# SCIENTIFIC MEMORANDUM
# Constantinos Simserides

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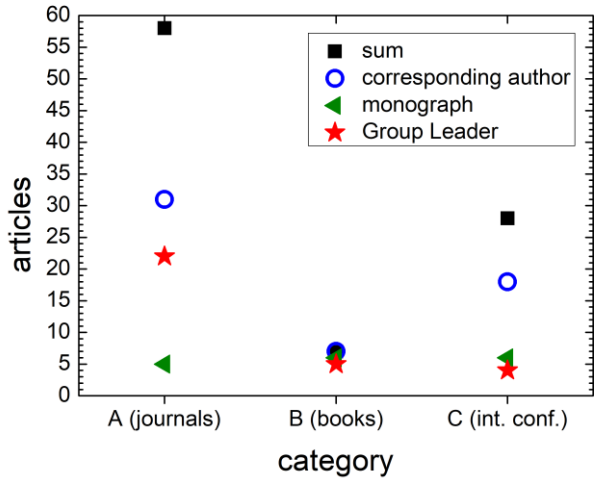



## Some numbers

| *number of authors in publication* | *Type A* | *Type B* | *Type C* | *Type D* | *Type E* |
|---|---|---|---|---|---|
| **monograph** | **5** | **6** | **6** | **0** | **1** |
| 2 authors | 13 | 0 | 1 | 2 | 1 |
| 3 authors | 17 | 1 | 13 | 3 | |
| 4 authors | 13 | 0 | 6 | 2 | |
| ≥ 5 authors | 10 | 0 | 2 | 1 | |
| **Group Leader in Athens** | **22** | **7** | **4** | **1** | |

| *my position in author list* | *Type A* | *Type B* | *Type C* | *Type D* | *Type E* |
|---|---|---|---|---|---|
| 1st author | 19 | 7 | 14 | 3 | 2 |
| 2nd author | 17 | 0 | 8 | 2 | |
| 3rd author | 9 | 0 | 4 | 1 | |
| 4th author | 8 | 0 | 0 | 1 | |
| ≥ 5th author | 5 | 0 | 2 | 1 | |
| *** corresponding author** | **31** | **7** | **18** | **3** | **2** |

| | | | | | |
|---|---|---|---|---|---|
| Total number of publications | 58 | 7 | 28 | 8 | 2 |

| Google Scholar 09/11/2024 | All | From 2019 |
|---|---|---|
| Citations | 1116 | 468 |
| h-index | 19 | 14 |
| i10-index | 36 | 18 |

**My counting of citations is the following (double citations, e.g., arXiv & Journal are taken as one):**

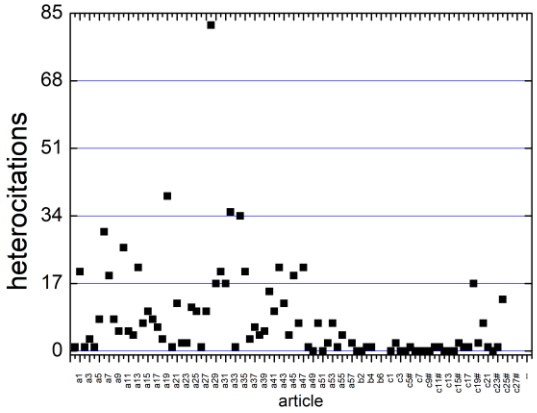
**705** Heterocitations

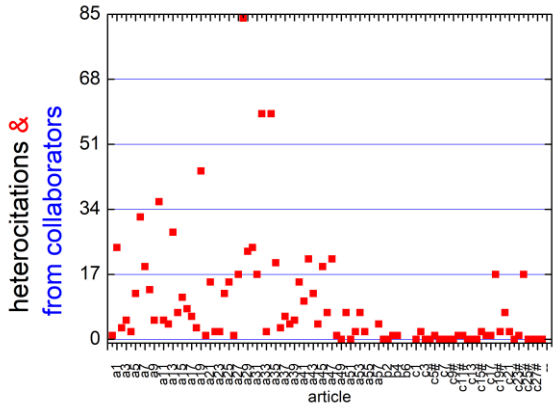
**14** Heterocitations in technical reports, abstracts, talks, collection, open-ebooks (list not complete)

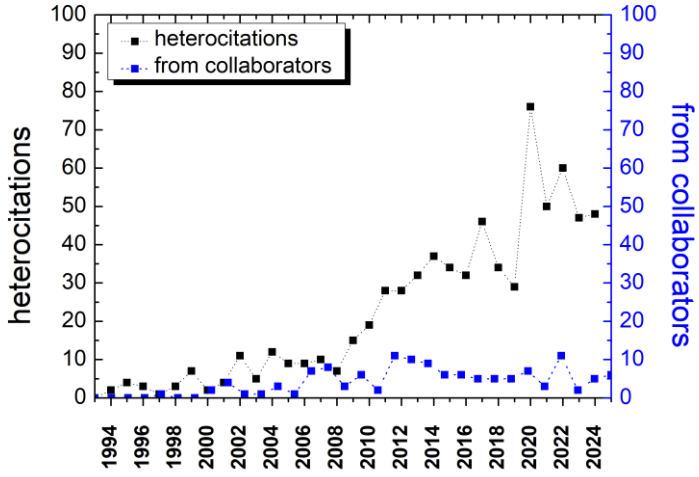
***130*** *Citations from collaborators*

***9*** *Citations from collaborators in technical reports and abstracts (list not complete)*

According to the data shown below,
my h-index (heterocitations only) is **17**
my h-index (heterocitations and citations from collaborators, excluding self-citations) is **17**




## A. 58 publications in international journals with referees

a58) Electronic structure, absorption spectra and oxidation dynamics in polyynes and dicyanopolyynes
L. Chalkopiadis, K. Lambropoulos and C. Simserides
Physical Chemistry Chemical Physics **26** (2024) 22149 - 22163 doi: 10.1039/D4CP02719A

The advent of femtosecond to attosecond experimental tools has made now possible to study such ultrafast carrier dynamics, e.g., the spatial and temporal charge density evolution, after an initial oxidation or reduction in molecules, candidates for atomic wires like polyynes and dicyanopolyynes. Here, we study the electronic structure and hole transfer in symmetric molecules containing carbon, nitrogen and hydrogen, the first members in the series of polyynic carbynes and dicyanopolyynes, using methods based on density functional theory (DFT): constrained DFT (CDFT), time-dependent DFT (TDDFT) and real-time TDDFT (RT-TDDFT), with Löwdin population analysis, comparing many levels of theory and obtaining convergence of the results. For the same purposes, we develop a Tight Binding (TB) variant using all valence orbitals of all atoms. This TB variant is applied here in linear molecules, but it is also adequate for electronic structure, charge transfer and charge transport of non-linear molecules and clusters of molecules. We calculate the electronic structure, the time-dependent dipole moment and the probabilities of finding the hole at each site, their mean over time values, the mean transfer rates from the oxidation site to other sites and the frequency content (using charge as well as dipole moment oscillations). We take into account zero-point motion. The initial conditions for RT-TDDFT are obtained by CDFT. For TB, we explore different initial conditions: we place the hole at a particular orbital or distribute it among a number of orbitals; it is also possible to include phase differences between orbitals. Finally, we compare with available experimental data.

a57) Charge transport in a double-stranded DNA: Effects of helical symmetry and long-range hopping
Sourav Kundu and **Constantinos Simserides**
Physical Review E **109** (2024) 014401 doi: 10.1103/PhysRevE.109.014401
Heterocitations 2, *From collaborators 2*

Within a tight-binding framework, we examine conformation-dependent charge transport properties of the DNA double-helix, including helical symmetry and the possibility of multiple charge conduction pathways. Using techniques based on the Green's function method, we inspect changes in the localization properties of DNA in the presence of long-range hopping, with varying disorder strength. We study three characteristic DNA sequences, two periodic and one random. We observe that, in all cases, due to disorder-induced delocalization, the localization length variation is similar. We also investigate the effect of backbone energetics on current-voltage (I-V) responses, using the Landauer-Büttiker formalism. We find that, in the presence of helical symmetry and long-range hopping, due to environmental effects, DNA can undergo a phase transition from semiconductor to insulator.

a56) Electronic Structure and Hole Transfer of All B-DNA Dimers and Homopolymers, via the Fishbone-Wire Model
**C. Simserides***, A. Orfanaki, N. Margariti, K. Lambropoulos
Materials **16** (2023) 3200 (25 pages) doi: 10.3390/ma16083200

We employ the Tight Binding Fishbone-Wire Model to study the electronic structure and coherent transfer of a hole (the absence of an electron created by oxidation) in all possible ideal B-DNA dimers as well as in homopolymers (one base pair repeated along the whole sequence with purine on purine). The sites considered are the base pairs and the deoxyriboses, with no backbone disorder. For the time-independent problem, we calculate the eigenspectra and the density of states. For the time-dependent problem after oxidation (i.e., the creation of a hole either at a base pair or at a deoxyribose), we calculate the mean-over-time probabilities to find the hole at each site and establish the frequency content of coherent carrier transfer by computing the Weighted Mean Frequency at each site and the Total Weighted Mean Frequency of a dimer or polymer. We also evaluate the main oscillation frequencies of the dipole moment along the macromolecule axis and the relevant amplitudes. Finally, we focus on the mean transfer rates from an initial site to all others. We study the dependence of these quantities on the number of monomers that are used to construct the polymer. Since the value of the interaction integral between base pairs and deoxyriboses is not well-established, we treat it as a variable and examine its influence on the calculated quantities.

a55) Charge transport properties of ideal and natural DNA segments, as mutation detectors
M. Mantela, K. Lambropoulos, **C. Simserides***
Physical Chemistry Chemical Physics **25** (2023) 7750 - 7762 doi: 10.1039/D3CP00268C
Heterocitations 4

DNA sequences of ideal and natural geometries are examined, studying their charge transport properties as mutation detectors. Ideal means textbook geometry. Natural means naturally distorted sequences; geometry taken from available databases. A tight-binding (TB) wire model at the base-pair level is recruited, together with a transfer matrix technique. The relevant TB parameters are obtained using a linear combination of all valence

orbitals of all atoms, using geometry, either ideal or natural, as the only input. The investigated DNA sequences contain: (i) point substitution mutations – specifically, the transitions guanine (G) ↔ adenine (A) – and (ii) sequences extracted from human chromosomes, modified by expanding the cytosine–adenine–guanine triplet [(CAG)n repeats] to mimic the following diseases: (a) Huntington's disease, (b) Kennedy's disease, (c) Spinocerebellar ataxia 6, (d) Spinocerebellar ataxia 7. Quantities such as eigenspectra, density of states, transmission coefficients, and the – more experimentally relevant – current–voltage (I–V) curves are studied, intending to find adequate features to recognize mutations. To this end, the normalised deviation of the I–V curve from the origin (NDIV) is also defined. The features of the NDIV seem to provide a clearer picture, being sensitive to the number of point mutations and allowing to characterise the degree of danger of developing the aforementioned diseases.

a54) Energy Transport along α-Helix Protein Chains:
External Drives and Multifractal Analysis
N. Sefidkar, S. Fathizadeh, F. Nemati and **C. Simserides**
Materials 15 (**2022**) 2779 doi: 10.3390/ma15082779
Special Issue **Computational Modeling and Simulation of Polymers and Biopolymers**
Heterocitations 1, *From collaborators 1*

Energy transport within biological systems is critical for biological functions in living cells and for technological applications in molecular motors. Biological systems have very complex dynamics supporting a large number of biochemical and biophysical processes. In the current work, we study the energy transport along protein chains. We examine the influence of different factors such as temperature, salt concentration, and external mechanical drive on the energy flux through protein chains. We obtain that energy fluctuations around the average value for short chains are greater than for longer chains. In addition, the external mechanical load is the most effective agent on bioenergy transport along the studied protein systems. Our results can help design a functional nano-scaled molecular motor based on energy transport along protein chains.

a53) Cyclo[18]carbon including Zero-Point Motion:
Ground State, First Singlet and Triplet Excitations, and Hole Transfer
K. Lambropoulos, A. M. Alvertis, A. Morphis and **C. Simserides**
Physical Chemistry Chemical Physics **24** (2022) 7779-7787 doi: 10.1039/D2CP00343K
Heterocitations 7

Recent synthesis of cyclo[18]carbon has spurred increasing interest in carbon rings. We focus on a comparative inspection of ground and excited states, as well as of hole transfer properties of cumulenic and polyynic cyclo[18]carbon via Density Functional Theory (DFT), time-dependent DFT (TD-DFT) and real-time time-dependent DFT (RT-TDDFT). Zero-point vibrations are also accounted for, using a Monte Carlo sampling technique and a less exact, yet mode-resolved, quadratic approximation. The inclusion of zero-point vibrations leads to a red-shift on the HOMO-LUMO gap and the first singlet and triplet excitation energies of both conformations, correcting the values of the 'static' configurations by 9% to 24%. Next, we oxidize the molecule, creating a hole at one carbon atom. Hole transfer along polyynic cyclo[18]carbon is decreased in magnitude compared to its cumulenic counterpart and lacks the symmetric features the latter displays. Contributions by each mode to energy changes and hole transfer between diametrically opposed atoms vary, with specific bondstretching modes being dominant.

a52) LCAO electronic structure of nucleic acid bases and other heterocycles and transfer integrals in B-DNA, including structural variability
M. Mantela, **C. Simserides***, and Rosa Di Felice*
Materials **14** (2021) 4930 (20 pages) doi: 10.3390/ma14174930
Special Issue **Computational Modeling and Simulation of Polymers and Biopolymers**
Heterocitations 2

To describe the molecular electronic structure of nucleic acid bases and other heterocycles, we employ the Linear Combination of Atomic Orbitals (LCAO) method, considering the molecular wave function as a linear combination of all valence orbitals, i.e., 2s, $2p_x$, $2p_y$, $2p_z$ orbitals for C,N, and O atoms and 1s orbital for H atoms. Regarding the diagonal matrix elements (also known as on-site energies), we introduce a novel parameterization. For the non-diagonal matrix elements referring to neighboring atoms, we employ the Slater–Koster two-center interaction transfer integrals. We use Harrison-type expressions with factors slightly

modified relative to the original. We compare our LCAO predictions for the ionization and excitation energies of heterocycles with those obtained from Ionization Potential Equation of Motion Coupled Cluster with Singles and Doubles (IP-EOMCCSD)/aug-cc-pVDZ level of theory and Completely Normalized Equation of Motion Coupled Cluster with Singles, Doubles, and non-iterative Triples (CR-EOMCCSD(T))/aug-cc-pVDZ level of theory, respectively, (vertical values), as well as with available experimental data. Similarly, we calculate the transfer integrals between subsequent base pairs, to be used for a Tight-Binding (TB) wire model description of charge transfer and transport along ideal or deformed B-DNA. Taking into account all valence orbitals, we are in the position to treat deflection from the planar geometry, e.g., DNA structural variability, a task impossible for the plane Hückel approach (i.e., using only $2p_z$ orbitals). We show the effects of structural deformations utilizing a 20mer evolved by Molecular Dynamics.

a51) Averaging method and coherence applied to Rabi oscillations in a two-level system
L. Chalkopiadis and **C. Simserides***
Journal of Physics Communications **5** (2021) 095006 (16 pages) doi: 10.1088/2399-6528/ac1abf
Related version at arXiv:2105.12127

