gap existing between ab initio approaches and continuum descriptions. We are developing pseudopotentials based on DFT-LDA but corrected for the band gap and effective masses using empirical functions. The method gives access to an accurate electronic quasiparticle structure. We do not attempt to calculate the total energy, which enables us to treat large nanostructures. I will present the construction of these potentials and the way the ensuing wave functions are used in a subsequent configuration interaction treatment of the excitation for the excitonic properties. I will present our recent efforts towards the reduction of empiricism in the correction of LDA and an improved scheme in the treatment of correlations in our configuration interaction treatment. I will briefly illustrate the capability of the method on specific examples and the good agreement we obtain with experiments

Timothy Boykin
(University of Alabama at Huntsville)

Physics and Numerics of Multi-Band Tight-Binding Nanostructure Models

The multi-band tight-binding approach is well-suited for nanostructure modeling. The localized-orbital basis allows for efficient treatment of surfaces and interfaces, enabling the efficient calculation of the electronic structure and transport properties of nanodevices and nanostructures. The NEMO and OMEN tools utilize the empirical tight binding models heavily and demonstrate that quantitative agreement with experimental data can be obtained without any material parameter adjustments. Examples include multimillion atom InAs/InGaAs/GaAs quantum dot systems, disordered Si/SiGe quantum wells, and Single impurity systems. Effective application of the method does, however, require some care. Because it automatically includes evanescent states, properties must be calculated in a

numerically stable manner. The basis, like all bases used in practical calculations, is incomplete, and hence calculation of effective masses and inclusion of the electromagnetic vector potential are different than in continuous quantum mechanics. To obtain the approximate bands of alloy nanowires, supercell techniques and methods based on Brillouin zone unfolding can be effectively employed. We discuss the physical and numerical aspects of these topics with special reference to the NEMO-3D and OMEN simulation packages.

Brad Foreman

(Hong Kong University of Science and Technology)

Construction of Nanostructure Envelope-Function Models from First Principles

This talk will provide an overview of the key issues involved in deriving and implementing a multi-band envelope-function model for semiconductor nanostructures from first principles. The general formalism allows the inclusion of spinor quasiparticle self-energies [1,2], but the numerical implementations described here [3,4,5] use the local-density approximation to density-functional theory and norm-conserving pseudopotentials without spin-orbit coupling.

The first step is the construction of a simple but accurate approximation for the self-consistent nanostructure pseudopotential [1,3]. Deviations of the bare ionic pseudopotentials from those of a virtual bulk reference crystal are treated as perturbations. The linear and quadratic responses to a set of elementary monatomic and diatomic perturbations are calculated self-consistently. These monatomic and diatomic building blocks are then assembled to obtain the nanostructure pseudopotential (in the quadratic-response approximation). The results are shown to be good to within a few meV for typical semiconductors.

In the second step, the approximate pseudopotential is used to construct a k.p or envelope-function Hamiltonian. This can be done in many different ways, corresponding to different choices of perturbation theory. The main method described here is a straightforward application of Luttinger-Kohn perturbation theory in which both the nanostructure pseudopotential and the k.p interaction are treated as perturbations [2,4]. However, other choices may be useful in, for example, eliminating spurious solutions [5] or extending the domain of validity of the model to a larger fraction of the Brillouin zone.

The predictions of the envelope-function model are compared directly with numerical LDA calculations (for superlattices containing about 100 atoms) and shown to be accurate to within a few meV. Various limitations of the resulting model are discussed. The final Hamiltonian incorporates numerous effects not considered in previous studies and sheds light on some controversial issues such as operator ordering. The chosen parameterization of k.p material properties in terms of atomic and diatomic building blocks may be useful in empirical models as well.

