STAND-ALONE PROJECT

FINAL REPORT

Project number P21685-N22

Project title[1] Wigner-Boltzmann Particle Simulations

Wigner-Boltzmann Teilchen Simulationen

Project leader D.Sc. Dr. Mihail Nedjalkov

1 Short title in English and German language

I. Summary for public relations work

The project's most significant results (scientific advances) from the project leader's point of view should be presented on a single page (DIN A4, 11 pt font, line spacing 1.5) in a way that is comprehensible to the general public. In this text, it is important to use as few technical terms as possible in order to ensure that the text is interesting and understandable to people not familiar with the field. The main point should be mentioned at the very start of the summary. Please keep descriptions of the issues addressed and results obtained short and succinct. Possible applications to or implications for social, cultural, ecological, medical, economic or technological areas should also be mentioned briefly.

The summary should be submitted both in **German** and in **English** (without special characters). The summaries will be made available via the FWF's project database. The FWF will not edit the summaries, meaning that the authors bear full responsibility for the content of these texts.

1. Zusammenfassung für die Öffentlichkeitsarbeit

Ziel des FWF Projektes P21685-N22 ist die Entwickelung von theoretischen und numerischen Ansätzen für eine Teilchen-basierte Simulation von Quantenphänomenen in Nanostrukturen. Teilchen-basierende Modelle sind inhärent Teil der klassischen Mechanik und verschaffen Einsicht in die Funktionsweise vieler Mikroelektronik-Bauteile, jedoch erfordert die hervortretende Nanoelektronik eine Wellen-basierte Quantenmechanik. Das Teilchenkonzept kann in der Quantenphysik mittels der Wigner-Funktion – ein Quantenanalog zur klassischen Verteilungsfunktion – beibehalten werden. Diese Übereinstimmung wird erweitert und formt den theoretischen Grundstein von ViennaWD: ein Modell was die Quantenevolution durch die Generierung/Vernichtung (G/V) von positiven und negativen Teilchen erklärt. Ein wichtiges Projekt-Ergebniss ist, dass der G/V Prozess eine stochastische Alternative zur Newtonischen Beschleunigung darstellt. Das Modell kann Phänomene, wie Dekohärenz, beschreiben die zwischen den reinem Quanten- und klassischem Transportregimen liegen. Aushängeschild-Projektergebnisse werden erzielt durch die Wigner-Untersuchung der Dekohärenz eines Elektronenzustandes durch Phononen. Das Überwiegen von klassischem oder Quantenverhalten ist von den involvierten physikalischen Größen abhängig. Das Skalierungstheorem wird hergeleitet, welches Einsicht in der Vernichtung von Quanteninformation verschafft und erklärt wieso aktuelle Nanometertransistoren noch durch klassische Methoden modelliert werden können. Zweitens, wird die Existenz von Klassen, physikalisch verschieden aber mathematisch äquivalenten Aufstellungen der Wigner-Boltzmann-Evolution, demonstriert. Numerische Untersuchungen zur Rolle von Grenzflächen in der Bildung von Elektronenzuständen in Nanotransistoren zeigen, dass zum Beispiel grobe aber spiegelnde Oberflächen die Zeitumkehrbarkeit beibehalten, während ebene, aber diffuse Oberflächen Dekohärenz verursachen. Anwendungen zur Untersuchung der Elektronendynamik der Einfang/Streuung um Oxid/Kanal Zentren von zweidimensionalen Nanobereich-MOSFETs haben Quanteneffekte aufgedeckt, wie Nichtlokalität, eine Blockierung der Kanalregion und Einfangkonstanten. Dieses etablierte das Modell als ein schlagkräftiges Forschungswerkzeug und beantwortet die grundlegende Herausforderung dieses Projektes: über-1D-hinausgehende-Quantenteilchen-basierte Simulationen. Eine MPI-Parallelisierung wurde fertiggestellt, um Aspekte des Speichers und der Laufzeit zu adressieren, um die Methode für stationäre, selbstkonsistente Anwendungen vorzubereiten. Im Rahmen von ViennaWD, wurden Teilchen-basierte Simulationswerkzeuge entwickelt die öffentlich zugänglich sind: http://viennawd.sourceforge.net/.

2. Summary for public relations work

The aim of FWF Project P21685-N22 is to develop a union of theoretical and numerical approaches for a particle-based simulation of quantum phenomena in nanostructures. While the particle concept is inherent to classical mechanics and particle-based models provide deep insight into phenomena governing generations of microelectronic devices, the emerging nanoelectronics require wave-based quantum mechanics. Nevertheless, the particle concept may be retained in the quantum world through use of the Wigner function, interpreted as a quantum analog of the classical distribution function. This correspondence is further expanded in what forms the basic theoretical pillar of ViennaWD: a model explaining the quantum evolution through generation/annihilation (g/a) of positive and negative particles. A very important project outcome is the result that the g/a process is a stochastic alternative to Newton's acceleration. It follows that the model bridges purely quantum with classical evolution: a wide range of phenomena existing between these ultimate transport regimes may be addressed, such as processes of decoherence: the environment-induced transition from a quantum to a classical state. Flagship project results are obtained from the Wigner study of an electron state Decoherence (WD) due to crystal lattice vibrations (phonons). These impact technologically important disciplines like nanoelectronics and quantum computing. It is shown that the domination of classical or quantum behavior depends on the scales of the involved physical quantities. A notion called scaling theorem is derived, which gives deep insight in the way of destruction of the quantum information and explains why the current nanometer transistors may be still modeled by classical methods. Secondly, the existence of classes of physically different, but mathematically equivalent setups of the Wigner–Boltzmann evolution is demonstrated. Numerical studies of the role of the interfaces on the formation of the electron state in nanotransitors show that e.g. rough but specular surfaces preserve the time reversability while flat but diffusive surfaces causes decoherence. Applications to trapping/scattering electron dynamics around oxide/channel centers of two dimensional nanoscale MOSFETs revealed quantum effects like non-locality, blocking of channel regions and capture constants. This established the model as a powerful research tool and answers the basic challenge of the project: quantum particle simulations beyond 1D structures. Optimization and large scale MPI parallelization have been successfully completed to address precision, memory and run time aspects preparing the method for stationary, self-consistent applications. The ViennaWD union is implemented in algorithms that form a suite of particle-based simulation tools, publicly available at http://viennawd.sourceforge.net/

II. Brief project report

- **To be written in the language of the original application**
- Target group: **peer reviewers**
- **Length:** not to exceed 16,000 characters (approx. 5 ½ pages) in total; please mention each point (approx. 2,000 words for each point or all together on 4 pages minimum, 11 pt font, line spacing 1.5, **no attachments apart from those mentioned in section III**)

1. Report on research work

1.1 Information on the development of the research project

- Overall scientific concept and goals;
- Was there a fundamental change in research orientation between the start and the end of the project? If so, what form did the change take, and what effect did it have on the work?

