Summary of professional accomplishments

1. **Paweł Scharoch**

2. **Diploma**

1980 – *Master of Science and Engineering in Fundamental Problems of Technology*, obtained at Wroclaw University of Technology, Faculty of Fundamental Problems of Technology.

1. 1986 – *PhD in Physics*, obtained at Wroclaw University of Technology, Faculty of Fundamental Problems of Technology. Thesis: *Quantum efficiency of internal photoelectric effect in narrow-gap semiconductors.*

3. **History of employment in research institutions**

Now, from October 1991
WROCLAW UNIVERSITY OF TECHNOLOGY, FACULTY OF FUNDAMENTAL PROBLEMS OF TECHNOLOGY; Senior Research Assistant in the Theory of Condensed Matter Physics Group (at present the Department of Theoretical Physics).

From 05.2008 to 31.06.2015
R&D CENTER OF TELEKOMUNIKACJA POLSKA S.A. (at present ORANGE LABS), part time; Chief Specialist in Research Department.

From 10.2001 to 01.2002
FRITZ-HABER INSTITUTE, THEORY DEPARTMENT, BERLIN –
Research practice.

From 10.1995 to 03.2000
INSTITUTE of TELECOMMUNICATION, WROCLAW BRANCH –
Part time.

From 05.1985 to 12.1991
INSTITUTE of TELECOMMUNICATION, WROCLAW BRANCH –
Research Assistant in the Department of Electromagnetic Hazards

From 02.1987 to 12.1988
UNIVERSITY OF DURHAM, GREAT BRITAIN –
Postdoc in the Semiconductor Theory Group.

4. **Scientific achievements within the subject of habilitation:** *'Ab initio' computational studies of structural, elastic and electronic properties of chosen semiconductor systems*

Mixed semiconductor systems have been a matter of much interest to scientists and technologists almost from the beginning of semiconductor physics development. However, for over than 20 years they are a subject of particularly intensive research stimulated by their properties which are interesting from application perspective, and on the other hand, by the rapid development of modern technologies. The subject of interest are first of all structural (e.g. crystal lattice, atomic distribution in mixed system), elastic and electronic parameters

(band structure), since they determine numerous application possibilities, e.g. in optoelectronics. The parameters are closely related to each other, e.g. strains or atomic distribution affect the electronic structure, atomic distribution affects elastic properties etc. An important role in the development of the field is attributed to *ab initio* theoretical studies, because of their **predictive power.** The computational investigations are much faster and much cheaper than real life experiments and allow to evaluate the mentioned above properties and consequently to point at the materials which should be subjected to further research.

I got interested in the area (the aspect of ab initio modeling, which is a subject of the habilitation application), about 5 years ago. During the first 3 years, the computational investigations were conducted within 4 Master of Science diploma projects. The experience gained at that time allowed to establish a collaboration with the group led by dr hab. Robert Kudrawiec from the Laboratory of Optical Spectroscopy of Nanostructures (LOSN), Department of Experimental Physics in the Faculty of Fundamental Problems of Technology at Wroclaw University of Technology. The collaboration resulted in 4 papers published over the last year, it will be continued and extended on various aspects of semiconductor systems physics.

Below, I present a brief characteristics of 11 papers containing results of *ab initio* studies which either were led by me or in which I actively participated, and also a detailed characteristics of my contribution.

H1). Winiarski, M.J., Polak, M., Scharoch, P.
Anomalous band gap bowing of $AlN_{1-x}P_x$ alloy
(2013) Journal of Alloys and Compounds, 575, pp. 158-161.

It is the first from a series of works devoted to *ab initio* investigations into structural and electronic properties of mixed systems. There were several objectives, first of all to explore the predictive power of *ab initio* methods, since to the authors knowledge, the material has not been synthesized yet. Thus, a superior aim was the investigation into the properties of a hypothetical alloy in ZB (zinc blende) structure. The side purpose was to test the tools and methodologies used in calculations of that kind, in particular the proposed quite recently the exchange-correlation energy functional MBJLDA (*Modified Becke Jonson Local Density Approximation*) which is supposed to provide a correct band gap. As far as methodologies are concerned, two approaches have been tested: the supercell method (SC) and the alchemical mixing approach (AM). The supercell method consists in the use of large cells which are multiples of primitive cells. For example, in ZB structure, the parent compounds *AlN* and *AlP* contain two atoms in a primitive cell. The supercell with all the lattice vectors doubled contains *8* primitive cells, i.e. *16* atoms, *8 Al* and *8 N* (or *P*). Computations for such a system are demanding but realistic and allow to study compounds with compositions varying at *12.5%* step, and with different atomic distribution which makes possible studying the effect of this distribution (clustered vs. uniform) on physical properties. In the AM approach (which is sometimes mistakenly called the virtual crystal approximation – VCR), in the primitive cell (*2* atoms only), in the anion position, a pseudopotential is placed, which is a specially constructed superposition of two pseudopotentials *N* and *P* (*N/P*), in proportions corresponding to compositions (the details of the construction are described in the paper). The method is much more effective than the SC but much less reliable, which has been shown in this and in the following papers.