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Physics and Numerics of Multiband k.p Nanostructure Models

The k.p method was introduced over 50 years ago for bulk semiconductors and with slow perturbations. Through an ad-hoc symmetrization and through an envelope-function theory by Burt and Foreman, the multiband k.p method has been extended to nanostructures. The continuum description makes it one of the most efficient method for calculating the band structure of large nanostructures. In this talk, we will compare various facets of the implementation of the theory: Luttinger-Kohn versus Burt-Foreman Hamiltonian, zincblende versus wurtzite, single-k point versus full-zone description, and application to quantum wells, wires and dots. Furthermore, we will discuss the calculation of optical and piezoelectric properties. Numerical implementations will also be discussed; in particular, we will present the finite-element-based method that our group has used and compare to plane-wave methods and compare various multiband models. The problem of spurious solutions will be addressed.

Marc-André Dupertuis
(Ecole Polytechnique Fédérale de Lausanne)

Symmetries in Nanostructures: From the Physical Aspects to the Computational Aspects

High symmetry effects in nanostructures have recently become a subject of high interest. On the one hand one is now realizing that for prominent applications such as efficient entangled photon generation quantum dot symmetry could be the missing ingredient [1,2]. On the other hand one has recently found that a group theoretical analysis of the fine structure splittings of excitonic complexes was able to disentangle and interpret in a powerful way the complete spectroscopy of C_{3v}-quantum dots [3], evidencing symmetry elevation and symmetry breaking, and providing a synthetic picture for all observed transitions, including the minor ones. The goal of the present work is first to demonstrate how to apply symmetry arguments at different levels to nanostructures, experimentally and numerically, by treating the seminal example of complexes in Cs- and C_{3v}-quantum wires and quantum dots. We have demonstrated that great gains could be obtained on two fronts: 1) physical insight and specific clear cut predictions based on symmetry, 2) enhancement by orders of magnitude of the efficiency and reliability of numerical k.p computations, including subsequent many-body CI calculations. We have used also such a fully symmetrized approach as a post-processing algorithm, alleviating in this case any need of recoding.

A second outcome of our work has been the development of what is, to the best of our knowledge, the most advanced group theoretical treatment of nanostructures for quantum dots/wires. Indeed the standard way of applying group theoretical considerations to the spectrum of a physical system is usually to classify its eigenspaces with irreps of the symmetry groups. This approach is global, i.e. not

depending on the complexity of the construction of eigenstates from primitive constituents, and is powerful. Nevertheless we shall show that it is possible to use also symmetry at an intermediate level in the theory, and that it is again extremely helpful. We have called this general and systematic method “Maximum Symmetrization and Reduction (MSR)” [4]. An essential step of MSR is a systematic Spatial Domain Reduction (SDR) technique, which allows to reduce a salar equation on the minimal domain with automatic incorporation of the possible non-trivial boundary conditions. For a vectorial or spinorial set of functions, the SDR technique must be completed by the use of an optimal basis, and leads to an essential set of Ultimately Reduced Envelope Function (UREF). The SDR method leads to a bunch of new useful analytical results about the values of the functions and their derivatives at critical points of the boundaries, or between the subdomains. The advantages of MSR are numerous: sharper insights on the symmetry properties of every eigenstate, minimal coupling schemes, analytically and computationally exploitable at the component function level, minimal computing domains.

Finally, we predict the emergence of a few novel structure-independent analytical ratios of polarization anisotropy for certain transitions in C3v-quantum wires and quantum dots, whilst others, in the same spectrum, remain structure-dependent. This is one example of the predictive power of the MSR approach, the experimental verification of such a beautiful phenomenon still remains a challenge.