The subject of Project P21685 'Wigner-Boltzmann Particle Simulations' is models and simulation of electron transport in semiconductor nanostructures. The physics of the electrons in such structures is characterized by a complicated interplay between coherent quantum effects, such as quantization and tunneling, and processes of decoherence, which impose classical behavior. The world between these ultimate transport regimes is filled with unexplored *mixed mode* phenomena, particularly due to a lack of simulation approaches, which treat quantum and classical behavior on equal footing. The idea is to use the Wigner phase space formulation of quantum mechanics in conjunction with classical phase space concepts for development of such approaches. The activities focus on development of ViennaWD (formerly WIENS): a union of theoretical models in conjunction with numerical approaches and algorithms for particle simulation. The ViennaWD union is implemented in simulation tools, especially suitable for transient processes with open boundary conditions where other quantum approaches fail. The major challenge is the development of the first two-dimensional (2D) Wigner-particle simulator of quantum phenomena in nanostructures. In particular, a 2D self-consistent classical particle simulator needs to be developed as a platform for the quantum counterpart. A widespread use of ViennaWD to electron transport in nanostructures is of importance to multiple applications: it brings physical insight to phenomena and processes, further develops the simulation method and provides engineers and designers with parameters for high-level models. The project strictly followed the envisaged plan concerning the investigation of the theoretical aspects and the subsequent implementation and application; there was no deviation in the research orientation and the goals were successfully reached.

1.2 Most important results and brief description of their significance (main points) with regard to the following:

- Contribution to the advancement of the field (e.g. did the results contribute to increasing the importance of the field? In what way?);

Breaking of new scientific / scholarly ground (to what extent and in what respects?);

- Most important hypotheses / research questions developed (what relevance did the project have for the development of hypotheses / research questions, e.g. were new hypotheses / research questions developed or old hypotheses disproved?);
- Development of new methods;
- Relevance for other (related) areas of science (transdisciplinary issues and methods).

The project contributed to the development of **(i)** Wigner-Boltzmann theory, **(ii)** concepts of an efficient particle model and its implementation, and **(iii)** the application to physical processes and structures. The most important contributions of the project, relating them to **(i)** to **(iii),** are presented in the following.

(i) Decoherence: the scaling theorem: The Wigner-Boltzmann (W-B) equation describes electron evolution as a competition between classical phonon scattering and the quantum interaction with the electric potential. The evolution mode which dominates will depend on the scales of the involved physical quantities. Dimensionless parameters corresponding to the relative strength of the energy scales of the device, the potential, the phonon energy, and the electron-phonon coupling are introduced. A notion called scaling theorem derives the dependencies of these parameters on the phonon coupling. It is shown that an increase in the phonon coupling shrinks the interval of coherence, where the electronic state remains unperturbed. Furthermore, higher-order derivatives of the potential become suppressed, retaining only the first-order derivative, i.e. the electric field. This gradually transforms, on a microscopic level, the Wigner equation into the classical Boltzmann counterpart. *The theorem provides deep insight into the mechanisms of decoherence causing electron localization. This result independently suggests the idea of a finite coherence length in **(ii)**.*

(i) Decoherence: simulations of entagled states: The mechanism of decoherence due to phonons is analyzed with the help of an initial Wigner state, obtained by a superposition of two wave packets. The state comprises two Gaussians separated by a pronounced oscillatory term. The latter is responsible for the interference effects, which distinguish a pure entangled state from a mixed state. Due to the negative values, the former can be interpreted as a set of particles to which a sign is attributed; negative particles are solely ascribed to the interference term. Simulations show that phonons effectively destroy the interference term by mixing the values in the Wigner state. If negative particles and positive particles appear in the same region, they compensate each other. *The process provides insight into how scattering destroys the reversibility, by introducing a time arrow in the evolution.* The initial coherence in the wave vector dispersion is pushed towards the equilibrium distribution, causing the transition of the entangled state to a mixed state, which can be interpreted as a classical state. *This analysis provides **(ii)** with concepts of positive and negative particles and brings their numerical annihilation to the fore, during the process of evolution.*

(i) Semi-discrete Wigner function: Due to the effect of phonons and/or boundaries, a finite coherence length *L* may be specified in nanostructures. With a finite-valued *L*, the Wigner theory is reformulated with a quantized momentum space. The Wigner potential can then interpreted as a generator of signed particles, with discrete momentum values. *This concept is inherent to the model **(ii)**, but challenges the continuous character of both Newton's acceleration and phonon scattering. These two problems have been carefully addressed in the project.*

(ii) Quantum particle attributes: Using the Monte Carlo theory for solving integral equations, the above concepts are incorporated while retaining most of the properties of classical particles, like trajectories and ensemble averages, in the following picture: the Wigner potential generates particle pairs with complementary signs according to certain rules. Particles contribute to the physical averages in the classical way, but their corresponding sign is accounted for. Furthermore, two particles with opposite sign, which meet in a cell of the phase space at the same time, annihilate each other. This gives rise to the concept of indistinguishable particles (IP), which are stored on a phase space grid at consecutive time steps, so that a number per cell replaces the ensemble of particle states within that cell. This greatly reduces the memory requirements of the algorithm. *The first Wigner 2D simulations, **(iii)** could only be realized computationally thanks to these ideas. A picture of an ensemble of signed particles, which are generated, annihilated and reside in a discrete momentum subspace may be associated to any quantum process where electrons evolve under the influence of an electric potential and interact with certain scattering sources. This novel interpretation of the quantum evolution is a powerful tool for the analysis and modeling in the nanoscale limit.*