We study Rabi oscillations in a two-level system within the semiclassical approximation as an archetype test field of the Averaging Method (AM). The population transfer between the two levels is approached within the first and the second order AM. We systematically compare AM predictions with the rotating wave approximation (RWA) and with the complete numerical solution utilizing standard algorithms (NRWA). We study both the resonance ($\Delta = 0$) and out-of-resonance ($\Delta \neq 0$) cases, where $\Delta = \omega - \Omega$, and $\hbar\Omega = E_2 - E_1$ is the two-level energetic separation, while $\omega$ is the (cyclic) frequency of the electromagnetic field. We introduce three types of dimensionless factors $\epsilon$, i.e., $\Omega_R/\Delta$, $\Omega_R/\Sigma$, and $\Omega_R/\omega$, where $\Omega_R$ is the Rabi (cyclic) frequency and $\Sigma = \omega + \Omega$ and explore the range of $\epsilon$ where the AM results are equivalent to NRWA. Finally, by allowing for a phase difference in the initial electron wave functions, we explore the prospects coherence can offer. We illustrate that even with equal initial probabilities at the two levels, but with phase difference, strong oscillations can be generated and manipulated.

a50) Effects of structural dynamics on charge carrier transfer in B-DNA: a combined MD and RT-TDDFT study
M. Mantela, A. Morphis, K. Lambropoulos, **C. Simserides***, R. Di Felice*
The Journal of Physical Chemistry B **125** (2021) 3986-4003
doi: 10.1021/acs.jpcb.0c11489
Heterocitations 7

Hole transfer along the axis of duplex DNA has been the focus of physical chemistry research for decades, with implications in diverse fields, from nanotechnology to cell oxidative damage. Computational approaches are particularly amenable for this problem, to complement experimental data for interpretation of transfer mechanisms. To be predictive, computational results need to account for the inherent mobility of biological molecules during the time frame of experimental measurements. Here, we address the structural variability of B-DNA and its effects on hole transfer in a combined Molecular Dynamics (MD) and Real-Time Time-Dependent Density Functional Theory (RT-TDDFT) study. Our results show that quantities that characterize the charge transfer process, such as the time-dependent dipole moment and hole population at a specific site, are sensitive to structural changes that occur on the nanosecond time scale. We extend the range of physical properties for which such a correlation has been observed, further establishing the fact that quantitative computational data on charge transfer properties should include statistical averages. Furthermore, we use the RT-TDDFT results to assess an efficient tight-binding method suitable for high-throughput predictions. We demonstrate that charge transfer, although affected by structural variability, on the average, remains strong in AA and GG dimers.

a49) Hole transfer in open carbynes
**C. Simserides***, A. Morphis, K. Lambropoulos
Materials **13** (2020) 3979
doi: 10.3390/ma13183979
Special Issue **Computational Modeling and Simulation of Polymers and Biopolymers**

We investigate hole transfer in open carbynes, i.e., carbon atomic nanowires, using Real-Time Time-Dependent Density Functional Theory (RT-TDDFT). The nanowire is made of *N* carbon atoms. We use the functional B3LYP and the basis sets 3-21G, 6-31G*, cc-pVDZ, cc-pVTZ, cc-pVQZ. We also utilize a few Tight-Binding (TB)

wire models, a very simple model with all sites equivalent and transfer integrals given by the Harrison $pp\pi$ expression (TBI) as well as a model with modified initial and final sites (TBImod) to take into account the presence of one or two or three hydrogen atoms at the edge sites. To achieve similar site occupations in cumulenes with those obtained by converged RT-TDDFT, TBImod is sufficient. However, to achieve similar frequency content of charge and dipole moment oscillations and similar coherent transfer rates, the TBImod transfer integrals have to be multiplied by a factor of four (TBImodt4times). An explanation for this is given. Full geometry optimization at the B3LYP/6-31G* level of theory shows that in cumulenes bond length alternation (BLA) is not strictly zero and is not constant, although it is symmetrical relative to the molecule center. BLA in cumulenic cases is much smaller than in polyynic cases, so, although not strictly, the separation to cumulenes and polyynes, approximately, holds. Vibrational analysis confirms that for $N$ even all cumulenes with coplanar methylene end groups are stable, for $N$ odd all cumulenes with perpendicular methylene end groups are stable, and the number of hydrogen atoms at the end groups is clearly seen in all cumulenic and polyynic cases. We calculate and discuss the DFT ground state energy of neutral molecules, the CDFT "ground state energy" of molecules with a hole at one end group, energy spectra, density of states, energy gap, charge and dipole moment oscillations, mean over time probabilities to find the hole at each site, coherent transfer rates, and frequency content, in general. We also compare RT-TDDFT with TB results.

a48) Hole Transfer in Cumulenic and Polyynic Carbynes
**C. Simserides***, A. Morphis, K. Lambropoulos
The Journal of Physical Chemistry **124** (2020) 12834−12849
doi: 10.1021/acs.jpcc.0c03763
Heterocitations 1

We study hole transfer in open cumulenic and polyynic nanowires made of $N$ carbon atoms, using Real-Time Time-Dependent Density Functional Theory (RT-TDDFT) and Tight-Binding (TB) wire models. For RT-TDDFT we mainly use functional B3LYP and basis sets cc-pVDZ, cc-pVTZ, cc-pVQZ, obtaining clear convergence; cc-pVTZ is the smallest basis set of sufficient quality; cc-pVQZ is better with higher computational cost. For TB we use a simplistic wire model where all sites are equivalent (TBI) and models with modified initial and final sites, mimicking the existence of one or two or three hydrogens at edge sites (TBImod, TBImodt4times). We compare the ground state energy, $E_{GS}$, obtained by DFT for cumulenic molecules with coplanar (*co*) or perpendicular (*pe*) methylene end groups as well as polyynic molecules starting with short (*sl*) or with long (*ls*) C-C bonds. For odd $N$, cumulenic *pe* molecules have lower $E_{GS}$ than cumulenic *co* molecules, that are probably transition states. We examine energy spectra, density of states, energy gap, charge oscillations, mean over time probabilities to find the hole at each site, coherent transfer rates, electric dipole moment and frequency content. DFT shows that due to the impact of end groups, there exists a cumulenic energy gap, smaller than the polyynic one. TBI and TBImod reproduce approximately the magnitude of the energy gap in the polyynic case at the limit of large $N$. TBImod is capable of predicting the same site occupations with the nicely converged RT-TDDFT ones for the cumulenic case. However, charge and dipole moment oscillations as well as transfer rates by RT-TDDFT are approximately four times faster than those by TBImod. The site occupations of polyynic *sl* and of polyynic *ls* molecules are modified relative to cumulenic molecules; the trends can be explained qualitatively.

a47) Tight-Binding modeling of nucleic acid sequences:
interplay between various types of order or disorder and charge transport
K. Lambropoulos* and **C. Simserides***
Symmetry **11** (2019) 968 (26 pages)
doi: 10.3390/sym11080968
invited Review to the Special Issue of Symmetry,
Symmetry and Asymmetry in Quasicrystals or Amorphous Materials,
with guest Editor Professor Enrique Macia.
Heterocitations 21

This review is devoted to tight-binding (TB) modeling of nucleic acid sequences like DNA and RNA. It addresses how various types of order (periodic, quasiperiodic, fractal) or disorder (diagonal, non-diagonal, random, methylation et cetera) affect charge transport. We include an introduction to TB and a discussion of its various submodels [wire, ladder, extended ladder, fishbone (wire), fishbone ladder] and of the process of renormalization. We proceed to a discussion of aperiodicity, quasicrystals and the mathematics of aperiodic substitutional sequences: primitive substitutions, Perron-Frobenius eigenvalue, induced substitutions, Pisot property. We discuss the energy structure of nucleic acid wires, the coupling to the leads, the transmission

coefficients and the current-voltage curves. We also summarize efforts aiming to examine the potentiality to utilize the charge transport characteristics of nucleic acids as a tool to probe several diseases or disorders.

a46) Quasi-periodic and fractal polymers: Energy structure and carrier transfer
M. Mantela, K. Lambropoulos, M. Theodorakou, and **C. Simserides***
Materials **12** (2019), 2177 (30 pages)
doi: 10.3390/ma12132177
Also at arXiv:1901.06273
Heterocitations 7

We study the energy structure and the coherent transfer of an extra electron or hole along aperiodic polymers made of $N$ monomers, with fixed boundaries, using B-DNA as our prototype system. We use a Tight-Binding wire model, where a site is a monomer (e.g., in DNA, a base pair). We consider quasi-periodic (Fibonacci, Thue–Morse, Double-Period, Rudin–Shapiro) and fractal (Cantor Set, Asymmetric Cantor Set) polymers made of the same monomer (I polymers) or made of different monomers (D polymers). For all types of such polymers, we calculate the highest occupied molecular orbital (HOMO) eigenspectrum and the lowest unoccupied molecular orbital (LUMO) eigenspectrum, the HOMO–LUMO gap and the density of states. We examine the mean over time probability to find the carrier at each monomer, the frequency content of carrier transfer (Fourier spectra, weighted mean frequency of each monomer, total weighted mean frequency of the polymer), and the pure mean transfer rate $k$. Our results reveal that there is a correspondence between the degree of structural complexity and the transfer properties. I polymers are more favorable for charge transfer than D polymers. We compare $k(N)$ of quasi-periodic and fractal sequences with that of periodic sequences (including homopolymers) as well as with randomly shuffled sequences. Finally, we discuss aspects of experimental results on charge transfer rates in DNA with respect to our coherent pure mean transfer rates.

a45) Periodic, quasiperiodic, fractal, Kolakoski, and random binary polymers:
Energy structure and carrier transport
K. Lambropoulos and **C. Simserides***
Physical Review E **99** (2019) 032415 (17 pages)
doi: 10.1103/PhysRevE.99.032415
Also at arXiv:1808.04764
Heterocitations 19
This article has been honored with the **Academy of Athens, Lycurgus Award, 2022, for original research in Theoretical Physics.**

We study periodic, quasiperiodic (Thue-Morse, Fibonacci, period doubling, Rudin-Shapiro), fractal (Cantor, generalized Cantor), Kolakoski, and random binary sequences using a tight-binding wire model, where a site is a monomer (e.g., in DNA, a base pair). We use B-DNA as our prototype system. All sequences have purines, guanine (G) or adenine (A), on the same strand, i.e., our prototype binary alphabet is {G,A}. Our aim is to examine the influence of sequence intricacy and magnitude of parameters on energy structure, localization, and charge transport. We study quantities such as autocorrelation function, eigenspectra, density of states, Lyapunov exponents, transmission coefficients, and current-voltage curves. We show that the degree of sequence intricacy and the presence of correlations decisively affect the aforementioned physical properties. Periodic segments have enhanced transport properties. Specifically, in homogeneous sequences transport efficiency is maximum. There are several deterministic aperiodic sequences that can support significant currents, depending on the Fermi level of the leads. Random sequences is the less efficient category.

a44) Periodic polymers with increasing repetition unit:
Energy structure and carrier transfer
K. Lambropoulos, C. Vantaraki, P. Bilia, M. Mantela, and **C. Simserides***
Phys. Rev. E **98** (2018) 032412 (14 pages + 23 pages Supplemental Material)
doi: 10.1103/PhysRevE.98.032412
Also at arXiv arXiv:1808.05614
Heterocitations 4

We study the energy structure and the transfer of an extra electron or hole along periodic polymers made of $N$ monomers, with a repetition unit made of $P$ monomers, using a tight-binding wire model, where a site is a monomer (e.g., in DNA, a base pair), for $P$ even, and deal with two categories of such polymers: made of the

same monomer (GC…, GGCC…, etc.) and made of different monomers (GA…, GGAA…, etc.). We calculate the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) eigenspectra, density of states, and HOMO-LUMO gap and find some limiting properties these categories possess, as $P$ increases. We further examine the properties of the mean over time probability to find the carrier at each monomer. We introduce the *weighted mean frequency* of each monomer and the *total weighted mean frequency* of the whole polymer, as a measure of the overall transfer frequency content. We study the pure mean transfer rates. These rates can be increased by many orders of magnitude with appropriate sequence choice. Generally, homopolymers display the most efficient charge transfer. Finally, we compare the pure mean transfer rates with experimental transfer rates obtained by time-resolved spectroscopy.

a43) Spectral and transmission properties of periodic 1D Tight-Binding lattices with a generic unit cell: an analysis within the transfer matrix approach
K. Lambropoulos, and **C. Simserides**
Journal of Physics Communications **2** (2018) 035013 (19 pages)
doi: 10.1088/2399-6528/aab065
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We report on the electronic structure, density of states and transmission properties of the periodic one-dimensional Tight-Binding (TB) lattice with a single orbital per site and nearest-neighbor hoppings, with a generic unit cell of $u$ sites. The determination of the eigenvalues is equivalent to the diagonalization of a real tridiagonal symmetric $u$-Toeplitz matrix with (cyclic boundaries) or without (fixed boundaries) perturbed upper right and lower left corners. We solve the TB equations via the Transfer Matrix Method, producing analytical solutions and recursive relations for its eigenvalues, closely related to the Chebyshev polynomials. We examine the density of states and provide relevant analytical relations. We attach semi-infinite leads, determine and discuss the transmission coefficient at zero bias and investigate the peaks number and position, and the effect of the coupling strength and asymmetry as well as of the lead properties on the transmission profiles. We introduce a generic optimal coupling condition and demonstrate its physical meaning.

a42) Electronic structure and charge transport properties of atomic carbon wires
K. Lambropoulos and **C. Simserides***
Physical Chemistry Chemical Physics **19** (2017) 26890 - 26897
doi: 10.1039/c7cp05134d
Heterocitations 21

Atomic carbon wires represent the ultimate one-atom-thick one-dimensional structure. We use a Tight-Binding (TB) approach to determine the electronic structure of polyynic and cumulenic carbynes, in terms of their dispersion relations (for cyclic boundaries), eigenspectra (for fixed boundaries) and density of states (DOS). We further derive the transmission coefficient at zero bias by attaching the carbynes to semi-infinite metallic leads, and demonstrate the effect of the coupling strength and asymmetry to the transparency of the system to incident carriers. Finally, we determine the current-voltage (I-V) characteristics of carbynes and study the effect of factors such as the weakening of the coupling of the system to one of the leads, the relative position of the Fermi levels of the carbyne and the leads, the leads' bandwidth and, finally, the difference in the energy structure between the leads. Our results confirm and reproduce some of the most recent experimental findings.

a41) RT-TDDFT study of hole oscillations in B-DNA monomers and dimers
M. Tassi, A. Morphis, K. Lambropoulos, and **C. Simserides**
Cogent Physics (2017)
doi: 10.1080/23311940.2017.1361077
Related version at arXiv arXiv:1704.07413 [physics.bio-ph]
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We employ Real-Time Time-Dependent Density Functional Theory to study hole oscillations within a B-DNA monomer (one base pair) or dimer (two base pairs). Placing the hole initially at any of the bases which make up a base pair, results in THz oscillations, albeit of negligible amplitude. Placing the hole initially at any of the base pairs which make up a dimer is more interesting: For dimers made of identical monomers, we predict oscillations with frequencies in the range $f \approx$ 20-40 THz, with a maximum transfer percentage close to 1. For dimers made of different monomers, $f \approx$ 80-400 THz, but with very small or small maximum transfer

percentage. We compare our results with those obtained recently via our Tight-Binding approaches and find that they are in good agreement.

a40) Electronic structure and carrier transfer in B-DNA monomer polymers and dimer polymers: Stationary and time-dependent aspects of wire model vs. extended ladder model
K. Lambropoulos, M. Chatzieleftheriou, A. Morphis, K. Kaklamanis, R. Lopp, M. Theodorakou, M. Tassi, and **C. Simserides***
Physical Review E **94** (2016) 062403 (22 pages)
doi: 10.1103/PhysRevE.94.062403
Related version at arXiv arXiv:1609.00235v1
Heterocitations 15