A few interesting results have been achieved. A dependence of the lattice constant on the composition calculated within the SC obeys Vegard's law (the linear dependence), but the same dependence calculated within the AM shows a significant bowing (Fig.1). This is an artefact of the AM computational method whose reasons have been investigated and discussed in the work (H4). A strong effect of atomic configuration on the band gap has been revealed, in particular an unusually big bowing in the clustered configuration with optimized geometry (Fig.6). Similarly as in the case of the lattice constant, a big discrepancy between the results obtained from the SC and AM methods can be observed.

All the calculations in this and the following projects have been done with the use of ABINIT package, in the Wroclaw Center for Networking and Supercomputing.

My contribution in this project consisted in calculations planning (including methodologies), interpreting the results and coediting the manuscript. I estimate this contribution to be **30%**.

H2). Scharoch, P., Winiarski, M.
An efficient method of DFT/LDA band gap correction
(2013) Computer Physics Communications, 184 (12), pp. 2680-2683.

In the calculations of electronic structure from first principles, the well-known "band gap problem" appears consisting in underestimation of the band gap in the Local Density and Generalized Gradient Approximations (LDA and GGA) of the exchange-correlation energy functionals. The reason is the convex behavior of the functionals under a fractional change in electronic density (the article contains the discussion of the effect). It is known however that for finite systems it is possible to evaluate the fundamental gap with a good accuracy from the difference in self-consistent energies for the excited and the ground states ($\Delta(SCF)$, *SCF* – Self Consistent Field). The application of the $\Delta(SCF)$ method in an infinite system is in principle impossible since, on the one hand, an excitation of a single electron leads to an infinitesimal change in the total energy (which together with the convexity of functionals is the reason for the underestimation of the band gap), and on the other hand, an excitation of one electron per primitive cell would lead to unphysically large excited densities and is technically impossible in the calculations. The ABINIT program allows to apply partial occupancies which made it possible to formulate an idea of constructing an excited state from partial occupancies with a Gaussian distribution centered e.g. on Γ point in the Brillouin zone (for a direct transition). The energies of excited states can then be calculated for small excitations of varying quantity and extrapolated to 1 electron per primitive cell. The total energy is normalized to a unit cell so the band gap can be evaluated as a difference in self-consistent energies for the excited (1 electron per unit cell) and the ground state. A parameter appears in the method, the half-width of the Gaussian (σ_k), which can be treated as a fitting parameter since the calculated band gap depends on the value of this parameter. This fact has been used in the construction of the band gap correction methods. It has been shown in the literature that in an infinite system the effect of functional convexity can be neutralized by the localization of electron in *r*-space. The method of such localization has been proposed in the context of the present work.

The following results have been obtained. It has been shown that for small excitations the total energy varies linearly with the value of the excited charge; it has been proved formally and confirmed in calculations that the $\Delta(SCF)$ method is equivalent to the $\Delta(EIG)$ where the band gap is calculated as an average of Kohn-Sham energies sampled with the same

distribution as in $\Delta(SCF)$; it has been shown that the correlation exists between σ_k, giving a correct band gap and experimental gap (although it is known that no such correlation exists between the LDA/GGA gap and the experimental gap), and on that basis two methods of E_g evaluation in the unknown system proposed. One of this method consists in applying the linear dependence of σ_k on the composition in an alloy, and the other (called "semi-empirical") consists in searching for the crossing point of the evaluated E_g dependence on σ_k with the established universal dependence $E_g(\sigma_k)$.

The paper has been regarded in the Institute of Low Temperatures and Structure Research in Wroclaw as one of most important achievements in the year 2013.

My contribution in the project consisted in formulating the idea, working out the theoretical background, proving the equivalence of $\Delta(SCF)$ and $\Delta(EIG)$ methods (from Janaks theorem), taking part in numerical calculations, proposing one of the methods of band gap evaluation (the semi-empirical), proposing the method of electron localization in *r*-space, writing the manuscript. I estimate the contribution to be **60%**.

H3). Scharoch, P., Winiarski, M.J., Polak, M.P.
Ab initio study of $In_xGa_{1-x}N$ - Performance of the alchemical mixing approximation
(2014) Computational Materials Science, 81, pp. 358-365.

The paper contains a description of the extended computational research of $In_xGa_{1-x}N$ system with the alchemical mixing method (AM) (* - see the footnote), including structural, elastic and electronic properties. One of the aims, apart from investigating into system properties (partly unknown, like elastic parameters in ZB structure), was testing the reliability of AM approximation and possible reasons of discrepancy between the results obtained with this method and the supercell (SC) one. A lot of experimental data have been collected in the paper for the purpose of comparison with calculations.

To a large extent, the work has a technical character (learning and practicing the research tools, testing the approximations, e.g.; for the calculation of electronic structure, the proposed recently MBJLDA functional has been used). An important achievement of the work has been a demonstration that the AM approximation leads to acceptable results for elastic constants but not for bowings of the lattice parameter and the band gap which are unphysical. It has been proved via an analysis of the projected densities of states in the AM and SC approaches that the bowings are mainly due to the lack of the local ionic relaxation in the AM approximation where atoms always occupy high symmetry positions of the primitive cell. This fact was an inspiration of the proposed later SC/AM method which was a combination of the SC and AM method (*1* or *2* alchemical atoms in a supercell).