(ii) Evolution duality: the concept of a discrete momentum space raises an important question relating to the second law of mechanics, where a constant force changes the momentum of a particle continuously. The answer to the question of how acceleration is accounted for by the particle sign algorithm becomes a proof of concept for the whole approach. The analysis is based on the equivalence of the Wigner and classical evolution for linear potentials. An initial peak of *N* particles is assumed, whose classical evolution corresponds to a continuous acceleration over a Newton trajectory. According to the quantum model, positive or negative particles are generated and annihilate each other at the discrete nodes. This happens by a generation of negative particles on the initial node where they annihilate, and of positive particles on the adjacent node to be occupied next. This results in a gradual transmission of the particles between the adjacent nodes The statistical averages giving the time evolution of the momentum are consistent with Newton's second law. *This establishes the Wigner particle generation/ annihilation concept as an alternative to the continuous process of Newton acceleration.*

(ii) Optimization: The model is compatible with and can be directly implemented on regular device MC platforms. This has been shown through a collaboration with the Sofia group of Prof. I.Dimov, where the algorithm has been implemented on the public GNU simulator *archimedes.* A comparison of benchmark test results between the latter and in-house obtained results demonstrated a good agreement, however it raised the need to improve the precision and address the memory demands of the model. *The algorithm has been optimized with a novel scheme for particle generation, while the memory problem has been solved by a MPI/open MP parallelization scheme based on spatial domain decomposition*.

(iii) Applications: Fig.1 shows a 2D quantum transient simulation of a Wigner packet representing a single charge in the channel of a realistic nanoscale MOSFET, in the presence of a discrete trap, introduced by a 2D square quantum well at the channel/oxide interface. The channel potential is provided by our partner in this research - the device simulation group from the University of Glasgow. The simulations clarify the dynamics of the charging process in terms of charging and dwelling times and dependences on the characteristics of the trap.

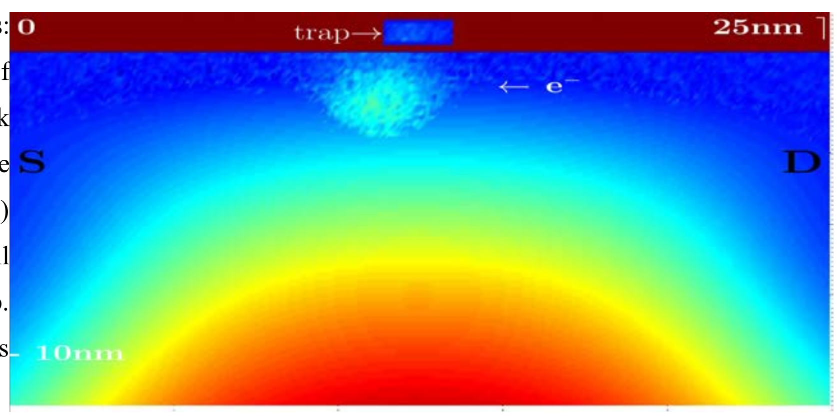

Figure 1: First Wigner 2D simulations: tunneling of an electron with energy of 0.15eV through the 1.5eV high, 0.2nm thick trap barrier. The trap is 1nm/2nm. The initially Gaussian electron density (light blue) spreads in the channel (dark blue). It is well visible how part of it penetrates in the trap. The relative electron density in the trap gives the capture probability.

The effect of a single impurity in the channel has been explored within the same approach. In particular, the long range Coulombic nature of the impurity is calculated by a self-consistent simulation, which allows a focus on the electron interacting with the internal kernel modeled by a square barrier. The results from two theories: the classical (phonon-less) Boltzmann and the quantum Wigner models are shown in Fig.2. The Boltzmann evolution can be easily anticipated and is used as a reference: as can be seen, the whole palette of package colours surrounds the centre. Only particles impinging on the surface of the dopant are scattered back. In contrast, in the quantum case the vicinity of the centre remains barely populated just like the region between the centre and the interface with the oxide, which remains blocked. Moreover, the non-local quantum interaction effectively destroys the far end of the packet, showing that it actually affects the transport in the whole cross section of the channel.

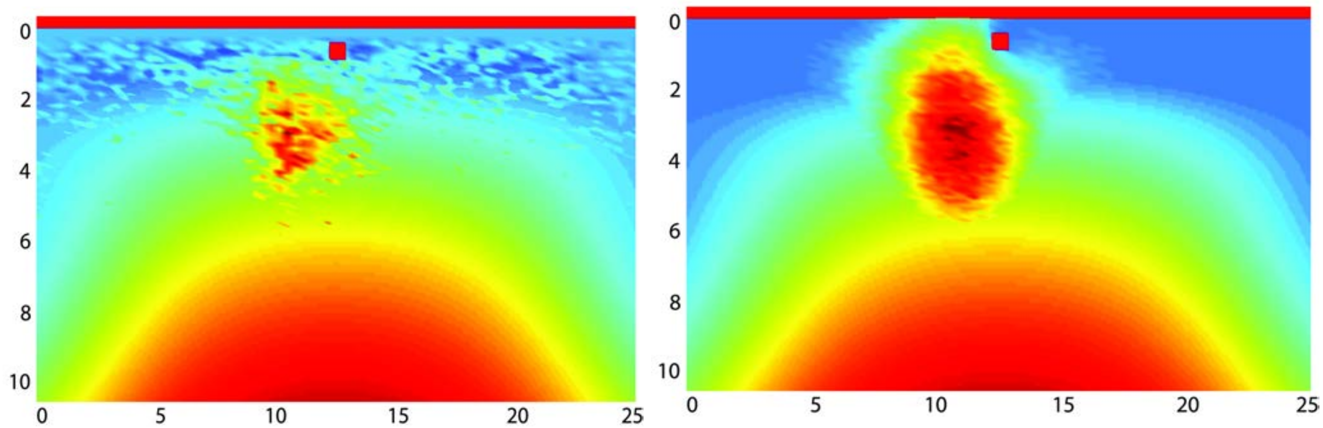

Figure 2: Wigner (left) and Boltzmann (right) evolution in the presence of a discrete dopant given by a 2D, 0.5eV high 0.3nms (red) square barrier at a distance of 0.4nm from the oxide.