We employ two Tight-Binding (TB) approaches to systematically study the electronic structure and hole or electron transfer in B-DNA monomer polymers and dimer polymers made up of $N$ monomers (base pairs): (I) at the base-pair level, using the on-site energies of base pairs and the hopping integrals between successive base pairs, i.e., a wire model and (II) at the single-base level, using the on-site energies of the bases and the hopping integrals between neighboring bases, i.e., an *extended* ladder model since we also include diagonal hoppings. We solve a system of $MD$ ("matrix dimension") coupled equations [(I) $MD = N$, (II) $MD = 2N$] for the time-independent problem, and a system of $MD$ coupled 1st order differential equations for the time-dependent problem. We perform a comparative study of stationary and time-dependent aspects of the two TB variants, using realistic sets of parameters. The studied properties include HOMO and LUMO eigenspectra, occupation probabilities, Density of States (DOS) and HOMO-LUMO gaps as well as mean over time probabilities to find the carrier at each site [(I) base pair or (II) base], Fourier spectra, which reflect the frequency content of charge transfer (CT) and pure mean transfer rates from a certain site to another. The two TB approaches give coherent, complementary aspects of electronic properties and charge transfer in B-DNA monomer polymers and dimer polymers.

a39) Wire and extended ladder model predict THz oscillations in DNA monomers, dimers and trimers
K. Lambropoulos, K. Kaklamanis, A. Morphis, M. Tassi, R. Lopp, G. Georgiadis, M. Theodorakou, M. Chatzieleftheriou, and **C. Simserides***
Journal of Physics: Condensed Matter **28** (2016) 495101 (19 pages)
doi: 10.1088/0953-8984/28/49/495101
Related version at arXiv arXiv:1609.00180v1
Heterocitations 5

We call monomer a B-DNA base pair and study, analytically and numerically, electron or hole oscillations in monomers, dimers and trimers. We employ two Tight Binding (TB) approaches: (I) at the base-pair level, using the on-site energies of the base pairs and the hopping parameters between successive base pairs i.e. a wire model, and (II) at the single-base level, using the on-site energies of the bases and the hopping parameters between neighbouring bases, specifically between (a) two successive bases in the same strand, (b) complementary bases that define a base pair, and (c) diagonally located bases of successive base pairs, i.e. an extended ladder model since it also includes the diagonal hoppings (c). For monomers, with TB II, we predict periodic carrier oscillations with frequency $f \approx$ 50-550 THz. For dimers, with TB I, we predict periodic carrier oscillations with $f \approx$ 0.25-100 THz. For trimers made of identical monomers, with TB I, we predict periodic carrier oscillations with $f \approx$ 0.5-33 THz. In other cases, either with TB I or TB II, the oscillations may be not strictly periodic, but Fourier analysis shows similar frequency content. For dimers and trimers, TB I and TB II are successfully compared giving complementary aspects of the oscillations.

a38) Lowest ionization and excitation energies of biologically important heterocyclic planar molecules
M. Mantela, A. Morphis, M. Tassi, and **C. Simserides***
Molecular Physics **114** (2016) 709-718
doi: 10.1080/00268976.2015.1113313
Heterocitations 4

We calculate the lowest ionization and excitation energies in a variety of biologically important molecules, i.e. π-conjugated systems like DNA and RNA bases and isomers plus related heterocyclic molecules. For approximately half of these molecules there are no experimental and theoretical/numerical data in the

literature, as far as we know. These electronic transitions are mainly but not exclusively of π and π-π* character, respectively. We perform symmetry-constrained Density Functional Theory (DFT) geometry optimization at the B3LYP/6-311++G** level of theory. At the DFT obtained ground-state geometries, we calculate vertical ionization energies with Ionization Potential Coupled Cluster with Singles and Doubles (IP-EOMCCSD) and vertical excitation energies with the Completely Renormalized Equation of Motion Coupled Cluster with Singles, Doubles, and non-iterative Triples (CREOMCCSD(T)) method. We also investigate whether a simple semi-empirical Hückel-type model approach with novel parametrization could provide reasonable estimates of the lowest π ionization and π-π* excitation energies. Our Coupled Cluster (CC) results are in very good agreement with experimental data, while the Hückel-type model predictions generally follow the trends with some deviation. Finally, we investigate the effect of basis set in IPEOMCCSD energies and we compare our CR-EOMCCSD(T) results with Time Dependent DFT (TDDFT) ones.

a37) Unbiased charge oscillations in B-DNA: monomer polymers and dimer polymers
K. Lambropoulos, M. Chatzieleftheriou, A. Morphis, K. Kaklamanis, M. Theodorakou, and **C. Simserides***
Physical Review E **92** (2015) 032725 (16 pages)
doi: 10.1103/PhysRevE.92.032725
Related older version also at arXiv:1504.02638
Δημοσιεύσαμε επίσης Publisher's Note: Unbiased charge oscillations in B-DNA: Monomer polymers and dimer polymers [Phys. Rev. E 92, 032725 (2015)]
K. Lambropoulos, M. Chatzieleftheriou, A. Morphis, K. Kaklamanis, M. Theodorakou, and **C. Simserides***
Physical Review E **93**, 069902(E) (2016)
doi: 10.1103/PhysRevE.93.069902
Heterocitations 6

We call monomer a B-DNA base-pair and examine, analytically and numerically, electron or hole oscillations in monomer- and dimer-polymers, i.e., periodic sequences with repetition unit made of one or two monomers. We employ a tight-binding (TB) approach at the base-pair level to readily determine the spatiotemporal evolution of a single extra carrier along a $N$ base-pair B-DNA segment. We study HOMO and LUMO eigenspectra as well as the mean over time probabilities to find the carrier at a particular monomer. We use the pure mean transfer rate $k$ to evaluate the easiness of charge transfer. The inverse decay length $\beta$ for exponential fits $k(d)$, where $d$ is the charge transfer distance, and the exponent $\eta$ for power law fits $k(N)$ are computed; generally power law fits are better. We illustrate that increasing the number of different parameters involved in the TB description, the fall of $k(d)$ or $k(N)$ becomes steeper and show the range covered by $\beta$ and $\eta$. Finally, both for the time-independent and the time-dependent problem, we analyze the *palindromicity* and the *degree of eigenspectrum dependence* of the probabilities to find the carrier at a particular monomer.

a36) THz and above THz electron or hole oscillations in DNA dimers and trimers
K. Lambropoulos, K. Kaklamanis, G. Georgiadis, and **C. Simserides***
Annalen der Physik (Berlin) **526** (2014) 249–258
doi: 10.1002/andp.201400067
Heterocitations 3

We propose a non conventional source or receiver of THz and above THz electromagnetic radiation. Specifically, we predict electron or hole oscillations in DNA dimers (two interacting DNA base-pairs or monomers), with frequency in the range $f \approx$ 0.25-100 THz (period $T \approx$ 10-4000 fs) i.e. potentially emitting electromagnetic radiation mainly in the mid- and far-infrared with wavelengths ≈ 3-1200 μm. The efficiency of charge transfer between the two monomers which make up the dimer is described with the maximum transfer percentage $p$ and the pure maximum transfer rate $pf$. For dimers made of identical monomers $p = 1$, but for dimers made of different monomers $p < 1$. Further, we extend the investigation to DNA trimers (three interacting DNA base-pairs or monomers). For trimers made of identical monomers the carrier oscillates periodically with $f \approx$ 0.5-33 THz ($T \approx$ 30-2000 fs); for 0 times crosswise purines $p = 1$, for 1 or 2 times crosswise purines $p < 1$. For trimers made of different monomers the carrier movement may be non periodic. Generally, increasing the number of monomers above three, the system becomes more complex and periodicity is lost; even for the simplest tetramer the carrier movement is not periodic.

a35) A systematic study of electron or hole transfer along DNA dimers, trimers and polymers
**C. Simserides***
Chemical Physics **440** (2014) 31-41
doi: 10.1016/j.chemphys.2014.05.024
Heterocitations 20
Related work at arXiv
arXiv:1402.0654 A systematic study of electron or hole transfer along DNA dimers, trimers and polymers
arXiv:1312.6842 Charge transfer along DNA dimers, trimers and polymers

A systematic study of carrier transfer along DNA dimers, trimers and polymers including poly(dG)-poly(dC), poly(dA)-poly(dT), GCGCGC..., ATATAT... is presented allowing to determine the spatiotemporal evolution of electrons or holes along a $N$ base-pair DNA segment. Physical quantities are defined including maximum transfer percentage $p$ and *pure* maximum transfer rate $pT$ when a period $T$ is defined; *pure* mean transfer rate $k$ and speed $u = kd$, where $d$ is the charge transfer distance. The inverse decay length $\beta$ for the exponential fit $k = k_0\exp(-\beta d)$ and the exponent $\eta$ for the power-law fit $k = k_0' N^{-\eta}$ are computed. $\beta \approx 0.2$ - 2 $\text{Å}^{-1}$, $k_0$ is usually $10^{-2}$-$10^{-1}$ PHz, generally $\approx 10^{-4}$-10 PHz. $\eta \approx 1.7$ - 17, $k_0'$ is usually $10^{-2}$-$10^{-1}$ PHz, generally $\approx 10^{-4}$-$10^{3}$ PHz. The results are compared with theoretical and experimental works. This method allows assess the extent at which a specific DNA segment can serve for charge transfer.

a34) Phase diagram and critical behavior of the random ferromagnet $Ga_{1-x}Mn_xN$
S. Stefanowicz, G. Kunert, **C. Simserides**, J. A. Majewski, W. Stefanowicz, C. Kruse, S. Figge, Tian Li, R. Jakieła, K. N. Trohidou, A. Bonanni, D. Hommel, M. Sawicki, and T. Dietl
Physical Review B **88** (2013) 081201(R) (4 pages)
doi: 10.1103/PhysRevB.88.081201
Also at: arXiv:1306.5141v1 [cond-mat.dis-nn] 21 Jun 2013
Heterocitations 34 (+1), *From collaborators 25 (+2)*

Molecular beam epitaxy has been employed to obtain $Ga_{1-x}Mn_xN$ films with $x$ up to 10% and Curie temperatures $T_C$ up to 13 K. The magnitudes of $T_C$ and their dependence on $x$, $T_C(x) \propto x^m$, where m = 2.2 ± 0.2 are quantitatively described by a tight binding model of superexchange interactions and Monte Carlo simulations of $T_C$. The critical behavior of this dilute magnetic insulator shows strong deviations from the clean case, in particular, (i) an apparent breakdown of the Harris criterion; (ii) a non-monotonic crossover in the values of the susceptibility critical exponent $\gamma_{eff}$ between the high temperature and critical regimes, and (iii) a smearing of the critical region, which can be explained either by the Griffiths effects or by macroscopic inhomogeneities in the spin distribution with a variance $\Delta x = (0.2 \pm 0.1)\%$.

a33) Density of states and extent of wave function: two crucial factors for small polaron hopping conductivity in 1D
M. Dimakogianni, **C. Simserides**, G. P. Triberis
Philosophical Magazine, **93** (2013) 2729-2748
doi: 10.1080/14786435.2013.785639
Heterocitations 1, *From collaborators1*
Also at arXiv:1209.1582v1 [cond-mat.dis-nn]
This article has been honored with the **Academy of Athens Georgios Th. Foteinos Award, 2014,** for original research in Experimental or Theoretical Physics.

We introduce a theoretical model to scrutinize the conductivity of small polarons in one-dimensional disordered systems, focusing on two crucial --as will be demonstrated-- factors: the density of states and the spatial extent of the wave function. The investigation is performed for any temperature up to 300 K and under electric field of arbitrary strength up to the polaron dissociation limit. To accomplish this task we combine analytical work with numerical calculations.

a32) Origin of low-temperature magnetic ordering in $Ga_{1-x}Mn_xN$
M. Sawicki, T. Devillers, S. Gałęski, **C. Simserides**, S. Dobkowska, B. Faina, A. Grois, A. Navarro-Quezada, K. N. Trohidou, J. A. Majewski, T. Dietl, A. Bonanni
Physical Review B **85** (2012) 205204 (4 pages)
doi: 10.1103/PhysRevB.85.205204

Also at arXiv:1202.6233v2 [cond-mat.mtrl-sci]
Heterocitations 35 (+1), *From collaborators 24 (+4)*

By use of highly sensitive millikelvin superconducting quantum interference device magnetometry, the magnitude of the Curie temperature as a function of the Mn concentration $x$ is determined for thoroughly characterized $Ga_{1-x}Mn_xN$. The interpretation of the results in the frame of tight-binding theory and of Monte Carlo simulations allows us to assign the spin interaction to ferromagnetic superexchange and to point out the limited accuracy of state-of-the-art *ab initio* methods in predicting the magnetic characteristics of dilute magnetic insulators.

a31) Near-Field Optical Properties of Quantum Dots, Applications and Perspectives
A. Zora, G. P. Triberis, **C. Simserides**
Recent Patents on Nanotechnology **5** (2011) pp. 188-224 (ISSN: 1872-2105)
Bentham Science Publishers
doi: 10.2174/187221051110503018 8
Heterocitations 17

Recent years have witnessed tremendous research in quantum dots as excellent models of quantum physics at the nanoscale and as excellent candidates for various applications based on their optoelectronic properties. This review intends to present theoretical and experimental investigations of the near-field optical properties of these structures, and their multimodal applications such as biosensors, biological labels, optical fibers, switches and sensors, visual displays, photovoltaic devices and related patents.

a30) Intrinsic optical bistability in a two-subband system in a semiconductor quantum well: Analytical results
S. G. Kosionis, A. F. Terzis, **C. Simserides**, E. Paspalakis
Journal of Applied Physics **109** (2011) 063109 (5 pages)
doi: 10.1063/1.3553871
Heterocitations 20 (+1), *From collaborators 4*

We study theoretically the conditions under which optical bistability is achievable in a two-subband system in a semiconductor quantum well. We consider the interaction of the two-subband system with a continuous wave electromagnetic field, which induces intersubband transitions. For the description of the system dynamics we use the effective nonlinear density matrix equations. We solve these equations analytically, in the steady state, for a GaAs/AlGaAs quantum well structure. For several combinations of the values of the parameters three real solutions of the population inversion arise and the phenomenon of optical bistability prevails.

a29) Linear and nonlinear optical properties of a two-subband system in a symmetric semiconductor quantum well
S. G. Kosionis, A. F. Terzis, **C. Simserides**, E. Paspalakis
Journal of Applied Physics **108** (2010) 034316 (5 pages)
doi: 10.1063/1.3457855
Heterocitations 17, *From collaborators6 (+1)*

We study the linear and nonlinear optical response of intersubband transitions in a semiconductor quantum well. We describe the coupling of the quantum well structure with the electromagnetic field by using the nonlinear density matrix equations, in the two-subband approximation. We provide proper approximate analytical solutions to these equations that are used for the closed-form determination of the optical susceptibilities $\chi^{(1)}$, $\chi^{(3)}$, and $\chi^{(5)}$. We also explore the dependence of $\chi^{(1)}$, $\chi^{(3)}$, and $\chi^{(5)}$ on the electron sheet density for a specific double GaAs/AlGaAs quantum well.

a28) Electronic parameters for charge transfer along DNA
L. G. D. Hawke, G. Kalosakas, **C. Simserides**
European Physical Journal E **32**, 291–305 (2010) doi: 10.1140/epje/i2010-10650-y
Also at arXiv:0908.1248v1 [physics.bio-ph]
Heterocitations 82 (+1), *From collaborators2*
Δημοσιεύσαμε επίσης Erratum to: Electronic parameters for charge transfer along DNA
L. G. D. Hawke, G. Kalosakas, and C. Simserides
European Physical Journal E **34** (2011) 118

doi: 10.1140/epje/i2011-11118-4

We systematically examine all the tight-binding parameters pertinent to charge transfer along DNA. The π molecular structure of the four DNA bases (adenine, thymine, cytosine, and guanine) is investigated by using the linear combination of atomic orbitals method with a recently introduced parametrization. The HOMO and LUMO wavefunctions and energies of DNA bases are discussed and then used for calculating the corresponding wavefunctions of the two B-DNA base-pairs (adenine-thymine and guanine-cytosine). The obtained HOMO and LUMO energies of the bases are in good agreement with available experimental values. Our results are then used for estimating the complete set of charge transfer parameters between neighboring bases and also between successive base-pairs, considering all possible combinations between them, for both electrons and holes. The calculated microscopic quantities can be used in mesoscopic theoretical models of electron or hole transfer along the DNA double helix, as they provide the necessary parameters for a tight-binding phenomenological description based on the _ molecular overlap. We find that usually the hopping parameters for holes are higher in magnitude compared to the ones for electrons. Our findings are also compared with existing calculations from first principles.