My contribution consisted in formulating the project theses, participation in numerical calculations, collecting the experimental data from the literature, explanation of the reasons of AM errors, and writing the paper. I estimate my contribution to be **50%**.

*) in the paper the name Virtual Crystal Approximation (VCA) has been used following the common practice in the literature. However, in later works it turned out that the VCA name in the related papers has a different meaning, close to the historically original one, on the ground of the single particle approximation and empirical psedopotentials. For this reason, in later works we decided to change the name of the approximation to *Alchemical Mixing* (AM), proposed by the authors of ABINIT package, and this name I use consequently throughout this document.

H4). Winiarski, M.J., Scharoch, P., Polak, M.P.
First principles prediction of structural and electronic properties of $Tl_xIn_{1-x}N$ alloy (2014) Journal of Alloys and Compounds, 613, pp. 33-36.

The work has been an attempt to study the properties of the alloy $Tl_xIn_{1-x}N$ which, to the authors knowledge, has not been investigated so far. Owing to the application of MBJLDA functional and fully relativistic pseudopotentials, a realistic prediction of the band-structure has been possible. The most important result has been presented in Fig.5, where a linear decrease in the band gap value with *TlN* content (from the value of about *0.7eV*) accompanied by a linear increase in the spin-orbit splitting (SOS) (from the value close to zero) can be seen. At the content of about $x=0.25$ the band gap approaches zero and SOS stabilizes at the value of about *1.4eV*. The possibility of obtaining different *Eg* and SOS through the content variation makes the material interesting from the point of view of optoelectronic applications (e.g. the possibility to eliminate the Auger transitions).

My contribution to the work consisted in the interpretation of the results and co-authoring the paper. I estimate the contribution to be **20%**.

H5). Polak, M.P., Scharoch, P., Kudrawiec, R., Kopaczek, J., Winiarski, M.J., Linhart, W.M., Rajpalke, M.K., Yu, K.M., Jones, T.S., Ashwin, M.J., Veal, T.D.
Theoretical and experimental studies of electronic band structure for $GaSb_{1-x}Bi_x$ in the dilute Bi regime
(2014) Journal of Physics D: Applied Physics, 47 (35).

This is the first from a series of papers which appeared as a result of collaboration with the group led by dr hab. Robert Kudrawiec from the Laboratory of Optical Spectroscopy of Nanostructures (LOSN), Department of Experimental Physics in the Faculty of Fundamental Problems of Technology at Wroclaw University of Technology. The contribution to the paper consisted in working out its theoretical part. Using the large scale *ab initio* calculations, a dependence of the $GaSb_{1-x}Bi_x$ band structure on the Bi content in the low content regime, up to *5%* (in particular, the positions of the band tops in Γ point and the band gap) has been evaluated. The aim was to compare the results of calculations with measurements done in LOSN by photoreflectance spectroscopy and to get from these calculations some additional information, particularly the absolute values of band offsets, important in applications. A representation of Projector Augmented Waves (PAWs) has been applied for geometry relaxation and HGH type pseudopotentials (*Hartwigsen, Goedecker i Hutter*) joined with the MBJLDA functional for the band structure calculations, which allowed to take into account the relativistic effects. Two original methods (to the authors knowledge) have been applied: the alchemical mixing joined with supercells (called SC-AM), and the method of *ab initio* energy gauge consisting in equating the value of Kohn-Sham potential in a supercell point distant from the Bi dopant (the method has been described in detail in the paper (H8)). The calculations have been performed on a *16*-atom supercell with one alchemical atom *Sb/Bi*, which has made it possible to achieve continuous change in compositions in the range of *0-12.5%*. A very good agreement of results with the experiment has been obtained, and following the discussion of the literature data, very reliable results concerning the band offsets have been achieved. Important was the conclusion that the incorporation of *Bi* modifies both the conduction and the valence bands (Fig.5), namely the bottom of the conduction band is lowered (*-26meV/%Bi*) while the top of the valence band is raised (*9.6meV/%Bi*). This is an

important contribution to the still lasting discussion about the effects of *Bi* dopant on the bands in III-V semiconductors.

There were 3 persons engaged in theoretical investigations*) (*ab initio* calculations), besides me Maciej Polak and Maciej Winiarski. My contribution into the theoretical part consisted in the participation in designing the methodology, authorship of new methods (SC-AM and the energy gauge), supervision over the calculations, discussion and interpretation of results, co-authorship of the theoretical part of the paper. I estimate the contribution to be **40 %**.

*) The project was realized under the leadership of dr hab. Robert Kudrawiec and covered the production of samples (under collaboration with a foreign partner), spectroscopic measurements and theoretical calculations. I estimate the contribution of the theoretical part to the whole work to be **33%.**

H6). Kudrawiec, R., Kopaczek, J., Polak, M.P., Scharoch, P., Gladysiewicz, M., Misiewicz, J., Richards, R.D., Bastiman, F., David, J.P.R.
Experimental and theoretical studies of band gap alignment in $GaAs_{1-x}Bi_x/GaAs$ quantum wells
(2014) Journal of Applied Physics, 116 (23).