The properties of the interfaces in novel devices, like DG-MOSFETs and Si gate-all-around transistors, is an area open for analysis with respect to their effect on the quantum state in the active region. The following analysis, based on the Wigner particle model, interchangeably uses the equivalent concepts of coherent regime, time reversibility, and quantum purity. A Gaussian packet is first simulated until it bounces back at an oblique angle from a flat, specular interface. Then, the time arrow is reversed and the simulation continues until reaching the initial time again. The Wigner solution in this case matches the initial packet, which indicates a coherent evolution. Further experiments gradually enable inelastic

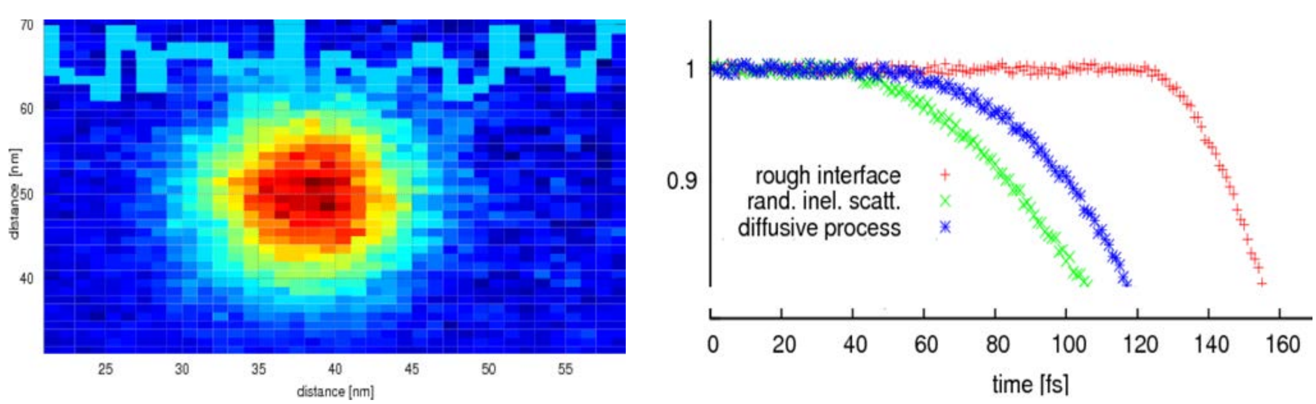

Figure 3: The evolution of an electron bouncing back from a rough specular interface (left) is coherent: by the purity (red curve) remains 1 for 130fs. The loss of quantum information begins much earlier in the case of a random reflection process.

and diffusive reflection, and surface roughness. The obtained results, as verified also by the calculated purity (see Fig.3), show that roughness alone cannot trigger irreversibility, and thus, induce classical behavior of the electrons. A random process is sufficient to cause decoherence even for flat surfaces. *The presented applications demonstrate not only the 2D aspects of the developed approach, but also establish the Wigner particle simulations a powerful method for analysis of mixed mode phenomena including transient processes with open boundaries.*

1.3 Information on the execution of the project, use of available funds and (where appropriate) any changes to the original project plan relating to the following:

- Duration;
- Use of personnel;
- Major items of equipment purchased;
- Other significant deviations.[3]

The submitted proposal envisaged two PhD positions, but only one has been approved, which assumed either a modification of the research line, or an extension of the project duration. The PI decided for the second option, which imposed a replanning of the budget aiming to both support an extended period of research and involvement of external collaborators in specific project activities. In accordance to this replanning, the PI began with only 80% of the initially requested salary, further reducing it as the project advanced. This allowed the project period to be extended by 50%, from 3 to 4.5 years, and also to support external collaborators, and working/conference visits. An additional problem arose from the PhD position: a highly-suitable candidate, selected at the beginning of the project, was hindered to take the position by bureaucratic requirements (as described in the first annual report) and the same happened later with two other candidates. For the first three years the position was only occupied for six months by a candidate, who, however, lost his interest in the research. As a consequence the software implementation schedule was heavily affected. Conversely, a correct step was the early engagement of a diploma student, Marek Pobjecky, who assisted with the code development. The main collaborator, Dr. Philipp Schwaha joined the project as a very motivated external researcher. While working for the software company Shenteq, he developed and applied a phonon decoherence (PD) simulator. The PD software is the only project related purchase classified as 'major items of equipment purchased' and can be freely downloaded from the homepage of ViennaWD. The project's PhD position was finally filled by Paul Ellinghaus. He rapidly progressed with the development and optimization of the software towards the project goals. Finally I acknowledge the valuable contributions from Prof. I.Dimov, Prof. Dragica Vasileska and Dr. J.M. Sellier in accordance with Section 5.

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3 The decision as to what should be regarded as a “significant deviation” is the responsibility of the project leader. As a guideline, any deviation of more than 25% from the original financial plan or work schedule should be accounted for.

2. Personnel development – Importance of the project for the research careers of those involved (including the project leader)

- Brief comments on the project's effects on the research careers of all project members, including special qualifications and special possibilities / opportunities opened up by the project.

2010 Dipl. Ing. P.Schwaha defended his doctorate. A chapter of his doctorate thesis unifies the first project related results.

2011 Dr. (Phys) M. Nedjalkov became Doctor of Science in Mathematics. A chapter of his big doctorate thesis is written along the lines of the project.

2015 Planned defence of P. Ellinghaus. His thesis will be based on the basic project outcomes.

3. Effects of the project beyond the scientific field

- Brief comments on specific effects beyond the research field, including activities outside the sphere of academia.

4. Other important aspects (examples)

- Project-related participation in national and international scientific / scholarly conferences, list of most important lectures held;
- Organisation of symposiums and conferences;
- Prizes/awards;
- Any other aspects.

A list of the 12 conferences, where project results were reported by talk or poster presentations is given in the 'Reviewed abstracts in conferences' section of the List of scientific publications.

Organisation of conferences:

2010 - *7th Int. Conf. Numerical Methods and Applications:* organizer of the special session: Monte Carlo and Quasi-Monte Carlo methods (item 1 in the section)

2013 - 9th Int. Conf. Large Scale Scientific Computing: organizer of the special session: Monte Carlo nethods: Theory, Applications and Distributed Computing. (item 7 in the section)

2014- 8*th Int. Conf. Numerical Methods and Applications:* organizer of the special session: Monte Carlo and Quasi-Monte Carlo methods (item 12 in the section)

III. Attachments

(lists may be as long as required)

1. Scholarly / scientific publications

Publications may only be listed if they relate directly to the project. **Up to three of the most important publications** should be highlighted as such (e.g. printed in bold letters).
Please note that funding for publication costs can be requested (under the original project number) for up to three years following completion of a project.