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Stefan Birner
(nextnano3)

Full-Band Envelope-Function Approach for Type-II Broken-Gap Superlattices

We present a novel charge self-consistent electronic structure scheme for InAs/GaSb type-II broken-gap superlattices [1, 2] that is based on the multiband $\mathbf{k}\cdot\mathbf{p}$ envelope function method. In broken-gap heterostructures (Fig. 1(a)), the standard multiband effective mass theory fails to yield the correct free carrier charge density because the separate occupation of electron and hole states is incompatible with a strong hybridization of conduction band and valence band states (Fig. 1(b)). In our method, we remain in the electron framework throughout and occupy all included subbands according to Fermi statistics. Subsequently, we subtract a positive background ionic charge that guarantees charge neutrality. With this procedure, we calculate optical transition energies of intrinsic InAs/GaSb superlattices as a function of the layer width. We find excellent agreement with experimental data in a regime where the superlattices exhibit a crossover in the energetic order of the lowest electron-like and the highest hole-like subbands. We discuss the implementation of this approach into the nextnano software [3] and review the current status of the nextnano project.

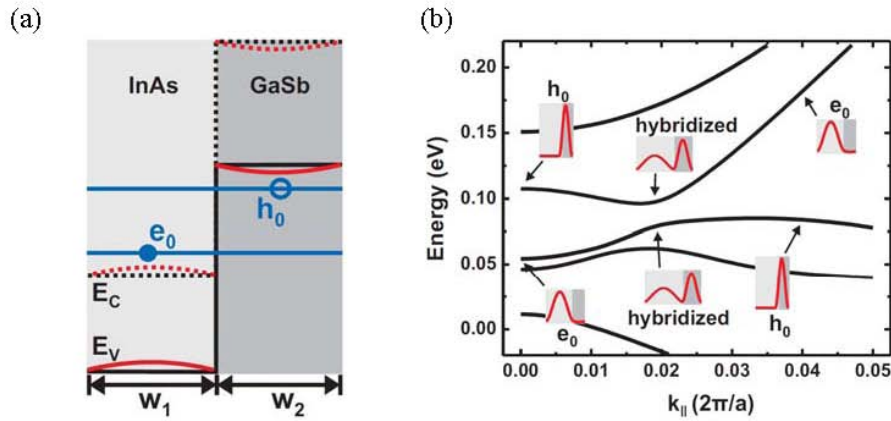


Fig. 1: (a) Band structure of InAs/GaSb superlattice with InAs and GaSb layer widths w_1 and w_2 , respectively. The broken gap ($E_G < 0$ eV) band edges in position space with qualitative zone center subband energies are sketched. Here, the energy of the electron ground state is lower than the hole ground state: $E(e_0) < E(h_0)$. In this case, a charge transfer between the different layers is expected that leads to a band bending as indicated. (b) Subband dispersions as a function of $k_{||}$ in the lateral direction of an InAs/GaSb superlattice with InAs and GaSb layer widths of $w_1 = 16$ nm and $w_2 = 8$ nm, respectively. The insets show probability densities of subband eigenstates at three different values of $k_{||}$ (0, 0.2, and 0.04 in units of $2\pi/a$, where a denotes the lattice constant of GaSb). The character of the individual eigenstates can be assigned from their localization in the InAs (light gray) or the GaSb (dark gray) layers. All energies are given relative to the zone center conduction band maximum in the InAs layer.

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Andrew Sunderland
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Parallel Symmetric Eigensolver Performance on High-End Computing Platforms

Eigenvalue and eigenvector computations arise in a wide range of scientific and engineering applications and usually represent a huge computational challenge. It is therefore imperative that appropriate, highly efficient and scalable parallel eigensolver methods are used in order to facilitate the solution of the most demanding scientific problems. This presentation will analyze and compare the performance of several of the latest eigensolver algorithms, including pre-release ScaLAPACK routines, on contemporary high-end systems such as the 11,328 core Cray XT4 UK system HECToR. The analysis will involve symmetric matrix examples obtained from current problems of interest from several large-scale scientific applications.