The next investigated system from the *Bi* diluted III-V semiconductors was $GaAs_{1-x}Bi_x$. As in the work (H5), the experimental tool was the photoreflectance spectroscopy, this time applied to the system of quantum wells $GaAs_{1-x}Bi_x/GaAs$. Such a sample configuration allowed to study VB-CB transitions between the first and the second levels in quantum wells, and the experimental data, when joined with the knowledge of geometrical parameters of wells, could be used to estimate the position of the band-–gap in the *Bi* diluted system ($GaAs_{1-x}Bi_x$) with respect to pure *GaAs* (*the band gap alignment*), or in other words, the band gap offsets.
The methodology of *ab initio* calculations was similar to that described in (H5), except that the *54*-atom supercell was applied (*3x3x3* primitive cells), first with *1* alchemical atom *As/Bi* (the content up to *3.7%*) and next with *1 Bi* atom and *1* alchemical atom (the contents *3.7-7.4%*). The configuration of the sample (quantum well) allowed to directly compare the band offsets obtained from measurement and from calculations. A very good agreement of experimental and theoretical results has been obtained (Fig.9), which again confirmed the reliability of the proposed method of band shift estimation, caused by incorporation of a dopant atom. An important qualitative and quantitative result was showing that the band gap bowing originates from the bowing of the valence band offset (*51-20meV/%Bi*) at almost linear dependence of the bottom of the conduction band (*-33meV/%Bi*), for compositions in the range *0-7.4%* .

Two persons were engaged in the *ab initio* theoretical investigations: I and Maciej Polak. My contribution*) was mainly of essential character, it consisted in designing the methodology, authorship of applied methods: SC-AM and the energy gauge, supervision over calculations, discussion about the results and the contribution to writing the theoretical part of the paper. I estimate the contribution to be **40 %.**

*) The project was realized under the leadership of dr hab. Robert Kudrawiec and covered the production of samples (under collaboration with a foreign partner), spectroscopic measurements and theoretical calculations. I estimate the contribution of the theoretical part to the whole work to be **33%.**

H7). Kopaczek, J., Kudrawiec, R., Polak, M.P., Scharoch, P., Birkett, M., Veal, T.D., Wang, K., Gu, Y., Gong, Q., Wang, S.

Contactless electroreflectance and theoretical studies of band gap and spin-orbit splitting in $InP_{1-x}Bi_x$ dilute bismide with $x \leq 0.034$
(2014) Applied Physics Letters, 105 (22)

Similarly as in the case of works (H5) and (H6), the *Bi* dilute III-V semiconductor, in this case *InP*, the electronic properties have been investigated both experimentally and theoretically. Owing to the experimental technique applied, the contactless electroreflectance, apart from the band gap it was possible for the first time to investigate the spin-orbit splitting as dependent on the *Bi* content. In *ab initio* calculations, the methodology described in (H5), with *54*-atom supercell and *1* alchemical atom *P/Bi* (compositions up to *3.7%*). A very good agreement of theoretical and experimental results has been obtained (Fig.2), including the spin-orbit splitting.

Two persons were engaged in the *ab initio* theoretical investigations: I and Maciej Polak. My contribution*) was mainly of essential character, consisted in designing the methodology, authorship of applied methods: SC-AM and the energy gauge, supervision over the calculations, discussion about the results and contribution to writing the theoretical part of the paper. I estimate the contribution to be **40 %.**

*) The project was realized under the leadership of dr hab. Robert Kudrawiec and covered the production of samples (under collaboration with a foreign partner), spectroscopic measurements and theoretical calculations. I estimate the contribution of the theoretical part to the whole work to be **33%.**

H8). Polak, M.P., Scharoch, P., Kudrawiec, R.
First-principles calculations of bismuth induced changes in the band structure of dilute Ga-V-Bi and In-V-Bi alloys: chemical trends versus experimental data
(2015) Semicond. Sci. Technol. 30 (2015) 094001

The work is the *ab initio* calculations based comparative study of the effect of the *Bi* dopant effect on electronic properties of semiconductor alloys of *Ga-V-Bi* and *In-V-Bi* type. The calculation results have been compared with numerous experimental data available in the literature and from our own measurements. The main objective of the work was to investigate the chemical trends in the behavior of parameters important from applications point of view, like the band gap, band offsets or spin orbit splitting. At the same time it was possible to check the quality of widely used approximations, i.e. VCA and band anticrossing model (BAC). The methodology similar to that described in (H5)-(H7) has been applied, except that the fully relativistic norm-conserving pseudopotentials have been generated (with the use of Atomic Pseudopotential Engine), and employed in the calculations. For the structure relaxation the LDA (*Perdew-Wang*) and for the band structure the MBJLDA functional have been used. The paper contains a detailed description of the energy gauge procedure. Precise methods of structure relaxation and adjusting the MBJLDA "C" parameter have been worked out. The *54*-atom supercell with *1* alchemical atom allowed to study the properties up to *3.7%* of the *Bi* content. Six alloys have been studied: $GaP_{1-x}Bi_x$, $GaAs_{1-x}Bi_x$, $GaSb_{1-x}Bi_x$, $InP_{1-x}Bi_x$, $InAs_{1-x}Bi_x$, and $InSb_{1-x}Bi_x$ and a very good agreement with the experiment has been obtained. The consistent methodologically calculations verified by experimental data allowed to formulate conclusions about chemical trends which are important from the point of view of modern optoelectronic devices design. The limitations of popular approximations VCA and BAC have been demonstrated. The paper got very good references in the journal Semiconductor Science and Technology.