a27) Control of Intersubband Quantum Well Transitions with Chirped Electromagnetic Pulses
E. Paspalakis, **C. Simserides**, A. F. Terzis
Journal of Applied Physics **107** (2010) 064306 doi: 10.1063/1.3329377
Heterocitations 10 (+1), *From collaborators7 (+1)*

We study the interaction of chirped electromagnetic pulses with intersubband transitions of a double semiconductor quantum well. We consider the ground and first excited subbands and give emphasis to controlled intersubband population transfer. The system dynamics is described by the nonlinear density matrix equations that include the effects of electron-electron interactions. These equations are solved numerically for various values of the electron sheet density for a realistic double GaAs/AlGaAs quantum well, and the efficiency of population transfer is discussed.

a26) Multi-spin-subband structure of dilute magnetic semiconductor quantum wells: Feedback mechanism
**C. Simserides***, K. Koumpouras
Superlattices and Microstructures **46** (2009) 889-899 doi:10.1016/j.spmi.2009.10.007
Heterocitations 1

Using a fully self-consistent envelope function approach, we focus on wide conduction band NMS (non-magnetic semiconductor)/DMS (dilute magnetic semiconductor)/NMS quantum wells, under weak external parallel magnetic field, where many spin-subbands are usually present. We concentrate on small values of the magnetic field because we want to investigate the influence of the feedback mechanism due to the difference of the concentrations of spin-up and spin-down carriers which could induce spontaneous spin-polarization i.e. in the absence of a magnetic field. We study the spin-subband structure, the spin-subband populations and the spin-polarization as functions of the sheet carrier concentration, $N_s$, for different values of the magnitude of the exchange interaction, $|J|$, between the itinerant carriers and the magnetic impurities. Our calculations for 0.01 T show that at 20 K the values of $|J|$ necessary to make this feedback mechanism sufficiently strong are too high compared to the $|J|$ values of common Mn-doped systems in the conduction band. However, the feedback mechanism will be sufficiently strong at low enough temperatures below 20 K for realistic values of $|J|$. Moreover, we explain how increasing the sheet carrier concentration the heterostructure is transformed from an almost square quantum well to a system of two coupled heterojunctions with an intermediate soft barrier.

a25) Ferromagnetic properties of p-(Cd,Mn)Te quantum wells: Interpretation of magneto-optical measurements by Monte Carlo simulations
A. Lipínska, **C. Simserides**, K. N. Trohidou, M. Goryca, P. Kossacki, A. Majhofer, and T. Dietl
Physical Review B **79** (2009) 235322
doi: 10.1103/PhysRevB.79.235322
Also at arXiv:0903.0406v1 [cond-mat.mtrl-sci]
Heterocitations 10, *From collaborators 5*

In order to single out dominant phenomena that account for carrier-controlled magnetism in p-Cd1−xMnxTe quantum wells we have carried out magneto-optical measurements and Monte Carlo simulations of time dependent magnetization. The experimental results show that magnetization relaxation is faster than 20 ns in

the paramagnetic state. Decreasing temperature below the Curie temperature $T_C$ results in an increase of the relaxation time but to less than 10 μs. This fast relaxation may explain why the spontaneous spin splitting of electronic states is not accompanied by the presence of non-zero macroscopic magnetization below $T_C$. Our Monte Carlo results reproduce the relative change of the relaxation time on decreasing temperature. At the same time, the numerical calculations demonstrate that antiferromagnetic spin-spin interactions, which compete with the hole-mediated long-range ferromagnetic coupling, play an important role in magnetization relaxation of the system. We find, in particular, that magnetization dynamics is largely accelerated by the presence of antiferromagnetic couplings to the Mn spins located outside the region, where the holes reside. This suggests that macroscopic spontaneous magnetization should be observable if the thickness of the layer containing localized spins will be smaller than the extension of the hole wave function. Furthermore, we study how a spin-independent part of the Mn potential affects $T_C$. Our findings show that the alloy disorder potential tends to reduce $T_C$, the effect being particularly strong for the attractive potential that leads to hole localization.

a24) Empirical LCAO parameters for pi molecular orbitals in planar organic molecules
L. G. D. Hawke, G. Kalosakas, **C. Simserides**
Molecular Physics **107** (2009) 1755–1771
doi: 10.1080/00268970903049089
Also at arXiv:0808.3984 [physics.chem-ph]
Heterocitations 11, *From collaborators 1*

We present a parametrization within a simplified LCAO model (a type of Hueckel model) for the description of π molecular orbitals in organic molecules containing π-bonds between carbon, nitrogen, or oxygen atoms with $sp^2$ hybridization, which we show to be quite accurate in predicting the energy of the highest occupied π orbital and the first π-π* transition energy for a large set of organic compounds. We provide four empirical parameter values for the diagonal matrix elements of the LCAO description, corresponding to atoms of carbon, nitrogen with one $p_z$ electron, nitrogen with two $p_z$ electrons, and oxygen. The bond-length dependent formula (proportional to $1/d^2$) of Harrison is used for the non-diagonal matrix elements between neighboring atoms. The predictions of our calculations have been tested against available experimental results in more than sixty organic molecules, including benzene and its derivatives, polyacenes, aromatic hydrocarbons of various geometries, polyenes, ketones, aldehydes, azabenzenes, nucleic acid bases and others. The comparison is rather successful, taking into account the small number of parameters and the simplicity of the LCAO method, involving only $p_z$ atomic orbitals, which leads even to analytical calculations in some cases.

a23) The π-π* molecular structure of flavin of FADH- enzymatic cofactor using the LCAO method
L. G. D. Hawke, **C. Simserides***, G. Kalosakas
Materials Science and Engineering B **165** (2009) 266–269
doi: 10.1016/j.mseb.2009.02.012
On the occasion of NN08
Heterocitations 2

The π–π* molecular structure (eigenenergies and eigenfunctions) of flavin tricyclic ring is calculated, using the linear combination of atomic orbitals (LCAO) method containing only $p_z$ atomic orbitals. In respect to FADH− position opposite to DNA lesion in photolyase, flavin's HOMO is found to be distributed in the central and distal side, while LUMO is localized in the distal side of flavin (the side that is closer to the adenine part of FADH− and farther than the DNA dimer lesion). LUMO1 as well as LUMO2 are mainly distributed in the proximal side of flavin (the side that is closer to the DNA dimer). Our findings are compared with previous theoretical results as well as with experimental values of known π–π* transitions.

a22) Principal thermodynamic properties of quasi two-dimensional carriers under in-plane magnetic field
**C. Simserides***
Journal of Physics: Condensed Matter **21** (2009) 015304 (6pp)
doi: 10.1088/0953-8984/21/1/015304
Heterocitations 2

An external magnetic field, $H$, applied parallel to a quasi-two-dimensional carrier system modifies quantitatively and qualitatively the density of states. We examine how this affects primary thermodynamic properties, namely, the entropy, $S$, the internal and free energy, $U$ and $F$, the magnetization, $M$, and the magnetic susceptibility, $\chi$m, using a self-consistent numerical approach. Although $M$ is mainly in the opposite

direction to $H$, the system is not linear. Hence, surprisingly, $\partial M/\partial H$ swings between negative and positive values, i.e. a diamagnetic to paramagnetic transition of entirely orbital origin is predicted. This phenomenon is important compared to the ideal de Haas–van Alphen effect, i.e. the corresponding phenomenon under perpendicular magnetic field. By augmenting temperature, the diamagnetic to paramagnetic transition fades away. The overall behaviour of entropy is also foreseen and consistently interpreted. While the entropy contribution to the free energy is very small at low temperatures, entropy shows a clear dependence on the external magnetic field.

a21) Effects of the task of categorizing FM direction on auditory evoked magnetic fields in the human auditory cortex
R. Koenig, C. Sielużycki, **C. Simserides**, P. Heil, H. Scheich
Brain Research **1220** (2008) 102-117
doi: 10.1016/j.brainres.2008.02.086
Heterocitations 12 (+1), *From collaborators 3*

We examined effects of the task of categorizing linear frequency-modulated (FM) sweeps into rising and falling on auditory evoked magnetic fields (AEFs) from the human auditory cortex, recorded by means of whole-head magnetoencephalography. AEFs in this task condition were compared with those in a passive condition where subjects had been asked to just passively listen to the same stimulus material. We found that the M100-peak latency was significantly shorter for the task condition than for the passive condition in the left but not in the right hemisphere. Furthermore, the M100-peak latency was significantly shorter in the right than in the left hemisphere for the passive and the task condition. In contrast, the M100-peak amplitude did not differ significantly between conditions, nor between hemispheres. We also analyzed the activation strength derived from the integral of the absolute magnetic field over constant time windows between stimulus onset and 260ms. We isolated an early, narrow time range between about 60ms and 80ms that showed larger values in the task condition, most prominently in the right hemisphere. These results add to other imaging and lesion studies which suggest a specific role of the right auditory cortex in identifying FM sweep direction and thus in categorizing FM sweeps into rising and falling.

a20) Room temperature photoluminescence of individual self-assembled quantum dots
A. Zora, **C. Simserides** and G. P. Triberis
Physica E: Low-dimensional Systems and Nanostructures **40** (2008) 1687-1689
doi: 10.1016/j.physe.2007.10.028
Proceedings of EP2DS 2007, Genova.
Heterocitations 1

We investigate the emission spectra of individual lens-shaped self-assembled quantum dots (QDs) in the high-temperature regime, in order to contribute to the fine structural analysis and to the appreciation of the QDs optical response. Our theoretical analysis results in an expression for the photoluminescence (PL) intensity of QDs in the linear regime, which reproduces satisfactorily the experimentally observed PL signal of individual lens-shaped In0.5Ga0.5As self-assembled quantum dots (QDs). Using the appropriate material parameters, the theoretical predictions for the interlevel spacing as well as for the dephasing time caused by electron longitudinal optical phonon interactions are in a good agreement with experiment.

a19) Electromagnetically induced population transfer between two quantum well subbands
E. Paspalakis, **C. Simserides**, S. Baskoutas, and A. F. Terzis
Physica E: Low-dimensional Systems and Nanostructures **40** (2008) 1301-1304
doi: 10.1016/j.physe.2007.08.078
Proceedings of EP2DS 2007, Genova.
Heterocitations 39, *From collaborators 5 (+1)*

We study theoretically the potential for control of the electron population in a single GaAs/AlGaAs quantum well that is coupled by strong pulsed electromagnetic fields. Using numerical calculations we present conditions that lead to high-efficiency intersubband population inversion.

a18) Quasi two-dimensional carriers in dilute-magnetic-semiconductor quantum wells under in-plane magnetic field

**C. Simserides*** and I. Galanakis
Physica E: Low-dimensional Systems and Nanostructures **40** (2008) 1214-1216
doi: 10.1016/j.physe.2007.08.061 Proceedings of EP2DS 2007, Genova.
- Also found at arXiv.org, arXiv:0708.2862v1 [cond-mat.mtrl-sci]
Heterocitations 3

Due to the competition between spatial and magnetic confinement, the density of states of a quasi two-dimensional system deviates from the ideal step-like form both quantitatively and qualitatively. We study how this affects the spin-subband populations and the spin-polarization as functions of the temperature, T, and the in-plane magnetic field, B, for narrow to wide dilute-magnetic-semiconductor quantum wells. We focus on the quantum well width, the magnitude of the spin-spin exchange interaction, and the sheet carrier concentration dependence. We look for ranges where the system is completely spin-polarized. Increasing T, the carrier spin-splitting, Uoo, decreases, while increasing B, Uoo increases. Moreover, due to the density of states modification, all energetically higher subbands become gradually depopulated.

a17) Theory of spontaneous emission of quantum dots in the linear regime
A. Zora, **C. Simserides** and G. P. Triberis
Journal of Physics: Condensed Matter **19** (2007) 406201 (9 pages)
doi: 10.1088/0953-8984/19/40/406201
Heterocitations 6

We develop a fully quantum-mechanical theory for the interaction of light and electron–hole excitations in semiconductor quantum dots. Our theoretical analysis results in an expression for the photoluminescence intensity of quantum dots in the linear regime. Taking into account the single-particle Hamiltonian, the free-photon Hamiltonian, the electron–hole interaction Hamiltonian, and the interaction of carriers with light, and applying the Heisenberg equation of motion to the photon number expectation values, to the carrier distribution functions and to the correlation term between the photon generation (destruction) and electron–hole pair, we obtain a set of luminescence equations. Under quasi-equilibrium conditions, these equations become a closed-set of equations. We solve them analytically, in the linear regime, and we find an approximate solution of the incoherent photoluminescence intensity. The validity of the theoretical analysis is tested by investigating the emission spectra in the high-temperature regime, interpreting the experimental findings for the emission spectra of a lens-shaped In0.5Ga0.5As self-assembled quantum dot. Our theoretical predictions for the interlevel spacing as well as for the dephasing time caused by electron–longitudinal optical phonon interactions are in good agreement with the experimental results.

a16) Spin-subband populations and spin polarization of quasi-two-dimensional carriers under an in-plane magnetic field
**C. Simserides***
Physical Review B **75** (2007) 195344 (7 pages)
doi: 10.1103/PhysRevB.75.195344
Heterocitations 8

Under an in-plane magnetic field, the density of states of quasi-two-dimensional carriers deviates from the occasionally stereotypic step-like form both quantitatively and qualitatively. Here we study how this affects the spin-subband populations and the spin-polarization as functions of the temperature, T, and the in-plane magnetic field, B, for narrow to wide dilute-magnetic-semiconductor quantum wells. We examine a wide range of material and structural parameters, focusing on the quantum well width, the magnitude of the spin-spin exchange interaction, and the sheet carrier concentration. Generally, increasing T, the carrier spin-splitting, Uosigma, decreases, augmenting the influence of the "minority"-spin carriers. Increasing B, Uosigma, increases and, accordingly, carriers populate "majority"-spin subbands while they abandon "minority"-spin subbands. Furthermore, in line with the density of states modification, all energetically higher subbands become gradually depopulated. We also indicate the ranges where the system is completely spin-polarized.

a15) Near-field magnetoabsorption of quantum dots
**C. Simserides***, A. Zora, G. Triberis
Physical Review B **73** (2006) 155313 (13 pages)
doi: 10.1103/PhysRevB.73.155313
Heterocitations 10, *From collaborators1*

We investigate the effect of an external magnetic field of variable orientation and magnitude (up to 20 T) on the linear near-field optical absorption spectra of single and coupled III-V semiconductor quantum dots. We focus on the spatial as well as on the magnetic confinement, varying the dimensions of the quantum dots and the magnetic field. We show that the ground state exciton binding energy can be manipulated utilizing the spatial and the magnetic confinement. The effect of the magnetic field on the absorption spectra, increasing the near-field illumination spot, is also investigated. The zero-magnetic-field "structural" symmetry can be destroyed varying the magnetic field orientation and this affects the near-field spectra. The asymmetry induced (except for specific orientations along symmetry axes) by the magnetic field, can be revealed in the near-field but not in the far-field spectra. We predict that near-field magnetoabsorption experiments, of realistic spatial resolution, will be in the position to bring to light the quantum dot symmetry. This exceptional symmetry-resolving power of the near-field magnetoabsorption, is lost in the far field. The influence of the Coulomb interactions on the absorption spectra is also discussed. Finally, we show that certain modifications of the magnetoexcitonic structure can be uncovered using a realistically acute near-field probe of ~ 20 nm.