Mikhail Nestoklon
(IOFFE institute)

Atomistic Modeling in Nanostructures: the $spds^$ Tight-Binding Model*

As high-performance computers are becoming more affordable, atomic-scale modeling is gaining importance as an investigative tool in materials science. Complementing *ab initio* and empirical approaches within atomic-scale simulations provide detailed information about the physical properties of materials. While first principles techniques like density functional theory (DFT) in the local density approximation (LDA) are well suited to predict structural properties and electronic bands over a large energetic region [1], the calculation of excited-state properties is still unsatisfactory. The necessity to accurately interpret the excited-state properties of semiconductor nanostructures has led to the development of various empirical approaches, ranging from empirical pseudopotentials (PP) [2] over kp models [3] to tight-binding (TB) methods [4].

Tight binding has existed for many years as a convenient and transparent model for the description of electronic structure in molecules and solids. Historic paper of Slater and Koster [5] provided the systematic procedure for formulating a tight binding Hamiltonian. Since the TB method uses only few basis functions, it is significantly more computationally efficient than methods based on plane-waves basis sets. Over the last 40 years a numerous applications of this approach were focused on diverse problems, following different philosophies and placing different levels of emphasis on the required level of accuracy. One of these philosophies is to determine the minimal basis of atomic orbitals suitable for accurate description of the electronic band structure of semiconductors. From interpretations of the electronic wavefunctions calculated with pseudopotential methods in terms of atomic symmetries it became obvious that d -symmetric contributions play a crucial role both for the valence band maximum at Γ and for the conduction states at X and L. This has led to basis extensions of earlier sp^3 [6] and sp^3s^* [4] TB models towards the inclusion of all five atomic d -states which are necessary for a reliable description of the valence bands and the first two conduction bands across the Brillouin zone [7], defining the empirical $sp^3d^5s^*$ TB model.

Tight-binding is perfectly suited for large-scale electronic structure calculations where a precise three-dimensional band structure is required. We illustrate this point from the study of spin properties in (110) quantum well systems that are a good example of pure interface physics where an accurate band structure description is required as well as an account on atomic structure at the interface. The second example we discuss concerns the modeling of the acceptor Mn state in GaAs bulk. Resent STM measurements have revealed unexpected features of shape of the localized hole state, the most evident one is significant anisotropy of surface local density of states in the presence of sub-surface Mn impurity. Some efforts have been devoted to get insight into the nature of this feature, but until now there is no consensus in the underlying mechanism [8, 9]. In this context we show that the $spds^*$ TB model is in agreement with the experimental observations, allowing to perform relatively easy and real-time calculation comparable in precision and physical details with best *ab initio* calculations.

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Semiconductor Nanowire Simulation for Technology Design

The recent fabrication of semiconductor wires with just a few nanometers in cross-section has upheld their strong position for applications in nanoelectronics and nanophotonics. Size-effects as well as surface chemistry play an important role for nanowires with this diameter [1]. Here, I will give an overview of our simulation tools within the Electronics Theory Group at Tyndall aiming at the determination of practical limits to electron device scaling. In particular, I will present our recent atomistic studies on scattering due to local oxidation [2] and electron-phonon coupling [3] and I will highlight the connection to and departure from effective continuum theories that can be used in nanowire transistor modelling [4].

The role of reduced dimensionality and of the surface on electron-phonon (e-ph) coupling in silicon nanowires is determined from first principles. Surface termination and chemistry is found to have a relatively small influence, whereas reduced dimensionality fundamentally alters the behaviour of deformation potentials. As a consequence, electron coupling to 'breathing modes' emerges that can not be described by conventional treatments of e-ph coupling. The nanowire deformation potentials are found to be highly anisotropic, leading mobilities in [110] wires to be 6 times larger than on [100] grown wires.

Also, using density functional theory in conjunction with a Green's function scattering method, it is found that the introduction of oxygen bridging and back bonds in narrow [110] Si nanowires does not significantly degrade hole transport for voltages up to several hundred millivolts relative to the valence band edge. As a result, the mean free paths are comparable to or longer than the wire lengths envisioned for transistor and other nanoelectronics applications. As in the case for e-ph scattering, transport along [100]-oriented nanowires is found to be less favorable.