My contribution was in designing the methodology, authorship of applied methods: SC-AM and the energy gauge, in discussion about the results and in writing the theoretical part of the paper. I estimate the contribution to be **35 %.**

H9). Zelazna, K., Polak, M.P., Scharoch, P., Serafinczuk' J., Gladysiewicz, M., Misiewicz, J., Dekoster, J., and Kudrawiec, R.
Electronic band structure of compressively strained $Ge_{1-x}Sn_x$ with x<0.11 studied by contactless electroreflectance
(2015) Appl. Phys. Lett. **106** , 142102

The $Ge_{1-x}Sn_x$ alloys have been a subject of intensive research over the last years because of their properties which are attractive for optoelectronic applications. It turns out that the *Sn* dopant in *Ge* results in advantageous changes in electronic properties, like an increase in carrier mobility and change of the band gap from indirect to direct. Knowledge of these properties is crucial for applications and still remains an open subject. Another important aspect is the effect of built-in compressive strain on the band structure. Such a strain appears in epitaxial layers of $Ge_{1-x}Sn_x$ on a pure *Ge* substrate. In the Laboratory of Optical Spectroscopy of Nanostructures (LOSN) at Wroclaw University of Technology the spectroscopic measurements have been performed with the contactless electroreflectance method which allowed to evaluate the energies of optical transitions from the light-hole, heavy-hole and spin-orbit splitting bands, and in particular an observation of the effect of the built-in biaxial strain. The measurements have been performed on the samples with various *Sn* content, up to about *10%*. The experimental results have been compared with the results of theoretical *ab initio* calculations. In the calculations, the *54*-atom supercells have been used in which *Ge* atoms have been successively replaced with *Sn* atoms, from *1* to *6* atoms, giving contents in the range *0-11%*. The applied methodology was similar to that described in works (H5)-(H8). The PAW potentials have been used for the structure relaxation and HGH pseudopotential joined with the MBJLDA functional for the band structure evaluation. A new element was a precise adjustment of the MBJLDA "C" parameter and the lattice constant of the *Ge* lattice to ideally reproduce the known from the literature band structure. For the mixed systems, the values of the parameters were taken from the linear interpolations between *Ge* and *Sn*. A special computer program has been written for finding the maximally uniform distribution of Sn atoms. Because of big requirements for computational recourses, the calculations were done for cubic cells and the values for the strained structures were evaluated from the Bir-Pikus theory.
A very good agreement between the calculations and the experimental data has been obtained, in particular the bowing parameters of the gaps HH-CB, LH-CB, SO-CB fit the ranges known from the literature.

Two persons were engaged in the *ab initio* theoretical investigations: I and Maciej Polak. In this project I was a main performer of the large scale calculations and to a large extent I designed the methodology. I also took part in the interpretation of results and writing the paper. I estimate my contribution in the theoretical *ab initio* investigations to be **60%.**[*)]

*) The project was realized under the leadership of dr hab. Robert Kudrawiec and covered the production of the samples (under collaboration with a foreign partner), spectroscopic measurements and theoretical calculations. I estimate the contribution of the theoretical part to the whole work to be **33%.**

Supervision of diploma works within the subject of habilitation

1) Paweł Szczepkowski, *'Ab initio' investigations into basic structural properties of $In_xAl_{1-x}N$ alloys using the supercell method*, MSc project (2011)

In this work, the first attempt was made to perform *ab initio* calculations for semiconductor alloys with the use of supercells. The basic structural and electronic properties were investigated.

2) Krzysztof Kołodziejski, *Ab initio calculations of deformation potentials in $In_xGa_{1-x}N$ within the coherent potential approximation,* MSc project (2012)

The work was an attempt of recognizing the Coherent Potential Approximation approach to investigate into the electronic properties of semiconductor alloys. Because of some technical difficulties the method has not been applied and the author concentrated on testing the method described in (H2)

3) Jakub Nowak, *The influence of temperature on indium segregation in alloys $In_XAl_{X-1}N$ – 'ab initio' calculations,* MSc project (2012).

The work was an attempt to perform the thermodynamics analysis of miscibility in semiconductor alloys, on the example of $In_XAl_{X-1}N$. Interesting results have been obtained, which became an inspiration for constructing a simplified method of miscibility analysis from first principles. The project is waiting for realization.

4) Maciej Polak, *'Ab initio' studies of material and electronic properties of chosen mixed III-V semiconductor*, Eng. Project (2013).

Within the project, the structural, elastic and electronic parameters have been calculated of a hypothetical semiconductor alloy $AlN_{1-x}P_x$, with the use of newest available methods and approximations. The experience gained has been used in the works (H1), (H3)-(H8)

5) Tomasz Woźniak, *'Ab initio' studies of geometrical and electronic structure of monolayers of chosen group-VI transition metal dichalcogenides*, Eng. Project (2014)

The work was a successful attempt to apply the methodology described in (H1), (H3)-(H8) for the analysis of structural and electronic properties of monolayers of the chosen group-VI transition metal dichalcogenides (like MoS_2)

6) Krzysztof Wittek, *'Ab initio' calculations of structural and elastic properties of semiconductor crystals GeSn, GeC oraz SnC,* Eng. Project (2014)

Within the project, the elastic constants of binary systems IV-IV have been evaluated. The results obtained with different methods (FD, DFPT with relaxed and unrelaxed ion) have been compared.