a14) A small polaron hopping model for multiphonon-assisted transport along DNA molecules, in the presence of disorder
G. Triberis, **C. Simserides*** and V. Karavolas
Physica E: Low-dimensional Systems and Nanostructures **32** (2006) 592–595
doi: 10.1016/j.physe.2005.12.111
Proceedings of MSS12 (12th International Conference on Modulated Semiconductor Structures)
Heterocitations 7

We discuss a small polaron hopping model, in order to explain the intense temperature ($T$) dependence of the electrical conductivity ($\sigma$) observed at high temperatures along the DNA molecules. The model takes into account the one-dimensional character of the system as well as the presence of disorder in the DNA double helix. Theoretical considerations based on percolation lead to analytical expressions for the high temperature multiphonon-assisted small polaron hopping conductivity, the maximum hopping distance and their temperature dependence. For example, experimental data for the $\lambda$-phage DNA, the poly(dA)-poly(dT) DNA, and the native wet-spun calf thymus Li-DNA, follow nicely the theoretically predicted behavior, $ln\sigma^{h} \sim T^{-2/3}$, over wide high-$T$ ranges. In contrast to some previously presented theoretical suggestions, our model leads to realistic values for the maximum hopping distances, supporting the idea of multiphonon-assisted hopping of small polarons between next nearest neighbors of the DNA molecular "wire". We also examine the low temperature case.

a13) Small polaron hopping transport along DNA molecules
G. P. Triberis, **C. Simserides** and V. C. Karavolas
Journal of Physics: Condensed Matter **17** (2005) 2681-2690
doi: 10.1088/0953-8984/17/17/016
Heterocitations 21, *From collaborators 7*

We present a small polaron hopping model for interpreting the strong temperature *(T)* dependence of the electrical conductivity, $\sigma$, observed at high (h) temperatures along DNA molecules. The model takes into account the one-dimensional character of the system and the presence of disorder in the DNA double helix. Percolation-theoretical considerations lead to analytical expressions for the high temperature multiphonon-assisted small polaron hopping conductivity, the hopping distance and their temperature dependence. The experimental data for lambda phage DNA *(λ*-DNA*)* and poly(dA)–poly(dT) DNA follow nicely the theoretically predicted behaviour *(*$\ln\sigma^{h} \sim T^{-2/3}$*)*. Moreover, our model leads to realistic values of the maximum hopping distances, supporting the idea of multiphonon-assisted hopping of small polarons between next nearest neighbours of the DNA molecular 'wire'. The low temperature case is also investigated.

a12) Properties of conduction-band dilute-magnetic-semiconductor quantum wells in an in-plane magnetic field: A density of states profile that is not step-like
**C. Simserides***
Physical Review B **69** (2004) 113302 (4 pages)
doi: 10.1103/PhysRevB.69.113302
Heterocitations 4

We examine how an in-plane magnetic field, *B*, modifies the density of states (DOS) in narrow-to-wide, conduction-band dilute magnetic semiconductor (DMS) quantum wells. We demonstrate that the DOS diverges significantly from the famous step-like 2DEG form and this causes severe changes to the physical properties e.g. to the spin-subband populations, the internal and free energy, the Shannon entropy and the in-plane magnetization, *M*. We predict a considerable fluctuation of *M* in cases of vigorous competition between spatial and magnetic confinement.

a11) Local optical absorption by confined excitons in single and coupled quantum dots
**C. D. Simserides***, U. Hohenester, G. Goldoni and E. Molinari
Physica Status Solidi B **224** (2001) 745-749
doi: 10.1002/(SICI)1521-3951(200104)224:3<745::AID-PSSB745>3.0.CO;2-9
Heterocitations 5
Proceedings of QD-2000 (International Conference on Semiconductor Quantum Dots)

We investigate optical near-field spectra of single and coupled semiconductor quantum dot. An enhanced role for the Coulomb correlations is predicted, and it is shown that the spectra depend crucially on the spatial resolution of the "local" probe. The intensity of certain optical peaks as a function of the resolution exhibits an unexpected non-monotonic behavior, which is identified as a fingerprint of Coulomb interactions in zero-dimensional nanostructures.

a10) Local absorption spectra of artificial atoms and molecules
**C. D. Simserides**, U. Hohenester, G. Goldoni and E. Molinari
Physical Review B **62** (2000) 13657-13666
doi: 10.1103/PhysRevB.62.13657
Heterocitations 26 (+1), *From collaborators 10*

We investigate theoretically the spatial dependence of the linear absorption spectra of single and coupled semiconductor quantum dots, where the strong three-dimensional quantum confinement leads to an overall enhancement of Coulomb interaction and, in turn, to a pronounced renormalization of the excitonic properties. We show that - because of such Coulomb correlations and the spatial interference of the exciton wavefunctions - unexpected spectral features appear whose intensity depends on spatial resolution in a highly non-monotonic way when the spatial resolution is comparable with the excitonic Bohr radius. We finally discuss how the optical near-field properties of double quantum dots are affected by their coupling.

a9) Local absorption spectra of single and coupled semiconductor quantum dots
**C. D. Simserides***, U. Hohenester, G. Goldoni and E. Molinari
Materials Science and Engineering B **80** (2001) 266-269
doi: 10.1016/S0921-5107(00)00652-8
Heterocitations 5
Proceedings of EXMATEC 2000 (5th International Workshop on Expert Evaluation & Control of Compound Semiconductor Materials & Technologies)

We study theoretically the local absorption spectra of single and double semiconductor quantum dots, in the linear regime. The three-dimensional confinement leads to an enhancement of the Coulomb correlations, while the spectra depend crucially on the size of the «local» probe. We show that because of such Coulomb correlations the intensity of certain optical peaks as a function of the resolution can exhibit an unexpected non-monotonic behavior for spatial resolutions comparable with the excitonic Bohr radius. We finally discuss the optical near-field properties of coupled quantum dots for different coupling strengths.

a8) Optical Spectra of Single Quantum Dots: Influence of Impurities and Few-Particle Effects
A. Hartmann, Y. Ducommun and E. Kapon, U. Hohenester, **C. Simserides** and E. Molinari
Physica Status Solidi A **178** (2000) 283-290
doi: 10.1002/1521-396X(200003)178:1<283::AID-PSSA283>3.0.CO;2-M
Heterocitations 8, *From collaborators 5*

The evolution of photoluminescence (PL) spectra of single GaAs/AlGaAs quantum dots (QD) is studied as a function of laser excitation power and temperature. At very low powers, where multi-exciton occupation of the QD can be excluded, an unexpected and pronounced spectral evolution is observed (large energy shifts and

appearance of multiple emission lines). A similar evolution is observed at low excitation powers with increasing temperature. A model, taking into account the influence of the shallow, residual impurities in the environment of each QD, explains the observed spectral evolutions in terms of photo-depletion of the QD and hopping of impurity-bound carriers back into the QD. Theoretical calculations of the PL due to N electrons + 1 hole (Ne+1h) QD states allow us to attribute the 2 meV spaced lines in the experimental spectra to the different charge states Ne + 1h, (N- 1)e + 1h, . .. of the QD.

a7) The density of states and the electron concentration of a double-heterojunction system subjected to an in-plane magnetic field
**C. D. Simserides***
Journal of Physics: Condensed Matter **11** (1999) 5131-5141
doi: 10.1088/0953-8984/11/26/314
Heterocitations 19

We calculate the electronic states of $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ double heterojunctions subjected to a magnetic field parallel to the quasi two-dimensional electron gas layer. We study the energy dispersion curves, the density of states, the electron concentration and the distribution of the electrons in the subbands.

The parallel magnetic field induces severe changes in the density of states, which are of crucial importance for the explanation of the magnetoconductivity in these structures. However, to our knowledge, there has been no systematic study of the density of states under these circumstances. We attempt a contribution in this direction.

For symmetric heterostructures, the depopulation of the higher subbands, the transition from a single-layer to a bilayer electron system and the domination of the bulk Landau levels in the centre the wide quantum well, as the magnetic field is continuously increased, are presented in the «energy dispersion picture» as well as in the «electron concentration picture» and in the «density of states picture».

a6) Electron scattering by optical phonons in $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ quantum wells
X. Zianni, **C. D. Simserides** and G. P. Triberis
Physical Review B **55** (1997) 16324-16330
doi: 10.1103/PhysRevB.55.16324
Heterocitations 30, *From collaborators 2*

The scattering of a quasi two dimensional electron gas by optical phonons in selectively doped AlGaAs/GaAs/AlGaAs quantum wells is systematically studied in order to determine the effect of phonon confinement. The electron states are calculated solving self-consistently Schroedinger and Poisson equations to obtain an accurate dependence upon the structure parameters and the temperature. We study the way the scattering is affected by the form of the phonons calculating the mobility using three models for the phonons. They are considered: (a) as 3d (b) as a set of confined and interface phonons and (c) as the normal modes of the heterostructure. The relaxation times for the electron energy subbands are calculated solving the system of Boltzmann equations. The effect of the temperature and the well width variation is also investigated. The results are in a good agreement with experimental measurements. The agreement is only slightly dependent on the model used for the phonons and becomes best when the effect of the heterostructure on the phonon modes is taken into account.

a5) Looking for the maximum low-temperature conductivity in selectively-doped $Al_xGa_{1-x}As$-GaAs-$Al_xGa_{1-x}As$ double heterojunctions
**C. D. Simserides** and G. P. Triberis
Journal of Physics: Condensed Matter **8** (1996) L421-L426
doi: 10.1088/0953-8984/8/30/002
Heterocitations 8, *From collaborators 4*

We use self-consistent numerical calculations to study the sheet electron concentration and the mobility as functions of the doping concentration, the spacer thickness, the well width and the Al mole fraction of a selectively doped $Al_xGa_{1-x}As$-GaAs- $Al_xGa_{1-x}As$ double heterojunction, using no arbitrary, *a priori*, assumptions, at low temperatures. For the first time we take into account two kinds of donor (shallow and deep) that coexist in the Si-doped $Al_xGa_{1-x}As$. We study all the significant scattering mechanisms. The model, based exclusively upon the knowledge of the material and structural parameters involved, allows as to obtain the maximum conductivity for any specific structure. Our results are in a very good agreement with experiment.

a4) A study on the temperature dependence of the quasi-two-dimensional electron concentration and mobility in $Al_xGa_{1-x}As/GaAs$ selectively doped heterostructures
**C. D. Simserides** and G. P. Triberis
Journal of Physics: Condensed Matter **7** (1995) 6317-6326
doi: 10.1088/0953-8984/7/31/014
Heterocitations 1, *From collaborators1*

From the early eighties, experiments based on the Hall effect, in various $Al_xGa_{1-x}As/GaAs$ selectively doped heterostructures, showed that up to a certain temperature the sheet electron concentration remains almost constant and then continuously increases up to room temperature. Conventional Hall experiments cannot separate the contribution of the bulk electrons from that of the quasi-two-dimensional electron gas (Q2DEG), not only as far as the Hall sheet electron concentration, $n_H$, is concerned but also the Hall mobility, $\mu_H$. However, the determination of the Q2DEG concentration and mobility, is an essential parameter for all these high-speed devices. Although experimental results on the mobility of the Si-doped bulk $Al_xGa_{1-x}As$ have been reported, there is a lack of such reports for the mobility of the Q2DEG. Only recently Schacham et al presented an experimental technique to separate the Q2DEG from the bulk contribution at room temperature.

Here, we present a quantitative analysis to interpret the temperature dependence of the Q2DEG sheet electron concentration versus the bulk sheet electron concentration, taking into account the fact that in the Si-doped $Al_xGa_{1-x}As$ two types of donors coexist, i.e. deep and shallow, which independently, and by different mechanisms, provide electrons to the bulk $Al_xGa_{1-x}As$ different conduction band minima (Γ, L, X) and to the Q2DEG. We calculate the electronic states, the ionized- donor concentrations, the Q2DEG and the bulk electron concentrations and the corresponding mobilities as a function of temperature. Our numerical results are in very good agreement with the experimental data.

a3) On the temperature dependence of the electronic states and the mobility in AlGaAs/GaAs heterostructures
**C. D. Simserides** and G. P. Triberis
Superlattices and Microstructures **14** (1993) 277-282
doi: 10.1006/spmi.1993.1139
Heterocitations 3, *From collaborators 2*
Proceedings of ICSMM-7 (7th International Conference on Superlattices, Microstructures and Microdevices)

Experiment shows that in AlGaAs/GaAs heterostructures the sheet electron concentration remains almost constant up to a certain temperature, while it increases at higher temperatures. We attempt an interpretation of this temperature dependence, taking into account the fact that in the bulk n-AlGaAs deep and shallow donors exist, which independently and by different mechanisms provide electrons to the different conduction band minima of the bulk n-AlGaAs, and contribute to the formation of the Q2DEG. We calculate the electronic states of this structure, the Q2DEG and the bulk concentrations, and the corresponding mobilities as a function of temperature. Our numerical results are in an excellent agreement with experimental data.

a2) Comments on the efficiency of Selectively-Doped Double-Heterojunction Structures
**C. D. Simserides** and G. P. Triberis
Physica Status Solidi B **184** (1994) K49-K52
doi: 10.1002/pssb.2221840234
Heterocitations 1, *From collaborators 2*

We present the form of the electron concentration during the transition from a "perfect" square well to a system of "two separated heterojunctions", in Selectively Doped Double Heterojunction structures. We also present a cartography of the surface $N_s = N_s(N_d,D_s)$, that is, of the dependence of the sheet electron concentration, $N_s$, from the doping concentration, $N_d$ and the spacer thickness, $D_s$. We project the iso-$N_s$ curves on the $(N_d,D_s)$ plane. The iso-$N_s$ map allows us to choose the most suitable combination of the $(N_d,D_s)$ values to obtain the desired $N_s$.

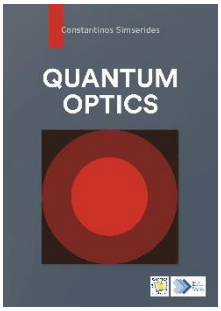
a1) A systematic study of electronic states in n-$Al_xGa_{1-x}As$/GaAs/n-$Al_xGa_{1-x}As$ selectively-doped double-heterojunction structures

**C. D. Simserides** and G. P. Triberis,
Journal of Physics: Condensed Matter **5** (1993) 6437-6446
doi: 10.1088/0953-8984/5/35/009
Heterocitations 20, *From collaborators 4*

The electron concentration, the wavefunctions and the energy levels of a n-$Al_xGa_{1-x}As$/GaAs/n-$Al_xGa_{1-x}As$ double heterojunction are evaluated by solving Schroedinger and Poisson equations self-consistently. We investigate, at zero temperature, the dependence of the sheet electron concentration, and the subband populations on the well width, spacer thickness and doping concentration, for Al mole fraction x = 0.3. We give physical interpretations to some interesting characteristics observed. The transition from a "perfect" square well to a system of "two separated heterojunctions" is systematically studied. Our results are in excellent agreement with previous experiments.