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Time	Wednesday 23 / 06 / 10	Thursday 24 / 06 / 10	Friday 25 / 06 / 10
Chair	Stanko Tomic	Max Migliorato	G.P. Srivastava
9.00 - 9.30	Stanko Tomic (STFC Daresbury Laboratory) <i>Welcome: Advance in Empirical Electronic Structure Methods for Nanostructures</i>	Aldo Di Carlo (University of Rome "Tor Vergata") <i>Multiscale Simulations of Nanostructured Devices with TiberCAD</i>	Bernd Witzigmann (Universität Kassel) <i>The Non-Equilibrium Green's Function Formalism for Optoelectronic Devices</i>
9.30 -10.00	Frederic Aniel (Université Paris-Sud) <i>The k.p Theory Beyond Standard 8-Band Theory Parametrization Strategies and its Applicability in Electronics and Optoelectronic Devices Design</i>		
10.00 - 10.30		Pawel Hawrylak (University of Ottawa) <i>QNANO: Computational Platform for Semiconductor Nanostructures</i>	Urs Aeberhard (Forschungszentrum Jülich) <i>Non-Equilibrium Green's Function Theory of Quantum Photovoltaic Devices</i>
10.30 - 11.00	Coffee		Coffee
11.00 - 11.30	Wlodek Zawadzki (Polish Academy of Sciences) <i>Effects of Spin-Orbit Interaction on Spin Properties of Electrons in III-V Semiconductor Heterostructures</i>	Coffee	Ned Ekins-Daukes (Imperial College London) <i>High Efficiency Quantum Well Solar Cells</i>
11.30 - 12.00		Lin-Wang Wang (Lawrence Berkeley National Laboratory) <i>LCBB Method for CMOS Device Simulations</i>	
12:00 - 12:30	Guido Goldoni (Università degli Studi di Modena e Reggio Emilia) <i>Few-Body Physics in Semiconductor Quantum Dots with the Configuration Interaction Approach</i>		Andrei Schliwa (Konrad-Zuse-Zentrum für Informationstechnik Berlin (ZIB)) <i>Application of Eighth-Band k.p Theory to the Electronic Structure of Quantum Dot</i>
12.30 - 13.00		Elisa Antolin (Universidad Politécnica de Madrid) <i>Intermediate Band Solar Cells</i>	
13.00 - 13:30	Lunch	Lunch	Jose Manuel Llorens Montolio (Instituto de Microelectrónica de Madrid) <i>Towards the Understanding of the Optical Properties of GaInAsSb/GaAs Self-Assembled Quantum Dots</i>
13.30 - 14.30			WORKSHOP CLOSES
Chair	Eoin O'Reilly	Eoin O'Reilly	
14.30 - 15.00	Vladimir Falko (Lancaster University) <i>Electrons in Bilayer Graphene: Lishitz Transition and Spontaneous Symmetry Breaking</i>	David Binks (University of Manchester) <i>Experimental Aspects of Multiple Exciton Generation</i>	
15.00 - 15.30		Guy Allan (Université Lille 1) Carrier Multiplication in Bulk and Nanocrystalline Semiconductors: Mechanism, Efficiency, and Interest for Solar Cells	
15.30 - 16.00	Bart Partoens (University of Antwerp) <i>Tight-Binding Description of Graphene, Graphene Multilayers and Graphite</i>		
16:00 - 16:15	Coffee	Coffee	
16.15 - 16.45	Michael Flatté (University of Iowa) <i>Empirical Tight-Binding and Real-Space Envelope-Function Calculations of Single-Donor Spin Dynamics</i>	Marco Califano (University of Leeds) <i>An Atomistic Semiempirical Pseudopotential Guide to Excitation and De-Excitation Processes in Semiconductor Nanocrystals</i>	
16:45 - 17:15			
17.15 - 19.00	Poster Session	Round Table Discussion (Chair: Stanko Tomic)	