Presentations on international conferences within the subject of habilitation

SPIE Conference, Dresden 2013.
P Scharoch, M Winiarski, M Polak
Semiconductor alloys for optoelectronic applications - 'Ab initio' modeling
(oral presentation: P Scharoch)

Energy Materials and Nanotechnology Coference, Quinqdao, 15-17 June, 2015.
P Scharoch
Ab initio modeling of semiconductor alloys for nanostructure-based optoelectronic applications
(*invited talk*)

Workshop on Bismuth Containing Semiconductors, Madison, 19-22 July 2015.
P Scharoch, MP Polak, M Gadysiewicz and R Kudrawiec
Ab initio Prediction of Non-Linear Variation of the Band Gap and Spin-Orbit-Splitting in Ge1-xSnx and its Comparison with Measurements of Direct Optical transitions in Compressively Strained Ge1-xSnx Layers with x<11%
(*oral presentation*: P Scharoch)

Workshop on Bismuth Containing Semiconductors, Madison, 19-22 July 2015.
M Gladysiewicz, M Polak, P Scharoch, M Wartak, R Kudrawiec
Electronic Band Structure and Material Gain of Ga(in)BiAs/GaAs Quantum Wells Grown on GaAs Calculated with 14-band and 8-band kp Model
(*oral presentation*: M Gladysiewicz)

Workshop on Bismuth Containing Semiconductors, Madison, 19-22 July 2015.
MP Polak, P Scharoch and R Kudrawiec
Influence of Bismuth on the Band Structure of Ga-V-Bi and In-V-Bi Dilute Alloys. DFT Compared with Experimental Data
(*oral presentation*: M Polak)

Compound Semiconductor Week, Santa Barbara, 28.06-2.07 2015.
M Gladysiewicz, M Polak, P Scharoch, M Wartak, R Kudrawiec
Theoretical Calculations of Electronic Band Structure and Material Gain of III-V-Bi Quantum Wells Grown on GaAs, InP, and GaSb Substrates
(*oral presentation*: M Gladysiewicz)

44th International School and Conference on Physics of Semiconductors "Jaszowiec 2015"
T Woźniak, M Winiarski, P Potasz, P Scharoch, A Wójs
'Ab initio' studies of geometrical and electronic structure of monolayers of chosen group-VI transition metal dichalcogenides
(*poster*)

43rd Congress of Polish Physicists – Kielce 2015r.
T Woźniak, P Scharoch
Ab initio study of the structural and electronic properties of chosen VIB transition metal dichalcogenides (oral presentation)

5. **Other scientific achievements**.

1) Sieradzki, A., Basta, M., Scharoch, P., Bigot, J.-Y. *Ultrafast Optical Properties of Dense Electron Gas in Silicon Nanostructures*(2014) Plasmonics, 9 (3), pp. 545-551.

The paper reports on investigations into ultrafast dynamics of carriers in silicon via measurements of time resolved reflection spectra with femtosecond resolution. My contribution consisted in the participation in discussion and interpretation of results, and in writing the paper. I estimate this contribution to **20%**.

2) Winiarski, M., Scharoch, P.
Ab initio study of basic material properties of Fe, Co, and Ni ferromagnetic crystals
(2010) Computational Materials Science, 48 (3), pp. 700-704.

The paper in a large part is a report on results obtained within the realization of MSc project by Maciej Winiarski under my supervision. The calculations have been done within the spin density functional theory (SDFT). The influence of the spin on structural and elastic properties has been investigated as well as some technical aspects of the effect of pseudopotential generation condition (the core model parameters) on magnetic properties. It has been shown that the core model parameters have a crucial effect on magnetization up to the case of its complete disappearance if the model core radius is too small.

My contribution to the work consisted in the supervision over the project, discussion and interpretation of results, and in writing a part of the manuscript. I estimate this contribution to be **40%.**

3) Scharoch, P.
Ab initio study of the temperature-dependent structural properties of Al(110)
(2009) Physical Review B - Condensed Matter and Materials Physics, 80 (12).

The work contains the proposition of methodology to study from first principles some subtle temperature structural effects observed in Al(110) surface. The experiment shows that the temperature dependent surface relaxation strongly depends on the distance from the surface, i.e. an anomalous expansion of the 2-3 interlayer distance is observed at 1-2 interlayer contraction and almost unchanged 3-4 distance. The computational study has been based on the assumption that the phenomenon is a superposition of 3 effects: the effect of the bulk-substrate thermal expansion, the asymmetry of potential in the direction perpendicular to the surface and the entropy induced effect. The inclusion of the last effect required the application of the Free Energy Surface (FES) concept which in principle is the quasiharmonic approximation applied to the surface. All the effects have been evaluated *ab initio*. The project was computationally very demanding and its realization lasted over 2 years (4 presentations on international conferences, including 2 oral presentations). The obtained results agreed very well with the available experimental data.