Please make sure that all publications are freely available on the Internet. For details, see the Open Access Policy of the FWF. (In the Life Sciences category, all refereed publications are to be made available through Europe PubMedCentral)

Please indicate at the end of every peer-review publication (in brackets) the Open Access (OA) type as following:

- Gold OA = published in Open Access Journal, with or without an author fee (see register of all Open Access Journals http://www.doaj.org/)
- Hybrid OA = published in a subscription journal but Open Access by an author fee (see http://en.wikipedia.org/wiki/Hybrid_open_access_journal)
- Green OA = self-archived electronic copy of the final "accepted manuscript" which might include an embargo period (see: http://www.fwf.ac.at/en/research-funding/open-access-policy/)
- Other OA = any other type of Open Access
- No OA = not published Open Access

1.1 Peer-reviewed publications / already published (journals, monographs, anthologies, contributions to anthologies, proceedings, research data, etc.)

Citations should be provided in a **commonly used format.** For each work, the publication list **must mention the following**:

- Author(s)
- Title
- Journal
- Issue
- Year
- Pages
- DOI or ISBN (for books)
- If Open Access: URL
- Open Access (OA) Type

LIST OF PEER-REVIEWED PUBLICATIONS PROJECT P 21685-N22

Wigner-Boltzmann Particle Simulations

Total 34: book chapters 3; in books 4; journals and proceedings 15; reviwed abstracts 12.

Book chapters:

3. S. Ahmed, M. Nedjalkov, D. Vasileska:
"*Comparative Study of Various Self-Consistent Event Biasing Schemes for Monte Carlo Simulations of Nanoscale MOSFETs*"; in "*Theory and Applications of Monte Carlo Simulations*", V. Chan (ed); Intech Open Access Publisher, 2013, ISBN: 978-953-51-1012-5, 109 - 133 doi:10.5772/53113.
http://dx.doi.org/10.5772/53113
Gold OA

2. P. Schwaha, M. Nedjalkov, S. Selberherr, I. Dimov:
"*Monte Carlo Investigations of Electron Decoherence due to Phonons*"; in "*Monte Carlo Methods and Applications*", K. K. Sabelfeld, I. Dimov (ed); De Gruyter, 2012, ISBN: 978-3-11-029347-0, 203 - 211.
http://www.iue.tuwien.ac.at/pdf/ib_2012/BC2012_Nedjalkov_1.pdf
Green OA

1. M. Nedjalkov, D. Querlioz, P. Dollfus, H. Kosina:
"*Wigner Function Approach*"; in "*Nano-Electronic Devices: Semiclassical and Quantum Transport Modeling*", D. Vasileska, S.M. Goodnick (ed); Springer, 2011, ISBN: 978-1-4419-8839-3, 289-358 doi:10.1007/978-1-4419-8840-9_5**.**
http://www.iue.tuwien.ac.at/pdf/ib_2010/BC2011_Kosina_1.pdf
Green OA

Contributions to books:

4. P. Schwaha, M. Nedjalkov, S. Selberherr, J. M. Sellier, I. Dimov, R. Georgieva:
"*Stochastic Alternative to Newton's Acceleration*";
in "*Large-Scale Scientific Computing*", I. Lirkov, S. Margenov, J. Wasniewski (ed); Springer, 2014, SBN: 978-3-662-43879-4, 178 - 185 doi:10.1007/978-3-662-43880-0_19.
http://www.iue.tuwien.ac.at/pdf/ib_2014/BC2014_Schwaha_1.pdf
Green OA

3. J.M. Sellier, M. Nedjalkov, I. Dimov, S. Selberherr:
"*The Role of Annihilation in a Wigner Monte Carlo Approach*";
in "*Large-Scale Scientific Computing*", I. Lirkov, S. Margenov, J. Wasniewski (ed); Springer, 2014, ISBN: 978-3-662-43879-4, 186 - 193 doi:10.1007/978-3-662-43880-0_20.
http://www.iue.tuwien.ac.at/pdf/ib_2014/BC2014_Sellier_1.pdf
Green OA

2. P. Schwaha, M. Nedjalkov, S. Selberherr, I. Dimov:
"*Phonon-Induced Decoherence in Electron Evolution*";
in "*Lecture Notes in Computer Science, Vol. 7116*", I. Lirkov, S. Margenov, J. Wasniewski (ed); Springer, 2012, ISBN: 978-3-642-29842-4, 472 - 479 doi:10.1007/978-3-642-29843-1_53.
http://www.iue.tuwien.ac.at/pdf/ib_2011/BC2012_Schwaha_1.pdf
Green OA

1. M. Nedjalkov, S. Selberherr, I. Dimov:
"*Stochastic Algorithm for Solving the Wigner-Boltzmann Correction Equation*";
in "*Lecture Notes in Computer Science, Vol. 6046*", I. Dimov, S. Dimova, N. T. Kolkovska (ed);
Springer, 2011, ISBN: 978-3-642-18465-9, 95 - 102.
http://www.iue.tuwien.ac.at/pdf/ib_2010/BC2011_Nedjalkov_Springer.pdf
Green OA

Contributions to journals and conference proceedings

15. P. Ellinghaus, M. Nedjalkov, and S. Selberherr
Efficient Calculation of the Two-Dimensional Wigner Potential full paper
in "*Proceedings of the 17th International Workshop on Computational Electronics*", IEEE Xplore (2014), 1-3, doi:10.1109/IWCE.2014.6865812
http://www.iue.tuwien.ac.at/pdf/ib_2014/CP2014_Ellinghaus_5.pdf
Green OA

14. P. Ellinghaus, M. Nedjalkov, and S. Selberherr
Implications of the Coherence Length on the Discrete Wigner Potential full paper
in "T*he 17th International Workshop on Computational Electronics* ", IEEE Xplore
(2014), 1-3, doi:10.1109/IWCE.2014.6865852
http://www.iue.tuwien.ac.at/pdf/ib_2014/CP2014_Ellinghaus_6.pdf
Green OA

13. P. Ellinghaus, M. Nedjalkov, and S. Selberherr
The Wigner Monte Carlo Method for Accurate Semiconductor Device Simulation
in "*Proceedings of the 19th International Conference on Simulation of Semiconductor Processes and Devices (SISPAD)*", (2014), 113-116, ISBN: 978-1-4799-5287-8
http://www.iue.tuwien.ac.at/pdf/ib_2014/CP2014_Ellinghaus_3.pdf
Green OA