## B. 6 books and 1 invited chapter (monograph) in a book


b7) Book: **Κβαντική Οπτική**.
**Κωνσταντίνος Σιμσερίδης**, (2023). Αριθμός σελίδων 418. Γλώσσα: Ελληνικά.
ISBN: 978-618-5726-65-2
Άδεια Χρήσης: Αναφορά Δημιουργού - Μη Εμπορική Χρήση - Παρόμοια Διανομή 4.0 Διεθνές (CC BY-NC-SA 4.0)
doi: http://dx.doi.org/10.57713/kallipos-185
Handle http://hdl.handle.net/11419/9253
Metadata in Greek:https://repository.kallipos.gr/handle/11419/9254?&locale=gr
Βιβλιογραφική Αναφορά: Σιμσερίδης, Κ. (2023). Κβαντική Οπτική [Προπτυχιακό εγχειρίδιο]. Κάλλιπος, Ανοικτές Ακαδημαϊκές Εκδόσεις.




b6) Book: **Quantum Optics**.
**Constantinos Simserides**, (2023). Number of pages 404. Language: English.
ISBN: 978-618-5726-66-9
Άδεια Χρήσης: Αναφορά Δημιουργού - Μη Εμπορική Χρήση - Παρόμοια Διανομή 4.0 Διεθνές (CC BY-NC-SA 4.0)
doi: http://dx.doi.org/10.57713/kallipos-186
Handle: http://hdl.handle.net/11419/9254
Metadata in English: https://repository.kallipos.gr/handle/11419/9254?&locale=en
Βιβλιογραφική Αναφορά: Σιμσερίδης, Κ. (2023). Κβαντική Οπτική (Αγγλική έκδοση) [Προπτυχιακό εγχειρίδιο]. Κάλλιπος, Ανοικτές Ακαδημαϊκές Εκδόσεις.


b5) Book: **Ισχυρή Δέσμευση σε Μόρια, Πολυμερή, Στερεά** [Μονογραφία].
**Κωνσταντίνος Σιμσερίδης**, (2023). Αριθμός σελίδων 347. Γλώσσα: Ελληνικά.
ISBN: 978-618-5726-51-5
Άδεια Χρήσης: Αναφορά Δημιουργού - Μη Εμπορική Χρήση - Παρόμοια Διανομή 4.0 Διεθνές (CC BY-NC-SA 4.0)
doi: http://dx.doi.org/10.57713/kallipos-165
Handle http://hdl.handle.net/11419/9114
Βιβλιογραφική Αναφορά: Σιμσερίδης, Κ. (2023). Ισχυρή Δέσμευση σε Μόρια, Πολυμερή, Στερεά [Μονογραφία]. Κάλλιπος, Ανοικτές Ακαδημαϊκές Εκδόσεις.

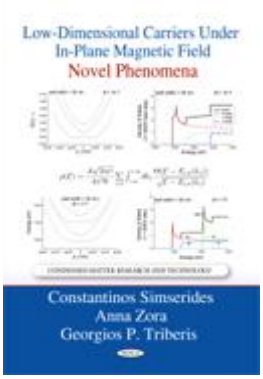

**b4) Book Βιβλίο**
**Καταστάσεις της Ύλης, Κωνσταντίνος Σιμσερίδης,**
**(States of Matter, Constantinos Simserides)**
ISBN 978-960-603-289-9, Αθήνα 2015 (Athens 2015)
Σύνδεσμος Ελληνικών Ακαδημαϊκών Βιβλιοθηκών (Hellenic Academic Libraries Link), Εθνικό Μετσόβιο Πολυτεχνείο, Ηρώων Πολυτεχνείου 9, 15780 Ζωγράφου www.kallipos.gr Creative Commons Αναφορά δημιουργού - Μη εμπορική χρήση - Όχι παράγωγα έργα (CC BY-NC-ND) 3.0.
http://repository.kallipos.gr/handle/11419/2117 Eudoxus ID: 320167
One of the suggested books for
[1] "States and properties of Matter", Physics Department, NKUA

**Contents in four chapters and 271 pages**: **1.** Introduction to the States of Matter **2.** Solids **3.** Chronological review. Alloys. Synthesis - Structure - Properties - Efficiency **4.** Real Gases and Liquids.
Heterocitations 1

**b3) Book Βιβλίο**

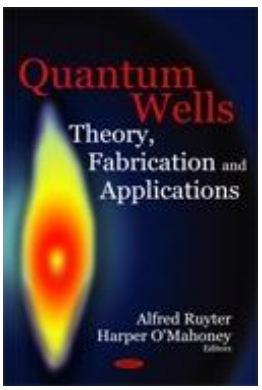

**Κβαντική Οπτική και Lasers, Κωνσταντίνος Σιμσερίδης,**
**(Quantum Optics and Lasers, Constantinos Simserides)**
ISBN: 978-960-603-073-4 Αθήνα 2015 (Athens 2015)
Σύνδεσμος Ελληνικών Ακαδημαϊκών Βιβλιοθηκών (Hellenic Academic Libraries Link), Εθνικό Μετσόβιο Πολυτεχνείο, Ηρώων Πολυτεχνείου 9, 15780 Ζωγράφου www.kallipos.gr 
http://repository.kallipos.gr/handle/11419/2108 Eudoxus ID:320166
One of the suggested books for
[1] "Quantum Optics and Lasers", Physics Department, NKUA
[2] "Special Topics in Physics", Department of Mechanical Engineering, Piraeus University of Applied Sciences
Heterocitations 1
**Contents in seven chapters and 324 pages**: **1.** Introduction to the quantum nature of light **2.** Interaction mechanisms between EM radiation and matter (*N*-level system) **3.** Semi-classical approach to the interaction between EM radiation and matter. EM radiation classically, *N*-level system quantum mechanically. **4.** Full quantum mechanical approach to interaction between EM radiation and matter. EM radiation and *N*-level system quantum mechanically. Quantization of EM field. **5.** Lasers **6.** Density Matrix **7.** Several other issues about the properties and the function of lasers.

**b2) Book**




**Low-Dimensional Carriers Under In-Plane Magnetic Field: Novel Phenomena**
**C. Simserides**, A. Zora, G.P. Triberis.
Nova Science Publishers, New York (www.novapublishers.com)
**Series:** Condensed Matter Research and Technology,
**Pub. Date:** 2010, **Pages:** 7 x 10. COB, 165 pp. 8 chapters
**Binding:** Hardcover **ISBN:** 978-1-61668-141-8
**Binding:** ebook **ISBN:** 978-1-61470-196-5
**Contents in 8 chapters and 165 pages: 1.** Quantum mechanics and thermodynamics of quasi two-dimensional carriers under in-plane magnetic field. **2.** Magnetoresistance oscillations **3.** Plasmons **4.** Photoluminescence: the N-type kink **5.** Thermodynamics and spin-subband structure of diluted magnetic semiconductor systems **6.** Diluted magnetic semiconductor quantum wells: temperature, magnetic field, carrier concentration and exchange interaction dependence **7.** Orbital thermodynamic properties **8.** A quasi zero-dimensional case: quantum dots under magnetic field of variable orientation

**b1) Invited chapter in the book**:




"Quantum Wells: Theory, Fabrication and Applications", Pages: pp.540
Nova Science Publishers, New York (www.novapublishers.com).
Editors: Alfred Ruyter and Harper O'Mahoney, Pub. Date: 2009,
Binding: Hardcover, ISBN: 978-1-60692-557-7
Binding: ebook, ISBN: 978-1-61470-723-3

Chapter title: "Quantum wells under in-plane magnetic field: Density of states and novel phenomena in thermodynamic properties, magnetization and spin-polarization." Pages 481-516.
Author: **C. Simserides***

**Chapters:**
**1.** Photodectors based on quantum-well structures: theory, properties and novel concepts by C. Rivera **2.** Recent developments of PbSe-based IV-VI semiconductor quantum well structures by S. Mukherjee, S. L. Elizondo, L. A. Elizondo, Z. Shi **3.** Coupled quantum well structures by L. Yang, Q. X. Zhao, M. Willander B Collective electronic excitations in systems exhibiting quantum well states by A. Politano **5.** Magneto-optical study of

semimagnetic single and double quantum well structures based on Cd(Mn)Se/CdMgSe material system by I.I. Reshina, S.V. Ivanov **6.** Optical gain in InGaAsN quantum well structures. summary of various approaches by M.S. Wartak **7.** Magnetoexciton dispersion in GaAs - (Ga, Al) As single and coupled quantum wells by Z.G. Koinov **8.** Bonding and antibonding states in natural molecules and double quantum wells by R. Gutierrez **9.** Spin slitting in modulation-doped semiconductor quantum wells by U. Ekenberg and D. M. Gvozdi **10.** Infinite quantum well: on the quantization problem by P. L. Garcia de Leon, J. P. Gazeau, D. Gitman, J. Queva **11.** Elementary excitations in artificially disordered electron systems: random multi-layers by Yu A. Pusep **12.** Quantum wells under in-plane magnetic field: density of states and novel phenomena in thermodynamic properties, magnetization and spin-polarization by **C. Simserides 13.** Effects of weak magnetic field on Rashba spin orbit interaction in spin dependent resonant transmission in a ZeSe/Zn1-xMnxSe heterostructure by A. John Peter Heterocitations to the book as a whole 2

## C. 28 publications in international conference proceedings, some of them in international journals with referees, 15 with referees #

c28) Proceedings of ANBRE21 (Arch Eng, Nano, Bio, Robotics & Energy). The 2021 International Conference on Advances in Biomaterials and Biomechanics in Bioengineering (ICBME21), Seoul National University, Korea, August 23-26, 2021.
**C. Simserides***, A. Morphis, K. Lambropoulos.
Hole Transfer in Open Cumulenic and Polyynic Carbyne Chains. Link here.
We studied in Simserides (2020a) and Simserides (2020b) hole transfer in open atomic, cumulenic and polyynic, carbon nanowires (Cretu (2013), Milani (2017)), employing Real-Time Time-Dependent Density Functional Theory (RT-TDDFT) and Tight-Binding (TB). The end-sites contain 1 or 2 or 3 hydrogen atoms. For DFT, CDFT, RT-TDDFT, we use the basis sets 3-21G, 6-31G*, cc-pVDZ, cc-pVTZ, cc-pVQZ and mainly the functional B3LYP. For TB, we try the following wire models: one simplistic with all sites equivalent and transfer integrals given by the Harrison $pp\pi$ expression (TBI), one with modified initial and final sites (TBImod) to include the presence of 1 or 2 or 3 hydrogen atoms at the edge-sites [this achieves similar site occupations in cumulenes with those obtained by converged RT-TDDFT], and one with TBImod transfer integrals multiplied by a factor of four (TBImodt4times) [this achieves also similar frequency content of charge and dipole moment oscillations and similar coherent transfer rates]. Full geometry optimization shows that in cumulenes the bond length alternation (BLA) is not zero and is not constant, although it is symmetrical relative to the molecule center. BLA in cumulenes is much smaller than in polyynes. Vibrational analysis shows which molecule conformations are stable. In Simserides (2020a) and Simserides (2020b) we discuss the DFT ground state energy of neutral molecules, the CDFT "ground state energy" of molecules with a hole at one end group, energy spectra, density of states, energy gap, charge and dipole moment oscillations, mean site occupations, coherent transfer rates, frequency content. Here we present a few aspects of those results.

c27#) Frequency Content of Carrier Oscillations along B-DNA Aperiodic and Periodic Polymers
M. Mantela, K. Lambropoulos, C. Vantaraki, P. Bilia, A. Morphis, and **C. Simserides***
PIERS (PhotonIcs and Electromagnetics Research Symposium, aka
Progress In Electromagnetics Research Symposium), 17-20 June 2019, Rome, Italy.
pp. 831-838, doi: 10.1109/PIERS-Spring46901.2019.9017899
URL: http://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=9017899&isnumber=9017213
**Honorable Mention Student Paper (Antennas & Microwave Technologies)** for the presenter **M. Mantela**
We study the frequency content of an extra carrier oscillation along B-DNA aperiodic and periodic polymers and oligomers made of $N$ monomers. In our work, we employ two variants of the Tight-Binding (TB) approach: a wire model and an extended ladder model including diagonal hoppings, as well as Real-Time Time-Dependent Density Functional Theory (RT-TDDFT). In the wire model, the site is a monomer, i.e., a base pair, while, in the extended ladder model, the site is a base. Initially, we focus on the Fourier Spectra of the probabilities to find the extra carrier at each monomer, having placed it at time zero at a specific monomer. We define the *weighted mean frequency* (WMF) of each site, a measure of its frequency content, using as weight the Fourier amplitude of each component of its frequency spectrum. The large-$N$ limits of the WMFs are constants in the THz domain. To obtain a measure of the overall frequency content of carrier oscillations in the polymer, we define the *total weighted mean frequency* (TWMF), averaging the WMFs of all sites weighting over the mean over time probabilities of finding the extra carrier at each site. The large-$N$ limit of the TWMFs are also constants in the THz domain. Generally, the frequency content of coherent carrier oscillations along B-DNA aperiodic and periodic polymers is in the THz domain.

c26#) Frequency Content of Carrier Oscillations along B-DNA Polymers
K. Lambropoulos, M. Mantela, **C. Simserides***
PIERS (Progress in Electromagnetics Research Symposium) Proceedings,
19- 22 November 2017, Singapore.
Volume 2018-November, 2018, Pages 186-193.
doi: 10.1109/PIERS-FALL.2017.8293134
We study the frequency content of an extra carrier oscillation along characteristic periodic B-DNA polymers made of $N$ monomers. We employ two variants of the Tight-Binding approach, a wire model and an extended ladder model including diagonal hoppings. In the former, the site is a monomer, i.e., a base pair, while, in the

latter, the site is a base. Initially, we focus on the Fourier Spectra of the probabilities to find the extra carrier at each monomer, having placed it at time zero at a specific monomer. Using the Fourier amplitude of each component of the frequency spectrum, we define the *weighted mean frequency* (WMF) for each site, a measure of its frequency content. To obtain a measure of the overall frequency content of carrier oscillations in the polymer, we define the *total weighted mean frequency* (TWMF), averaging the WMFs of all sites weighting over the probabilities of finding the extra carrier at each site. The frequency content is generally in the THz domain. Finally, we also give an example of an aperiodic sequence, the (A,T) Cantor dust.

c25#) THz oscillations in DNA monomers, dimers and trimers

K. Lambropoulos, K. Kaklamanis, G. Georgiadis, M. Theodorakou, M. Chatzieleftheriou, M. Tassi, A. Morphis and **C. Simserides***

36th PIERS (Progress in Electromagnetics Research Symposium) Proceedings, 6-9 July 2015, Prague, pp 879-883

We call *monomer* a B-DNA base-pair and study electron or hole oscillations in *monomers*, *dimers* and *trimers*. We employ two Tight Binding (TB) approaches: (I) at the base-pair level, using the on-site energies of the base-pairs and the hopping parameters between successive base-pairs and (II) at the single-base level, using the on-site energies of the bases and the hopping parameters between neighboring bases. With (II), for monomers, we predict oscillations with frequency $f \approx$ 50-550 THz. With (I), for dimers, we predict oscillations with $f \approx$ 0.25-100 THz, for trimers made of identical monomers $f \approx$ 0.5-33 THz. In other cases, the oscillations may be not strictly periodic, but Fourier analysis shows similar frequency content. For dimers, we compare approaches (I) and (II). Finally, we present calculations with (III) Real-Time Time-Dependent Density Functional Theory (RT-TDDFT) for the adenine-thymine (A-T) and the guanine-cytosine (G-C) base-pairs. It seems that a non conventional source or receiver of electromagnetic radiation with $f$ from fractions to THz to just below PHz could be envisaged.

c24#) Theory of ferromagnetism driven by superexchange in dilute magnetic semiconductors

**C. Simserides***, J.A. Majewski, K.N. Trohidou, T. Dietl

European Physical Journal Web of Conferences **75**, 01003 (2014)

http://dx.doi.org/10.1051/epjconf/20147501003

doi: 10.1051/epjconf/20147501003

On the occasion of JEMS 2013, Rhodes, Greece

Heterocitations 13 (+1), *From collaborators 4*

Also at arXiv:1308.4517v1 [cond-mat.mtrl-sci] 21 Aug 2013

Magnetic properties of $Ga_{1-x}Mn_xN$ are studied theoretically by employing a tight binding approach to determine exchange integrals $J_{ij}$ characterizing the coupling between Mn spin pairs located at distances $R_{ij}$ up to the 16th cation coordination sphere in zinc-blende GaN. It is shown that for a set of experimentally determined input parameters there are no itinerant carriers and the coupling between localized $Mn^{3+}$ spins in GaN proceeds via superexchange that is ferromagnetic for all explored $R_{ij}$ values. Extensive Monte Carlo simulations serve to evaluate the magnitudes of Curie temperature $T_C$ by the cumulant crossing method. The theoretical values of $T_C(x)$ are in quantitative agreement with the experimental data that are available for $Ga_{1-x}Mn_xN$ with randomly distributed $Mn^{3+}$ ions with the concentrations $0.01 \le x \le 0.1$.