I have been the only author of the work (contribution **100%**).

4) Scharoch, P., Peisert, J., Tatarczyk, K.
Thermodynamics of fcc Al crystal from first principles - Performance of local density and generalized gradient approximations
(2007) Acta Physica Polonica A, 112 (3), pp. 513-521.

In the work, the quasiharmonic approximation has been applied to study Al crystal thermodynamics. The approximation consists in the evaluation of phonon frequencies as functions of the lattice parameter. It is possible because at an artificial isotropic strain the atoms are always in equilibrium positions in spite of the fact that the crystal as a whole is not. The incorporation of volume dependent phonons into the free energy formula makes the free energy volume dependent which is called the free energy surface (FES). The FES minimum position corresponding to crystal equilibrium depends on temperature and exhibits the crystal thermal expansion. The results of this work were used in the described above project (3). An interesting side result of this work was a comparison of various approaches to phonon dispersion calculations (direct vs. DFPT). An interesting conclusion was that the crystal thermal expansion is not connected with the nonlinearity of interactions (according to some opinions) but is a purely entropic effect.

The subject of the work was my idea and in large part was realized under my supervision by Krzysztof Tatarczyk within his MSc project. However, for the purpose of realization of the project (3) I did all the calculations myself (except the phonons from DFPT). I estimate my contribution to be **40%**.

5) Scharoch, P.
The semiempirical method for finding thermal characteristics of simple crystals
(2004) Acta Physica Polonica A, 106 (4), pp. 487-495.

An interesting direction of *ab initio* methods application is joining them with the known empirical models, like in the case of crystal thermodynamics the Einstein or the Debye model. The *ab initio* calculations provide in this case some quantities appearing in the models which lead to significant reduction of parameters which are fitted to the experiment. The methods are simplified tools of fast analysis of physical parameters where the costly large scale computations are avoided. In the presented work, the Einstein model of crystal dynamics has been used in which the dynamics is represented by one frequency only and the dependence of this frequency on crystal volume (modeled by the exponential function). The volume dependence of the static total energy has been evaluated *ab initio* and approximated by the Murnaghan equation of state. The two parameters appearing in the model (Einstein frequency and Grüneisen number) have been fitted to chosen experimental data giving the thermodynamic characteristics in a large range of temperatures and pressures. The description, although simplified, showed a very good agreement with the experimental data.

I have been the only author of the work (contribution **100%**).

6) Scharoch, P., Neugebauer, J., Scheffler, M.
Al(111)-(√3×√3)R30: On-top versus substitutional adsorption for Rb and K
(2003) Physical Review B - Condensed Matter and Materials Physics, 68 (3), art. no. 035403, pp. 354031-354035.

The project was realized during the 3-month practice in the Fritz-Haber Institute in Berlin. It has been shown via *ab initio* studies that in ordered structures *Al(111)-(√3×√3)R30* the observed experimentally transition at temperatures *250K* (*Rb*), 2*20K* (*K*) from "on-top" to "substitutional" is irreversible, which means the "on-top" state at low temperatures is metastable.

The project was a continuation of works conducted in FHI concerning the properties of ordered structures of alkali metals on *Al* surface. I have done the *ab initio* calculations and I have written the manuscript of the paper. I estimate my contribution to be **40%**.

7) Scharoch, P., Parliński, K., Kiejna, A.
Ab initio calculations of phonon dispersion relations in aluminium
(2000) Acta Physica Polonica A, 97 (2), pp. 349-354.

The paper reports on *ab initio* calculations of phonon dispersion relations in *fcc Al* crystal with the use of a direct method and PHONON software written by Prof. Krzysztof Parlinski.

I have done the calculations and I estimate my contribution to be **40%.**

8) Kiejna, A., Peisert, J., Scharoch, P.
Quantum-size effect in thin Al(110) slabs
(1999) Surface Science, 432 (1), pp. 54-60.

An infinite crystal surface in *ab initio* calculations is modeled with the use of infinite slabs "cut out" from the bulk crystal and separated by vacuum layers (to avoid interaction between adjacent slabs). A single slab contains two surfaces which are the subject of interest. Unfortunately in metals the quantum size effect (QSE) appears which manifests itself by special oscillations of electron density in the direction normal to the surface. This is a physical effect but unwanted in *ab initio* surface studies because it leads to false results for surface characteristics. In the work, the effect of QSE has been studied on various surface characteristics (geometry relaxation, work function, surface energy), via checking the convergence of results with respect to the number of layers. It has been shown that the QSE may have a significant influence even up to 15-16 layers.

In the project I took part in the calculations, discussion of results and writing the paper. I estimate my contribution to be **30%**.

9) Beattie, Alan R., Abram, R.A., Scharoch, P.
Hole impact ionization rates in InP and In0.53Ga0.47As
(1992) Semiconductor Science and Technology, 7 (3 B), pp. B512-B516.

In the work, the computer codes I have written, during the postdoctoral fellowship in Durham University (the works 11 and 12 described below), have been used to evaluate the overlap integrals necessary for calculations of the Auger transitions matrix elements. I estimate my contribution to be **20%**.