12. J. M. Sellier, M. Nedjalkov, I. Dimov, S. Selberherr:
"*A benchmark study of the Wigner Monte Carlo method*";
Monte Carlo Methods and Applications, **20** (2014), 43 - 51 doi:10.1515/mcma-2013-0018.
http://www.iue.tuwien.ac.at/pdf/ib_2013/JB2014_Sellier_2.pdf
Green OA

11. M. Nedjalkov, P. Schwaha, S. Selberherr, J. M. Sellier, D. Vasileska:
"*Wigner Quasi-Particle Attributes - An Asymptotic Perspective*";
Applied Physics Letters, 102 (2013), 163113-1 - 163113-4 doi:10.1063/1.4802931.
http://www.iue.tuwien.ac.at/pdf/ib_2012/JB2013_Nedjalkov_1.pdf
Green OA

10. P. Schwaha, D. Querlioz, P. Dollfus, J. Saint-Martin, M. Nedjalkov, S. Selberherr:
"*Decoherence effects in the Wigner function formalism*";
Journal of Computational Electronics, **12** (2013), 388 - 396 doi:10.1007/s10825-013-0480-9.
http://www.iue.tuwien.ac.at/pdf/ib_2013/JB2013_Schwaha_1.pdf
Green OA

9. J. M. Sellier, M. Nedjalkov, I. Dimov, S. Selberherr:
"*Decoherence and Time Reversibility: The Role of Randomness at Interfaces*";
Journal of Applied Physics, **114** (2013), 174902-1 - 174902-7 doi:10.1063/1.4828736.
http://www.iue.tuwien.ac.at/pdf/ib_2013/JB2013_Sellier_1.pdf
Green OA

8. S. Amoroso, L. Gerrer, A. Asenov, J. M. Sellier, I. Dimov, M. Nedjalkov, S. Selberherr:
"*Quantum Insights in Gate Oxide Charge-Trapping Dynamics in Nanoscale MOSFETs*";
in "*Proceedings of the 18th International Conference on Simulation of Semiconductor Processes and Devices (SISPAD)*", (2013), IEEE Xplore, 25 - 28, ISBN: 978-1-4673-5733-3; doi: 10.1109/SISPAD.2013.6650565
http://www.iue.tuwien.ac.at/pdf/ib_2013/CP2013_Nedjalkov_2.pdf
Green OA

7. J. M. Sellier, M. Nedjalkov, I. Dimov, S. Selberherr:
"*Two-dimensional Transient Wigner Particle Model*";
in "*Proceedings of the 18th International Conference on Simulation of Semiconductor Processes and Devices (SISPAD)*", (2013), IEEE Xplore (2013) Print ISBN: 978-1-4673-5733-3 doi: 10.1109/SISPAD.2013.6650660
http://www.iue.tuwien.ac.at/pdf/ib_2013/CP2013_Nedjalkov_1.pdf
Green OA

6. P. Schwaha, J. M. Sellier, M. Nedjalkov, I. Dimov, S. Selberherr:
"*The Ultimate Equivalence Between Coherent Quantum and Classical Regimes*";
"*Proceedings of the 16th International Workshop on Computational Electronics (IWCE 2013)*", (2013), 152 - 153. ISBN 978-3-901578-26-7
http://www.iue.tuwien.ac.at/pdf/ib_2012/CP2013_Schwaha_1.pdf
Green OA

5. M. Nedjalkov, S. Selberherr, D.K. Ferry, D. Vasileska, P. Dollfus, D. Querlioz, I. Dimov, P. Schwaha:
"*Physical Scales in the Wigner-Boltzmann Equation*";
Annals of Physics, 328 (2012), 220 - 237 doi:10.1016/j.aop.2012.10.001.
http://dx.doi.org/10.1016/j.aop.2012.10.001
Hybrid OA

4. M. Nedjalkov, P. Schwaha, S. Selberherr, D.K. Ferry, D. Vasileska, P. Dollfus, D. Querlioz:
"*Role of the Physical Scales on the Transport Regime*"; full paper
in "*The 15th International Workshop on Computational Electronics*", IEEE Xplore, 2012, ISBN: 978-1-4673-0705-5, 1 - 3 doi:10.1109/IWCE.2012.6242848.
http://www.iue.tuwien.ac.at/pdf/ib_2011/BC2012_Nedjalkov_1.pdf
Green OA

3. P. Schwaha, M. Nedjalkov, S. Selberherr, I. Dimov:
"*Particle-Grid Techniques for Semiclassical and Quantum Transport Simulations*"; full paper
in "*The 15th International Workshop on Computational Electronics*", IEEE Xplore, 2012, ISBN: 978-1-4673-0705-5, 1 - 3 doi:10.1109/IWCE.2012.6242860.
http://www.iue.tuwien.ac.at/pdf/ib_2011/BC2012_Schwaha_2.pdf
Green OA

2. M. Nedjalkov, P. Schwaha, S. Selberherr, D.K. Ferry:
"*Phonon Decoherence in Wigner-Boltzmann Transport*";
Poster: International Winterschool on New Developments in Solid State Physics, Mauterndorf, Austria; 12.02.2012 - 17.02.2012; in "*Proceedings of International Winterschool on New Developments in Solid State Physics*", (2012), 61 - 62.
http://www.iue.tuwien.ac.at/pdf/ib_2011/CP2012_Nedjalkov_1.pdf
Green OA

1. M. Nedjalkov, H. Kosina, P. Schwaha:
"*Device Modeling in the Wigner Picture*";
Journal of Computational Electronics, **9** (2010), 218 - 223 doi:10.1007/s10825-010-0316-9.
http://www.iue.tuwien.ac.at/pdf/ib_2010/JB2010_Nedjalkov_1.pdf
Green OA

Reviewed abstracts for conference presentations

12. Paul Ellinghaus, Mihail Nedjalkov, and Siegfried Selberherr
Optimized Particle Regeneration Scheme for the Wigner Monte Carlo Method,
Talk: Eighth International Conference on Numerical Methods and Applications
20 - 24.08.2014, Borovets, Bulgaria; in '*Book of Abstracts' (2014), 12.*
http://www.iue.tuwien.ac.at/pdf/ib_2014/CP2014_Ellinghaus_4.pdf
Green OA

11. I. Dimov, M. Nedjalkov, J. M. Sellier, S. Selberherr:
"*Neumann Series Analysis of the Wigner Equation Solution*";
Talk: European Conference on Mathematics for Industry (ECMI), Taormina, Italy; (invited)
09-14.06. 2014; in "*Abstracts of the 18th European Conference on Mathematics for Industry*", (2014), 459.
http://www.iue.tuwien.ac.at/pdf/ib_2013/CP2014_Nedjaklov_3.pdf
Green OA