c23#) Temperature dependence of the emission spectra of individual self-assembled quantum dots

A. Zora, **C. Simserides** and G. P. Triberis

Journal of Physics: Conference Series **245** (2010) 012037

doi: 10.1088/1742-6596/245/1/012037

On the occasion of Quantum Dot 2010

Heterocitations 1

We have developed a quantum-mechanical theory for the interaction of light and electron-hole excitations in semiconductor quantum dots. Our theoretical analysis results in an expression for the photoluminescence intensity in the non-linear regime. The validity of the theoretical results is tested analyzing experimental data reported for the temperature dependence of the emission spectra of an individual lens-shaped In0:4Ga0:6As self-assembled quantum dot in a wide temperature range up to 300 K. Our theoretical predictions for the redshift of the emission peak with increasing temperature, in the range 2-300 K, agree with the experiment.

c22#) Reducing influence of antiferromagnetic interactions on ferromagnetic properties of p-(Cd,Mn)Te quantum wells
**C. Simserides***, A. Lipińska, K.N. Trohidou, T. Dietl
Physica E: Low-dimensional Systems and Nanostructures **42** (2010) 2694-2697
doi: 10.1016/j.physe.2009.10.062
On the occasion of MSS-14
Also at arXiv:1308.4525v1 [cond-mat.mes-hall]

In order to explain the absence of hysteresis in ferromagnetic p-type (Cd,Mn)Te quantum wells (QWs), spin dynamics was previ- ously investigated by Monte Carlo simulations combining the Metropolis algorithm with the determination of hole eigenfunctions at each Monte Carlo sweep. Short-range antiferromagnetic superexchange interactions between Mn spins –which compete with the hole-mediated long-range ferromagnetic coupling– were found to accelerate magnetization dynamics if the the layer containing Mn spins is wider than the vertical range of the hole wave function. Employing this approach it is shown here that appreciate magnitudes of remanence and coercivity can be obtained if Mn ions are introduced to the quantum well in a delta-like fashion.

c21) Effects of Detuning on Control of Intersubband Quantum Well Transitions with Chirped Electromagnetic Pulses
K. Blekos, **C. Simserides**, A. F. Terzis, E. Paspalakis
AIP Conference Proceedings **1288**, 137 (2010)
doi: 10.1063/1.3521346
Proceedings of ICO-PHOTONICS-DELPHI 2009, 7-9 OCT 2009, Emerging trends and Novel Materials in Photonics
Heterocitations 1, *From collaborators 1*

We study the interaction of a chirped electromagnetic pulse with intersubband transitions of a double semiconductor quantum well. We specifically consider the interaction of the ground and first excited subbands with the electromagnetic field and use the nonlinear density matrix equations for the description of the system dynamics. These equations are solved numerically for various values of the electron sheet density for a realistic double GaAs/AlGaAs quantum well, and the efficiency of population transfer is discussed with emphasis given to the effects of the detuning of the central frequency of the electromagnetic field from resonance.

c20#) The effect of the size of self-assembled individual quantum dots on their PL spectra
A. Zora, **C. Simserides**, G. P. Triberis
Physica Status Solidi C **5** (2008) 3806-3808 doi: 10.1002/pssc.200780185
On the occasion of the 3rd MNN 2007
Heterocitations 7

Based on an analytical expression for the photoluminescence (PL) intensity of individual quantum dots (QDs) in the linear regime, we investigate its dependence upon the size of self-assembled InGaAs QDs. We prove that decreasing the QD size, the PL-emission spectrum moves to higher energy, due to the confinement-induced blueshift of the electronic levels and the redshift from the increased Coulomb interaction caused by the compression of the exciton radii. This shift is in agreement with experimental results. Moreover, we show that larger dots provide more intense PL spectra.

c19#) Magneto-optics of quantum dots in the near field
**C. Simserides***, A. Zora, G. Triberis
International Journal of Modern Physics B **21** (2007) 1649-1653
doi: 10.1142/S0217979207043361
Proceedings of the 17th International Conference on High Magnetic Fields in Semiconductor Physics
Heterocitations 2

We examine a quantum dot (QD) illuminated in the near field with sub-wavelength spatial resolution, while simultaneously it is subjected to a magnetic field of *variable orientation* and *magnitude*. The magnetic field *orientation* can *conserve* or *destroy* the zero-magnetic-field ("structural") symmetry. The asymmetry induced by the magnetic field -except for specific orientations along symmetry axes- can be uncovered in the near-field (NF)

but not in the far-field (FF) spectra. We predict that NF magneto-absorption experiments of realistic spatial resolution could reveal the QD symmetry. This exceptional *symmetry-resolving* power of the near-field optics, is lost in the far field.

c18) Controlled Intersubband Population Dynamics in a Semiconductor Quantum Well
E. Paspalakis, **C. Simserides,** A. F. Terzis
AIP Conference Proceedings **963** (2007) 533
doi: 10.1063/1.2827038
Proceedings of ICCMSE 2007 (International Conference in Computational Methods in Science and Engineering 2007)
Heterocitations 17

We examine the intersubband transition dynamics of a single semiconductor quantum well when the ground and the first excited subbands are coupled by strong electromagnetic fields, with emphasis given to controlled intersubband population inversion. The system dynamics is described by the nonlinear density matrix equations that include the effects of electron electron interactions. We present analytical results for the electromagnetic field that can lead to high-efficiency population inversion in the system. The validity of the analytical results is tested with numerical solutions of the density matrix equations for various values of the electron sheet density for a realistic GaAs/AlGaAs quantum well.

c17) Near-field magneto-optics of quantum dots
A. Zora, **C. Simserides***, G. Triberis
AIP Conference Proceedings **893** (2007) 893-894
doi: 10.1063/1.2730179
28th International Conference on the Physics of Semiconductors, Vienna, Austria, July 24-28 2006
Heterocitations 1

Encouraged by the latest experimental developments as well as by the theoretical interest on the near-field (NF) optics of semiconductor quantum dots (QDs), we present our most recent theoretical results on the NF optical absorption and photoluminescence (PL) of single and coupled III-V QDs subjected additionally to an external magnetic field of variable orientation and magnitude. The zero-magnetic-field "structural" QD symmetry can be destroyed varying the magnetic field orientation. The asymmetry induced by the magnetic field -except for specific orientations along symmetry axes- can be uncovered in the near-field but not in the far-field spectra. Hence, we predict that NF magnetoabsorption experiments, of realistic spatial resolution, will be in the position to bring to light the QD symmetry.

c16) The effect of a categorical discrimination task on the auditory M100 peak latency
R. König, C. Sielużycki, **C. Simserides**, H. Scheich,
International Congress Series **1300** (2007) 45-48
doi: 10.1016/j.ics.2007.01.062
Proceedings of **BIOMAG 2006** (15th International Conference on Biomagnetism)
Heterocitations 1

The rationale of this magnetoencephalographic (MEG) study was the quest for temporal aspects of the fMRI-characterized hemispheric asymmetries of auditory cortex functions during the processing of simple linearly frequency-modulated (FM) tones. We searched for parameters which distinguish a stimulus-related task condition—the categorical discrimination of direction (upward versus downward) of frequency modulation—from mere exposure to the same FM tones. We found that the M100-peak latency after FM tones was significantly shorter in the task condition than in the exposure condition, in the left but not in the right hemisphere.

c15#) High temperature electrical conductivity due to small polaron hopping motion in DNA molecules
G. P. Triberis, V. C. Karavolas and **C. D. Simserides**
Journal of Physics: Conference Series **10** (2005) 210–213
doi: 10.1088/1742-6596/10/1/052
Proceedings of the 2nd Conf. on Microelectronics, Microsystems and Nanotechnology 2004

Heterocitations 2

We present a small polaron hopping model to interpret the high-temperature electrical conductivity measured along the DNA molecules. The model takes into account the one-dimensional character of the system and the presence of disorder in the DNA double helix. The experimental data for the lambda phage DNA ($\lambda$-DNA) and the poly(dA)-poly(dT) DNA follow nicely the theoretically predicted behavior leading to realistic values of the maximum hopping distances supporting the idea of multiphonon-assisted hopping of small polarons between next nearest neighbors of the DNA molecular "wire".

c14#) Spin-polarization and magnetization of conduction-band dilute-magnetic-semiconductor quantum wells with non-step-like density of states

**C. Simserides***

Journal of Physics: Conference Series **10** (2005) 143–146

doi: 10.1088/1742-6596/10/1/035

Proceedings of the 2nd Conf. on Microelectronics, Microsystems and Nanotechnology 2004

We study the magnetization, $M$, and the spin polarization, $\zeta$, of n-doped non-magnetic-semiconductor (NMS) / narrow to wide dilute-magnetic-semiconductor (DMS) / n-doped NMS quantum wells, as a function of the temperature, $T$, and the in-plane magnetic field, $B$. Under such conditions the density of states (DOS) deviates from the occasionally stereotypic step-like form, both quantitatively and qualitatively. The DOS modification causes an impressive fluctuation of $M$ in cases of vigorous competition between spatial and magnetic confinement. At low $T$, the *enhanced* electron spin-splitting, $U_{\sigma\sigma}$, acquires its bigger value. At higher $T$, $U_{\sigma\sigma}$ decreases, augmenting the influence of the spin-up electrons. Increasing $B$, $U_{\sigma\sigma}$ increases and accordingly electrons populate spin-down subbands while they abandon spin-up subbands. Furthermore, due to the DOS modification, all energetically higher subbands become gradually depopulated.

c13) Temperature dependent magnetization and magnetic phases of conduction-band dilute-magnetic-semiconductor quantum wells with non-step-like density of states

**C. Simserides***

AIP Conference Proceedings **772** (2005) 341-342

doi: 10.1063/1.1994128

ICPS27 (27th International Conference on the Physics of Semiconductors) proceedings published by AIP

We investigate the magnetization of II-VI non-magnetic-semiconductor (NMS) / narrow to wide dilute-magnetic-semiconductor (DMS) / NMS quantum wells. These structures are appropriate for conduction-band spintronics. We employ an in-plane magnetic field, $B$, in order to induce non-step-like density of states. Finally, we tune the spin polarization by varying the temperature, $T$, and $B$, i.e. we investigate the magnetic phases of these NMS/DMS/NMS structures.

c12) Do stimuli or tasks determine lateralized auditory cortex responses? An MEG study

C. Sielużycki, R. König, **C. Simserides**, H. Scheich

International Journal of Bioelectromagnetism, IJBEM **7** (2005) 185-188

[Proceedings of the Joint Meeting of 5th International Conference on Bioelectromagnetism and 5th International Symposium on Noninvasive Functional Source Imaging within the Human Brain and Heart (BEM & NFSI), University of Minnesota, Twin Cities campus in Minneapolis, Minnesota, USA, 12-15/5/2005].

http://www.ijbem.org/volume7/number2/185-188.pdf

We studied hemispheric differences of the evoked magnetic fields induced by frequency modulated tones (FMs) and pure sinusoidal tones, by means of magnetoencephalography (MEG). Seven subjects were exposed to three conditions: 1) passive listening to sinusoidal 1 kHz tones (*sine-exposure* condition), 2) passive listening to linear FMs (*FM-exposure* condition), and 3) directional categorization (up versus down) of FMs (*FM-task* condition). The underlying question was whether different stimuli determine the hemispheric activation of auditory cortex, or rather the task performed by the subjects. With binaural presentation we observed an N100m-latency difference between hemispheres for FMs and a smaller difference for sinusoidal tones. The right-hemispheric response to FMs was faster than the left one, both during task end exposure. We also observed different frequency content of the raw (non-averaged) data recorded for the three different conditions. Specifically, the FM-task condition produced a distinct spectral content compared to the two exposure conditions with tones and FMs, which induced a similar spectral pattern.

c11#) Magnetic field effects on the near field spectra of quantum dots
A. Zora, **C. Simserides***, G. Triberis
Physica Status Solidi A **202** (2005) 619–624
doi: **10.1002/pssa.200460440**
Proceedings of EXMATEC04 (7th Expert Evaluation & Control of Compound Semiconductor Materials & Technologies)
Heterocitations 1
We theoretically investigate the linear near field absorption spectra of semiconductor quantum dots under magnetic field of variable orientation. We examine if the application of the magnetic field alone is sufficient to cause – increasing the spot illuminated by the near field probe – "unexpected" features to the absorption spectra.

c10#) Near field spectroscopy of quantum dots under magnetic field
A. Zora, **C. Simserides*** and G. Triberis
International Journal of Modern Physics B **18** (2004) 3717-3721
doi: 10.1142/S0217979204027347
Proceedings of SEMIMAG16 (16th Internat. Conference on High Magnetic Fields in Semiconductor Physics)
Heterocitations 1
We present the basic steps for the study of the linear near field absorption spectra of semiconductor quantum dots under magnetic field of variable orientation. We show that the application of the magnetic field alone is sufficient to induce -increasing the spot illuminated by the near field probe- interesting features to the absorption spectra.

c9#) Magnetization and magnetic phases of conduction-band dilute-magnetic-semiconductor quantum wells with non-step-like density of states
**C. Simserides***
International Journal of Modern Physics B **18** (2004) 3745-3748
doi: 10.1142/S0217979204027384
Proceedings of SEMIMAG16 (16th Internat. Conference on High Magnetic Fields in Semiconductor Physics)
We study the magnetization and the magnetic phases of II-VI-based n-doped non-magnetic-semiconductor (NMS) / narrow to wide dilute-magnetic-semiconductor (DMS) / n-doped NMS quantum wells under in-plane magnetic field. The parallel magnetic field is used as a tool, in order to achieve non-step-like density of states in these -appropriate for conduction-band spintronics- structures.

c8) An MEG study of directional categorization of frequency-modulated tones
**C. Simserides**, R. König, and H. Scheich
Proceedings of the 14th International Conference on Biomagnetism (BIOMAG 2004),
E. Halgren, S. Ahlfors, M. Hämäläinen, and D. Cohen (eds.), pp. 543-544.
Boston: Biomag 2004 Ltd.

c7) Task-dependent activation of the auditory cortex by frequency-modulated tones: an MEG study
**C. Simserides***, R. König, and H. Scheich
Biomedizinische Technik **48** (2004) 205-207
Proceedings of NFSI-2003
(4th International Symposium on Nonivasive Functional Source Imaging)
Frequency modulations (FM) play a fundamental role in human speech and likewise in animal vocalization. Moreover, interest in the activation pattern of the human auditory cortex in response to FM tones is due to the fact that processing of FM tones as well as of speech prosodies may be based on common auditory mechanisms. The aim of this study is to provide information about the processing of FM tones as well as *the* dependence of the corresponding cortical activation on a directional decision task. This is achieved by the use of the MEG

technique that, unlike fMRI, is capable of tracking brain dynamics with an unequalled high temporal resolution in the millisecond range along with a yet satisfying spatial resolution.