10) Beattie, A.R., Abram, R.A., Scharoch, P.
Realistic evaluation of impact ionisation and Auger recombination rates for the ccch transition in InSb and InGaAsP
(1990) Semiconductor Science and Technology, 5 (7), art. no. 018, pp. 738-744.

In the work, the computer codes I have written, during the postdoctoral fellowship in Durham University (the works 11 and 12 described below), have been used to evaluate the overlap integrals and threshold energies necessary for calculations of the Auger transition probabilities. I estimate my contribution to be **20%**.

11) Beattie, A.R., Scharoch, P., Abram, R.A.
Impact ionisation threshold energy surfaces for anisotropic band structures in semiconductors
(1989) Semiconductor Science and Technology, 4 (9), art. no. 003, pp. 715-723.

The work has been done during the postdoctoral fellowship in Durham University (UK). Using the methods described below (12), the threshold surfaces have been evaluated (in the Brillouin Zone) for Auger transitions of *ccch* and *chlh* type in *InSb, InAs, InP, GaAs and GaSb*. I estimate my contribution to be **30%.**

12) Scharoch, P., Abram, R.A.
A method of determining the overlap integrals used in calculations of Auger transition rates in semiconductors
(1988) Semiconductor Science and Technology, 3 (10), art. no. 002, pp. 973-978.

The work has been done during the postdoctoral fellowship in Durham University (UK). The main objective was to work out an effective method of calculation of the overlap integrals necessary in calculations of Auger transitions in semiconductors matrix elements. The method is based on kp approximation with the effect of interaction of distant bands taken into account via Löwdin procedure. A very good agreement has been obtained with the overlap integrals calculated with the use of much more computationally demanding non-local Chelikowski-Cohen pseudopotentials. My contribution consisted in working out the models, their implementation, testing and taking part in writing the manuscript of the paper. I estimate the contribution to be **60%**.

13) Scharoch, P., Pawlikowski, J.M.
Quantum efficiency of internal photoeffects in narrow-gap semiconductors. II. Calculation results in comparison with experimental data
(1984) Journal of Applied Physics, 55 (6), pp. 1487-1491.

In the work, the model and programs have been used described below (14) for the calculation of quantum efficiency of an internal photoelectric effect in narrow gap semiconductors (*InSb i* $Cd_xHg_{1-x}Te$). An interesting dependence of results on electronic density has been obtained determined by appearing in the model screening constant. The paper contains also the results of conducted by me experiment and its comparison with calculations. I estimate my contribution to be **60%**.

14) Scharoch, P., Szatkowski, J., Pawlikowski, J.M.
Quantum efficiency of internal photoeffects in narrow-gap semiconductor: A model
(1982) Journal of Applied Physics, 53 (8), pp. 5710-5714.

The paper contains a description of the model and its implementation for the calculation of quantum efficiency of an internal photoelectric effect, where for energies greater than *2Eg* (*Eg* – the band gap) the Auger type transitions play an important role leading to the increase in the quantum efficiency above 1. The work was realized within the PhD project under supervision of Prof. J.M. Pawlikowski. I estimate my contribution to be **50%.**

15) Kaluski, M., Macher, M., Scharoch, P., Stasierski, L,
EM field estimation in the vicinity of multiple panel antenna systems for FM and TV broadcasting

(1996) Electromagnetic Compatibility 1996 - Thirteenth International Wroclaw Symposium Pages: 79-84

The paper is one of the results of my long-–lasting collaboration with the Institute of Telecommunication (and later R&D TPSA and Orange Labs), during which I worked on numerical modeling of electromagnetic fields around transmitting antenna and various structures dissipating EM fields. I estimate my contribution to be **20%.**

Supervision of other diploma works

1) Krzysztof Tatarczyk, *From ab initio dynamics to thermodynamics of chosen polyatomic systems*, (2000)

2) Tomasz Dobrzycki, *Phonon dispersion relations in (110) aluminum wall*, (2002)

3) Jarosław Pytowski, *Dynamics and thermodynamics of low dimensional periodic atomic structures–'ab initio' calculations*, (2004)

4) Łukasz Głowacki, *Dielectric and dynamic properties of AlAs – 'ab initio' calculations*, (2008)

5) Maciej Winiarski, *'Ab initio' investigations into basic properties of ferromagnetic crystals Fe,Co and Ni in equilibrium state*, (2009)

6) Wojciech Golubiński, *Evaluation of basic properties of metallic hydrogen – 'ab initio' calculations*, (2010)

7) Grzegorz Kinal, *Construction of the user interface for the program to analyze the electromagnetic fields around UHF and VHF transmitting antenna*. (2008), Eng. Project.

8) Bartłomiej Dochniak, *Construction and testing of the numerical models of spatial radiation characteristics of UHF and VHF antenna elements.* (2009), Eng. Project.

Oral presentations at international conferences

1. Scharoch P, Peisert J, Neugebauer J; *Understanding the temperature dependent surface multilayer relaxation of Al(110); an ab initio approach;* 2nd Workshop on ab-initio phonon calculation, Kraków 2007;
2. Scharoch P; *Thermal properties from first principles with the use of the Free Energy Surface concept*. 27th Max Born Symposium, Multiscale Modeling of Real Materials, Wroclaw 2010.

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