10. J.M. Sellier, M.Nedjalkov, I.Dimov, S.Selberherr,
The Multi-Dimensional Transient Challenge: The Wigner Particle Approach
Invited Talk: International Workshop on Computational Electronics (IWCE), Paris, France
03-06.06.2014 in "*Proceedings of the 17th International Workshop on Computational Electronics (IWCE 2014)*", (2014), 119-120. ISBN 978-2-9547858-0-6
http://www.iue.tuwien.ac.at/pdf/ib_2014/CP2014_Nedjalkov_1.pdf
Green OA

9. P. Ellinghaus, M. Nedjalkov, and S. Selberherr
Efficient Calculation of the Two-Dimensional Wigner Potential
Talk: International Workshop on Computational Electronics (IWCE), Paris, France, 03-06.06.2014 ; in "*Proceedings of the 17th International Workshop on Computational Electronics (IWCE 2014)*", (2014), 19-20. ISBN 978-2-9547858-0-6
http://www.iue.tuwien.ac.at/pdf/ib_2014/CP2014_Ellinghaus_1.pdf
Green OA

8 P. Ellinghaus, M. Nedjalkov, and S. Selberherr
Implications of the Coherence Length on the Discrete Wigner Potential
Talk: International Workshop on Computational Electronics (IWCE), Paris, France,
03-06.06. 2014 ; in "*Proceedings of the 17th International Workshop on Computational Electronics (IWCE 2014)*", (2014), 155-156. ISBN 978-2-9547858-0-6
http://www.iue.tuwien.ac.at/pdf/ib_2014/CP2014_Ellinghaus_2.pdf
Green OA

7. P. Schwaha, M. Nedjalkov, S. Selberherr, I. Dimov, R. Georgieva:
"*Stochastic Alternative to Newton's Acceleration*";
Talk: International Conference on Large-Scale Scientific Computations (LSSC), Sozopol, Bulgaria;
03 - 07.06. 2013 in "*Abstracts International Conference on Large-Scale Scientific Computations (LSSC)*", (2013), 77- 78.
http://www.iue.tuwien.ac.at/pdf/ib_2012/CP2013_Nedjalkov_2.pdf
Green OA

6. J. M. Sellier, M. Nedjalkov, I. Dimov, S. Selberherr:
"*The Role of Annihilation in a Wigner Monte Carlo Approach*";
Talk: International Conference on Large-Scale Scientific Computations (LSSC), Sozopol, Bulgaria;
03 - 07.06.2013; in "*Abstracts International Conference on Large-Scale Scientific Computations (LSSC)*", (2013), 78.
http://www.iue.tuwien.ac.at/pdf/ib_2012/CP2013_Nedjalkov_1.pdf
Green OA

5. M. Nedjalkov, P. Schwaha, S. Selberherr, D.K. Ferry, D. Vasileska, P. Dollfus, D. Querlioz:
"*Role of the Physical Scales on the Transport Regime*";
Talk: International Workshop on Computational Electronics (IWCE), Madison, WI, USA;
22 - 25.05.2012; in "*Proceedings of the 15th International Workshop on Computational Electronics (IWCE 2012)*", (2012), 47 - 48.
http://www.iue.tuwien.ac.at/pdf/ib_2011/CP2012_Nedjalkov_3.pdf
Green OA

4. P. Schwaha, M. Nedjalkov, S. Selberherr, I. Dimov:
"*Particle-Grid Techniques for Semiclassical and Quantum Transport Simulations*";
Poster: International Workshop on Computational Electronics (IWCE), Madison, WI, USA;
22 - 25.05.2012; in "*Proceedings of the 15th International Workshop on Computational Electronics (IWCE 2012)*", (2012), 177 - 178.
http://www.iue.tuwien.ac.at/pdf/ib_2011/CP2012_Nedjalkov_2.pdf
Green OA

3. P. Schwaha, M. Nedjalkov, S. Selberherr, I. Dimov:
"*Monte Carlo Investigations of Electron Decoherence due to Phonons*";
Talk: Seminar on Monte Carlo Methods (MCM), Borovets;
29.08.2011 - 02.09.2011; in "*Abstracts IMACS Seminar on Monte Carlo Methods (MCM)*", (2011), 48.
http://www.iue.tuwien.ac.at/pdf/ib_2011/CP2011_Schwaha_1.pdf
Green OA

2. P. Schwaha, M. Nedjalkov, S. Selberherr, I. Dimov:
"*Phonon-Induced Decoherence in Electron Evolution*";
Talk: International Conference on Large-Scale Scientific Computations (LSSC), Sozopol, Bulgaria;
06 - 10.06.2011; in "*Abstracts Intl. Conf. on Large-Scale Scientific Computations*", (2011), 74 - 75.
http://www.iue.tuwien.ac.at/pdf/ib_2010/CP2011_Schwaha_1.pdf
Green OA

1. M. Nedjalkov, S. Selberherr, I. Dimov:
"*Stochastic Algorithm for Solving the Wigner-Boltzmann Correction Equation*";
Talk: International Conference on Numerical Methods and Applications (NM&A), Borovets;
20 - 24.08. 2010; in "*Abstracts of the International Conference on Numerical Methods and Applications (NM&A)*", (2010), B-43.
http://www.iue.tuwien.ac.at/pdf/ib_2010/CP2010_Nedjalkov_3.pdf
Green OA

There are no entries relevant for sections 1.2 to 4.

1.2 Non peer-reviewed publications / already published (journals, monographs, anthologies, contributions to anthologies, research reports, working papers / preprints, proceedings, research data, etc.)

Citations should be provided in a **commonly used format.** For each work, the publication list **must mention the following**:

- Author(s)
- Title
- Journal
- Issue
- Year
- Pages
- DOI or ISBN or URL / if applicable
- Open Access / if applicable
- Open Access (OA) Type

1.3 Planned publications

(journals, monographs, anthologies, contributions to anthologies, proceedings, research data, etc.)

Author(s)			
Title			
Sources			
URL (if applicable)			
Peer Review	yes ☐	no ☐	
Status	in press/accepted ☐	submitted ☐	in preparation ☐

2. Most important academic awards

(Specific academic awards, honours, prizes, medals or other merits)

Name of award	n=national / i=international

3. Information on results relevant to commercial applications

- Type of commercial application:

1. Patent
2. Licensing
3. Copyrights (e.g. for software; no publications)
4. Others

5.