c6#) Not-step-like Density of States and carrier distribution of conduction-band, narrow-to-wide Dilute Magnetic Semiconductor quantum wells under in-plane magnetic field
**C. Simserides***
Physica E: Low-Dimensional Systems & Nanostructures **21** (2004) 956-960
doi: 10.1016/j.physe.2003.11.170
Proceedings of MSS11 (11th International Conference on Modulated Semiconductor Structures)
We analyze the important changes induced to the density of states (DOS) of narrow to wide conduction band Dilute Magnetic Semiconductor (DMS) quantum wells subjected to an in-plane magnetic field, B. We show quantitatively that the DOS diverges significantly from the famous step-like 2DEG form, by providing results for many values of B an grades of spatial localization. This introduces changes to the pertinent electronic properties. The self-consistent approach is indispensable and the eigenvalue problem has to be solved for each subband index i, spin σ, and in-plane wavevector e.g. $k_x$. We can select the appropriate parameters so that the structure is populated by carriers of spin down or exploit the effect of the depopulation of the higher spin-subbands to eliminate carriers with spin up.

c5#) The Density of States and the pertinent Electronic Properties of the quasi 2DEG in Simple and DMS structures subjected to an in-plane magnetic field
**C. Simserides***
Journal of Computational Electronics **2** (2003) 459-463
doi: 10.1023/B:JCEL.0000011471.69323.17
Heterocitations 1
Proceedings of IWCE-9 (9th International Workshop on Computational Electronics)
We analyze the important changes induced to the density of states (DOS) of a quasi two-dimensional-electron-gas (2DEG), when it is subjected to an in-plane magnetic field, B. The DOS diverges significantly from the famous step-like form and this introduces changes to the pertinent electronic properties. In order to calculate the DOS it is indispensable to use a self-consistent approach. The eigenvalue problem has to be solved for each subband index i and in-plane wavevector, $k_x$, when the quasi 2DEG is parallel to the xy-plane and B is applied along the y-axis. Although the modification of the DOS is usually ignored, we show here that not only the general shape of the DOS varies, but this effect is also quantitative.

c4) Auditory Cortex Response to Frequency-Modulated Tones Investigated with MEG
R. König, **C. Simserides**, and H. Scheich
Proceedings of the **International Conference on Auditory Cortex**, Shaker Verlag, Aachen, Germany (2003) p.30 (13-17 September 2003, Magdeburg, Germany)

c3) Conduction band narrow to wide Diluted Magnetic Semiconductor layers
under in-plane magnetic field: not step-like Density of States and consequences
**C. Simserides***
Proceedings of **MSS11** (2003) p.299 (booklet version)
(11th International Conference on Modulated Semiconductor Structures,
Nara, Japan, 14-18 July 2003)

c2) Local optical absorption by confined excitons in single and coupled quantum dots
**C. Simserides***, U. Hohenester, G. Goldoni and E. Molinari
Proceedings of the **ICPS-25** edited by N. Miura and T. Ando, Springer Berlin (2001) p.1117
(25th International Conference on the Physics of Semiconductors,
17-22 September 2000 Osaka, Japan).
Heterocitations 2

c1) Electronic properties of n-$Al_xGa_{1-x}As$/GaAs/n-$Al_xGa_{1-x}As$ double heterojunctions
**C. D. Simserides** and G. P. Triberis
Proceedings of the **4th-ICFSI**, World Scientific Publishing, London, England (1993) (4th International Conference on the Formation of Semiconductor Interfaces, 14-18/6/1993, Julich, Germany)

## D. 8 topical conference proceedings or international schools proceedings

In the following list extended or simple abstracts are not included.

d8) K. Lambropoulos, K. Kaklamanis, G. Georgiadis, and **C. Simserides,** Charge oscillations in the mid-to-far infrared and charge transfer in DNA, 9th Conference of the Hellenic Society for Computational Biology and Bioinformatics (HSCBB14), Agricultural University of Athens in 10-12 October 2014

d7) L. G. D. Hawke, G. Kalosakas, **C. Simserides**, Tight-binding parameters for charge transport in DNA, 5th Conference of the Hellenic Society for Computational Biology and Bioinformatics, 17-19 October 2010, Alexandroupolis, Greece

d6) A. Hartmann, Y. Ducommun and E. Kapon, U. Hohenester, **C. Simserides** and E. Molinari, Few-particle effects in the optical spectra of single semiconductor quantum dots, 11th International Winterschool on New Developments in Solid State Physics: Low-Dimensional Systems: Fundamentals and Applications, 21-25 February 2000, Mauterndorf, Salzburg, Austria

d5) V. Piazza, **C. D. Simserides***, W. Wegscheider and F. Beltram, Changing the density of states and the magnetoresistance of double heterojunctions by an in-plane magnetic field, Advanced Materials for Industrial Applications. Διεθνές θερινό σχολείο που οργανώθηκε από το Τμήμα Φυσικής του Αριστοτελείου Παν. Θεσσαλονίκης στην Καβάλα (20-27/6/1999)

d4) Ξ. Ζιάννη, **Κ. Δ. Σιμσερίδης** και Γ. Π. Τριμπέρης, Μελέτη της σκέδασης ηλεκτρονίων από οπτικά φωνόνια σε ημιαγώγιμες ετεροδομές, 11ο Πανελλήνιο Συνέδριο Φυσικής Στερεάς Κατάστασης, Σεπτέμβριος 1995, Ξάνθη. *Πρακτικά XI ΠΣΦΣΚ*.

d3) **Κ. Δ. Σιμσερίδης**, Ξ. Ζιάννη και Γ. Π. Τριμπέρης, Συστηματική μελέτη της ηλεκτρονιακής ευκινησίας σε επιλεκτικά εμπλουτισμένες διπλές ετεροεπαφές $Al_xGa_{1-x}As/GaAs$, 11ο Πανελλήνιο Συνέδριο Φυσικής Στερεάς Κατάστασης, Σεπτέμβριος 1995, Ξάνθη. *Πρακτικά XI ΠΣΦΣΚ*.

d2) **Κ. Δ. Σιμσερίδης** και Γ. Π. Τριμπέρης, Θερμοκρασιακή εξάρτηση των ηλεκτρονικών καταστάσεων και της ευκινησίας σε ετεροδομές AlGaAs/GaAs, 10ο Πανελλήνιο Συνέδριο Φυσικής Στερεάς Κατάστασης, Σεπτέμβριος 1994, Δελφοί. *Πρακτικά X ΠΣΦΣΚ*.

d1) **Κ. Δ. Σιμσερίδης** και Γ. Π. Τριμπέρης, Μια συστηματική μελέτη των ηλεκτρονικών καταστάσεων επιλεκτικά ντοπαρισμένων διπλών ετεροεπαφών τύπου n-AlxGa1-xAs/GaAs/n-AlxGa1-xAs, 9ο Πανελλήνιο Συνέδριο Φυσικής Στερεάς Κατάστασης, Σεπτέμβριος 1993, Ρίο, Πάτρα. Πρακτικά IX ΠΣΦΣΚ.

## E. 2 popular science publications

e1) **C. Simserides***, K. Lambropoulos. The future of nanotechnology and nanoscience and their applications. Physics News magazine, of Hellenic Physicists Association, Issue **22**, April 2018, pp. 28-37.

e2) **C. Simserides***. To become wise, start from names: Commutation and Anticommutation, InScience March 12, 2022 https://www.inscience.gr/2022/03/12/

Article link https://www.inscience.gr/2022/03/12/%ce%b1%cf%81%cf%87%ce%ae-%cf%83%ce%bf%cf%86%ce%af%ce%b1%cf%82-%ce%bf%ce%bd%ce%bf%ce%bc%ce%ac%cf%84%cf%89%ce%bd-%ce%b5%cf%80%ce%af%cf%83%ce%ba%ce%b5%cf%88%ce%b9%cf%82-%ce%bc%ce%b5%cf%84%ce%ac%ce%b8/

## F. 1 co-supervision of book translation

f1) Φυσικοχημεία Kurt W. Kolasinski,
Επιμέλεια: Παναγιώτης Γιαννακουδάκης, **Κωνσταντίνος Σιμσερίδης**
Μετάφραση: Χριστίνα Βανταράκη, Φανή Πινακίδου,
Έτος έκδοσης εντύπου 2020. ISBN 9789605863463.
Original Textbook:
Physical Chemistry - How Chemistry Works, 2017, Wiley, 726 pages.

## Sketch of PhD of Constantinos Simserides

### Electronic states and mobility of selectively doped heterostructures $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$

**Chapter A : Introduction.**
A1. Introduction to physics of semiconductor devices.
A2. Slater theorem (envelope function equation) and consequences.
A3. From Schrödinger equation through effective mass approach to effective mass equation.
A4. Applying BenDaniel-Duke equation.

**Chapter B. Electronic states of a double heterojunction at temperature $T$ = 0 K.**
B1. Introduction.
B2. Description of the system.
B3. Theoretical calculations.
B4. Results.

**Chapter Γ. Temperature dependence of electronic states.**
Γ1. Introduction.
Γ2. Formulation of the problem.
Γ3. Application to heterostructure.
Γ4. Results and discussion.

**Chapter Δ. General transport theory. Electron mobility and structure conductivity.**
Δ1. Introduction to the study of electron mobility.
Δ2. General transport theory - Boltzmann equation.
Δ3. General transport theory - Subband mobility and structure mobility.

**Chapter E. Screening on quasi-two-dimensional electron gas.**
E1. General theory (one subband in the well). Results.
E2. Comparison of TF-RPA results.
E3. General theory (many subband in the well).
E4. Results with many subbands in the well.

**Chapter ΣT. Alloy disorder.**
ΣT1. Introduction to alloy disorder
ΣT2. Matrix elements.
ΣT3. One subband in the well.
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**Chapter Z. Ionized donors.**
Z1. Introduction to ionized donor scattering
Z2. Matrix elements.
Z3. One subband in the well.
Z4. Ionized donors scattering. Results.

**Chapter H. Interface roughness.**
H1. Introduction to interface roughness scattering
H2. Matrix elements.
H3. One subband in the well.
H4. Interface roughness scattering. Results.

**Chapter Θ. Acoustic phonons and results with all scattering mechanisms.**
Θ1. Introduction to acoustic phonon scattering.
Θ2. Matrix elements.
Θ3. One subband in the well.
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**Appendices**

Π1 Proof of Slater theorem.
Π2 Electron eigenstates in a quantum well of potential energy $U(\boldsymbol{r}) = U(z)$
Π3 The density of eigenstates of quasi-two-dimensional electron gas.
Π4 The spatial density of occupied states at temperature *T*.
Π5 Proof of equation (Δ2.14).
Π6 Derivation of relation similar to equation (Δ3.6) in 3 dimensions.
Π7 The temperature dependence of polarizability.
Π8 The matrix elements for alloy disorder scattering.
Π9 Proof of equation (Π9.1)
Π10 The matrix elements for ionized donors scattering

**References**

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## Constantinos Simserides Ph.D. Summary in English

Electronic states and mobility of selectively doped $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ heterostructures

We use self-consistent numerical calculations to study the sheet electron concentration and the mobility as functions of the doping concentrations, the spacer thickness, the well width and the Al mole fraction of selectively doped $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ double heterojunctions, using no restrictive, a priori, assumptions. For the first time we take into account two kinds of donors (shallow and deep) that coexist in the Si-doped AlxGa1-xAs. We study all the significant scattering mechanisms. The model, based exclusively upon the knowledge of the material and structural parameters involved, allows us to obtain the maximum conductivity for any specific structure. The transition from a "perfect square quantum well" to a system of "two separated heterojunctions" is systematically studied. We also present a quantitative analysis of the temperature dependence of the quasi-two-dimensional electron concentration taking into account that in the Si-doped $Al_xGa_{1-x}As$ shallow and deep donors coexist. These donors provide electrons not only to the quasi-two-dimensional electron gas but also to the different conduction band minima of the bulk $Al_xGa_{1-x}As$. Our numerical results are in very good agreement with the experiment.

## ΣΧΕΔΙΑΓΡΑΜΜΑ ΔΙΔΑΚΤΟΡΙΚΗΣ ΔΙΑΤΡΙΒΗΣ του Κωνσταντίνου Σιμσερίδη

### Ηλεκτρονιακές καταστάσεις και ευκινησία επιλεκτικά εμπλουτισμένων ετεροδομών $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$

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Α2. Θεώρημα Slater (Εξίσωση Περιβάλλουσας Συναρτήσεως) και συνέπειες.
Α3. Από την εξ. Schrödinger μέσω της Προσέγγισης Ενεργού Μάζας στην εξίσωση Ενεργού Μάζας.
Α4. Εφαρμογή της εξίσωσης BenDaniel-Duke.

**Κεφάλαιο Β. Ηλεκτρονιακές καταστάσεις διπλής ετεροεπαφής σε θερμοκρασία T = 0K.**

Β1. Εισαγωγή.
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Β3. Θεωρητικοί υπολογισμοί.
Β4. Αποτελέσματα.

**Κεφάλαιο Γ. Θερμοκρασιακή εξάρτηση των ηλεκτρονιακών καταστάσεων.**

Γ1. Εισαγωγή.
Γ2. Μορφοποίηση του προβλήματος.
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**Κεφάλαιο Δ. Γενική Θεωρία Μεταφοράς. Ευκινησία των ηλεκτρονίων και αγωγιμότητα της δομής.**
Δ1. Εισαγωγή στη μελέτη της ηλεκτρονιακής ευκινησίας.
Δ2. Γενική Θεωρία Μεταφοράς - Εξίσωση Boltzmann.
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Ε1. Γενική Θεωρία (μία υποζώνη στο πηγάδι). Αποτελέσματα.
Ε2. Σύγκριση αποτελεσμάτων TF-RPA.
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Ε4. Αποτελέσματα με πολλές υποζώνες στο πηγάδι.

**Κεφάλαιο ΣΤ. Αταξία Κράματος.**
ΣΤ1. Εισαγωγή στη σκέδαση από αταξία κράματος.
ΣΤ2. Στοιχεία πίνακα.
ΣΤ3. Μία υποζώνη στο πηγάδι.
ΣΤ4. Πολλές υποζώνες στο πηγάδι.
ΣΤ5. Σκέδαση από αταξία κράματος. Αποτελέσματα.

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Ζ2. Στοιχεία πίνακα.
Ζ3. Μία υποζώνη στο πηγάδι.
Ζ4. Σκέδαση από ιονισμένους δότες. Αποτελέσματα.

**Κεφάλαιο Η. Τραχύτητα Ενδοεπιφανειών.**
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Η3. Μία υποζώνη στο πηγάδι.
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**Κεφάλαιο Θ. Ακουστικά Φωνόνια και αποτελέσματα με όλους τους μηχανισμούς σκέδασης.**
Θ1. Εισαγωγή στη σκέδαση από ακουστικά φωνόνια.
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**Παραρτήματα**
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Π2 Ιδιοκαταστάσεις ηλεκτρονίου σε κβαντικό πηγάδι δυναμικής ενέργειας $U(\boldsymbol{r}) = U(z)$
Π3 Η πυκνότητα ιδιοκαταστάσεων ψευδο-διδιαστάτου ηλεκτρονιακού αερίου.
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Π5 Απόδειξη της σχέσης (Δ2.14).
Π6 Εξαγωγή της ανάλογης σχέσης με την εξ.(Δ3.6) στις 3 διαστάσεις.
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Π8 Τα στοιχεία πίνακα για τη σκέδαση από αταξία κράματος.
Π9 Απόδειξη της σχέσης (Π9.1)
Π10 Τα στοιχεία πίνακα για τη σκέδαση από ιονισμένους δότες.

**Αναφορές**

Σημείωση : Αντί του όρου «ψευδο-δισδιάστατο» θα μπορούσαμε να χρησιμοποιήσουμε τους όρους «οιονεί δισδιάστατο» (πιο αρχαιοπρεπές) ή «σχεδόν δισδιάστατο» (πιο απλά). Επίσης χρησιμοποιήθηκε η λέξη «ηλεκτρονιακή» (δηλαδή των ηλεκτρονίων) αντί της λέξης «ηλεκτρονική» (που είναι γενικότερη).

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