Type of commercial application		
Subject / title of the invention / discovery		
Short description of the invention / discovery		
Year		
Status	granted ☐	pending ☐
Application reference (or patent number)		

4. Publications for the general public and other publications

(Absolute figures, separate reporting of national / international publications)

- Type of dissemination activities:

  1 Self-authored publications on the World Wide Web
  2 Editorial contributions in the media (print, radio, TV, www, etc.)
  3 (Participatory) contributions within science communication
  4 Popular science contributions (books, lectures, exhibitions, films, etc.)

	national	**International**
Self-authored publications on the www		
Editorial contributions in the media		
(Participatory) contributions within science communication		
Popular science contributions		

5. Development of collaborations

Indication of the most important collaborations (no more than 5) that took place (i.e. were initiated or continued) in the course of the project. Please provide the name of the collaboration partner (name, title, institution) and a few words about the scientific content. Please **categorise** each collaboration arrangement as follows:

N				Nationality of collaboration partner (please use the ISO-3-letter country code)
	G			Gender — **F** (female) **M** (male)
		E		Extent — **E1** **low** (e.g. no joint publications, but mention in acknowledgements or similar); **E2** **medium** (collaboration e.g. with occasional joint publications, exchange of materials or similar, but no longer-term exchange of personnel); **E3** **high** (extensive collaboration with mutual hosting of group members for research stays, regular joint publications, etc.)
			D	Discipline — **W** **within the discipline** (within the same scientific field) **I** **interdisciplinary** (involving two or more disciplines) **T** **transdisciplinary** (collaborations outside the sciences)

N	G	E	D	Name	Institution
BGR	M	E3	W	Prof. Ivan Dimov	IICT, Bulgarian Academy of Sciences
BGR	M	E3	W	Dr. Jean Michel Sellier	IICT, Bulgarian Academy of Sciences
USA	F	E3	W	Prof. Dragica Vasileska	Dept. of EE, Arizona State University
FRA	M	E2	W	Prof. Philippe Dollfus	University of Paris-Sud
GBR	M	E2	W	Prof. Asen Asenov	University of Glasgow

Prof. Dimov is an advisor of ViennaWD with contributions to the development of the Monte Carlo approach and the particle algorithm. The collaboration with Dr. Sellier (from the group of Prof. Dimov) relates to the implementation of the particle-sign algorithm in his device Monte Carlo simulator *archimedes* and an extension of the algorithm for the first two-dimensional applications. Prof. Vasileska is an advisor of ViennaWD with a basic contribution to the development of the CEMC simulator. The collaboration with the groups of Prof. Asenov and Prof. Dollfus relates to applications and analysis of the simulation results.

Note: General scientific contact and occasional meetings should not be considered collaborations for the purposes of this report.

6. Development of human resources in the course of the project

(Absolute figures with an indication of status (in progress / completed)

Note: It is not possible to assign a *venia* thesis / work (*Habilitation*) to a single project; here it is necessary to mention those *venia* theses for which the project was important. A similar caveat applies to Ph.D. and diploma theses: The FWF does not support thesis work, but instead funds the scientific work that forms the basis for such theses.

	In progress	**Completed**	**Gender**	
			f	**m**
Full professorship				
Venia thesis (*Habilitation*) / Equivalent senior scientist qualification **Doctor of Science thesis**		2011		M
Postdoc				
Ph.D. theses				
Master's theses				
Diploma theses				
Bachelor's theses				

Note: Doctor of Science degree is the highest scientific qualification existing in some countries. It is obtained after a Doctor degree and after a subsequent Habilitation. The PI obtained his D.Sc. degree in Mathematics from the Bulgarian Academy of Sciences in 2011. According to the regulations of BAS the degree is given for:*"work of an exceptional standard, containing original contributions to the advancement of knowledge and learning which has given the candidate international distinction in their field. Candidates must be able to demonstrate a sustained contribution to their subject, as evidenced by seminal publications."*

7. Applications for follow-up projects

(Please indicate the status of each project and the funding organisation)

7.1 Applications for follow-up projects (FWF projects)

Please indicate the project type (e.g. stand-alone project, SFB, DK, etc.)

Project number (if applicable)	**P26628-N27**		
Project type	**stand-alone**		
Title / subject	**Electro-Thermal Dynamics in Nanostructures**		
Status	granted ☐	pending ☒	in preparation ☐
Application reference (if a patent is applied)			

7.2 Applications for follow-up projects (Other national projects)

(e.g. FFG, CD Laboratory, K-plus centres, funding from the Austrian central bank [OeNB], Austrian federal government, provincial agencies, provincial government or similar sources)

Funding agency	Please choose an item: Wählen Sie ein Element aus.		
Other national funding agencies			
Project number (if applicable)			
Project type			
Title / subject			
Status	granted ☐	pending ☐	in preparation ☐
Total costs (granted)			

7.3 Applications for follow-up projects (international projects) (e.g. EU, ERC or other international funding agencies)

Country	**EU**		
Funding agency	**FP7**		
Project number (if applicable)	**318458**		
Project type	**ICT**		
Title / subject	**SUPERTHEME**		
Status	granted ☒	pending ☐	in preparation ☐
Total costs (granted)	**4.792.541,00 Eur** http://www.supertheme.eu/content/dam/supertheme/en/documents/supertheme-d1_1.pdf		

IV. Cooperation with the FWF

Please rate the following aspects with regard to your interaction with the FWF. Please provide any **additional comments (explanations)** on the supplementary sheet with a reference to the corresponding question/aspect.

Scale:
-2 highly unsatisfactory
-1 unsatisfactory
0 appropriate
+1 satisfactory
+2 highly satisfactory
X not used

Rules
(i.e. guidelines for: funding programme, application, use of resources, reports)

		Rating
Application guidelines	Length	**2**
	Clarity	**2**
	Intelligibility	**2**

Procedures (submission, review, decision)

	Advising	**2**
	Duration of procedure	**0**
	Transparency	**1**

Project support

Advising	Availability	**2**
	Level of detail	**2**
	Intelligibility	**2**

Financial transactions (credit transfers, equipment purchases, personnel management)	**2**

Reporting / review / exploitation

Effort	**1**
Transparency	**1**
Support in PR work / exploitation	**1**

Comments on cooperation/interaction with the FWF: