AMaSiS 2024:

Applied Mathematics and Simulation for Semiconductor Devices

Weierstrass Institute Berlin, September 10 – 13, 2024

AMaSiS 2024 is an interdisciplinary workshop dedicated to the mathematical modeling and numerical simulation of semiconductor devices. AMaSiS 2024 aims at bringing together experts from mathematics, physics, engineering, and materials science for discussions on computational materials science and electronic structure theory, quantum and semiclassical transport, simulation of semiconductor devices, and upscaling from quantum mechanics and particle systems to continuum scale models.

Weierstrass Institute for Applied Analysis and Stochastics

Berlin Mathematics Research Center MATH+

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The organizers,

Patricio Farrell,
Annegret Glitzky,
Markus Kantner,
Matthias Liero,
Michael O'Donovan,
and Josef Weinbub

1 General Information

1.1 Venues

The Tutorials 1 and 2 on September 10 will be held at the Lecture Hall 0007 of the Humboldt-Universität zu Berlin in Hausvogteiplatz 5-7, 10117 Berlin. The nearest underground stations are **Hausvogteiplatz**, served by line U2 and **Stadtmitte**, served by lines U2 and U6.
The scientific worshop takes place from September 11 – 13 and will be held at the Leibniz Headquarters in Chausseestraße 111, 10115 Berlin. The nearest underground station is **Naturkundemuseum**, served by line U6.
Please see www.bvg.de for more information on public transport in Berlin.

1.2 Workshop Dinner and Lunch

The workshop dinner will take place at the restaurant Tapas y Más, Neue Grünstraße 17-18, 10179 Berlin on Thursday, September 12 at 6.30 pm.

Here are a few places to have lunch near the venue at the Leibniz Headquarters:

- Mensa HU Nord – canteen of the Humboldt-Universität zu Berlin (canteen card needed, can be obtained at the canteen for 1.50 euros)
- Speisekombinat – pizza, pasta, and grilled meat
- Pascarella – fine Italian dining
- Cô Chu – Vietnamese cuisine
- Mmaah - Korean BBQ Express – Korean street food
- The Fresh Seeds – healthy fast food
- CousCous – vegan and vegetarian food
- Chelany – South-Asian cuisine
- Polish Dainty – savoury Polish cuisine

2 Detailed Schedule

Tuesday, September 10

08:15–09:10	Arrival & Registration
09:10–09:15	Tutorial Welcome
09:15–10:45	**Tutorial 1A** Jesús Carrete Montaña, U Zaragoza: *Thermal conductivity calculations with the Boltzmann transport equation and machine-learning force fields*
10:45–11:15	Coffee Break
11:15–12:45	**Tutorial 1B**
12:45–14:00	Lunch Break
14:00–15:30	**Tutorial 2A** Michele Simoncelli, U Cambridge: *From density-functional theory to dual wave-particle transport and device simulation*
15:30–16:00	Coffee Break
16:00–17:30	**Tutorial 2B**

Wednesday, September 11

08:15–09:00	Arrival & Registration
09:00–09:20	Opening
09:20–10:30	**Numerical Methods A** Mathieu Luisier: *Theory and algorithms for extreme-scale nano-device simulations* Christoph Jungemann: *Simulation of nanowire NMOSFETs based on the Boltzmann equation with Godunov-type stabilization*
10:30–11:00	Coffee Break
11:00–12:30	**Drift-diffusion A** Ansgar Jüngel: *Memristor drift-diffusion systems for brain-inspired neuromorphic computing* Dilara Abdel: *Modeling and simulation of vacancy-assisted charge transport in innovative semiconductor devices* Claire Chainais-Hillairet: *A drift-diffusion-Poisson system on a moving domain: Some theoretical and numerical results*
12:30–14:00	Lunch Break
14:00–15:30	**UV-Light and Alloy Disorder** Bernd Witzigmann: *Numerical simulation of carrier injection efficiency in ultraviolet light-emitting diodes* Marcel Filoche: *Accounting for nanoscale disorder in semiconductors with the localization landscape theory* Michael O'Donovan: *Multi-scale simulation of electronic and transport properties in (Al,Ga)N quantum well systems for UV-C emission*
15:30–16:00	Coffee Break
16:00–17:15	**2D Materials** William Vandenberghe: *Dielectric, magnetic, and contact properties of two-dimensional materials* Vittorio Romano: *Optimal control of a semiclassical Boltzmann equation for charge transport in graphene* Poster Pitching
17:30–19:00	Poster Session

Thursday, September 12

09:00–10:30	**Numerical Methods B** Zlatan Akšamija: *Numerical simulation of charge transport in doped conjugated polymers for organic electronics* Evelyne Knapp: *Parameter extraction for large-area semiconductor devices* Clément Jourdana: *Uniform accuracy towards numerical approximations for a Bloch model*
10:30–11:00	Coffee Break
11:00–12:30	**Spin-Qubit Devices** Chris Anderson: *Computational aspects of simulations of Si based quantum devices* Félix Beaudoin: *Technology computer-aided design of spin qubits in semiconductors* Abel Thayil: *Valley-splitting in Si/SiGe quantum wells*
12:30–14:00	Lunch Break
14:00–15:50	**Quantum Transport** Alberto Tibaldi: *Small-signal and noise analysis of nanodevices based on a quantum transport model* Cristina Medina Bailón: *Quantum corrections in EMC: From multisubband to quantum transport* Vito Dario Camiola: *Quantum MEP hydrodynamical model for charge transport* Orazio Muscato: *Wigner–Boltzmann Monte Carlo simulation of thermionic cooling devices based on resonant-tunneling AlGaAs/GaAs heterostructure*
15:50–16:20	Coffee Break
16:20–17:30	**Photovoltaics** Nicola Courtier: *Continuum-level modelling and simulation of electronic-ionic interactions in perovskite solar cells* Urs Aeberhard: *Simulation of advanced solar cells - beyond the limitations of the drift- diffusion picture*
18:30	Workshop Dinner

Friday, September 13

09:00–10:30	**Drift-diffusion B** Giuseppe Alì: *On the mathematical modelling of semiconductor laser diodes* Maxime Herda: *Numerical analysis of a finite volume scheme for charge transport in perovskite solar cells* Julien Moatti: *High-efficiency and reliable schemes for drift-diffusion systems*
10:30–11:00	Coffee Break
11:00–12:30	**Materials Modeling** Costanza Lucia Manganelli: *Strain engineering in CMOS micro- electronics. How to tailor* Nella Rotundo: *Perturbation approach and existence and uniqueness analysis for the forward lateral photovoltage scanning problem* Balázs Bámer: *Cluster-based multivariate spline model for dopant activation in SiC*
12:30	Closing

3 Poster Session (in Alphabetical Order)

Wednesday, September 11:

- Lasse Ermoneit (WIAS Berlin, Germany)
  Simulation and optimal control of single-electron shuttling in a SiGe quantum bus
- Jürgen Fuhrmann (WIAS Berlin, Germany)
  Development of numerical methods and tools for drift-diffusion simulations
- Annegret Glitzky (WIAS Berlin, Germany)
  Electrothermal models for organic semiconductor devices
- Yiannis Hadjimichael (WIAS Berlin, Germany)
  Strain distribution in zincblende and wurtzite GaAs nanowires bent by a one-sided (In, Al)As shell
- Christine Keller (WIAS Berlin, Germany)
  A drift-diffusion model to describe ion channel dynamics
- Hendrik Leenders (RWTH Aachen, Germany)
  Numerical methods for solving the Boltzmann transport equation in 2D material devices
- Steffen Maass (Technische Universität Berlin, Germany)
  Monolithic coupling of a CatMAP based microkinetic model for heterogeneous electrocatalysis and ion transport with finite ion sizes
- Tuan Tung Nguyen (Technische Universität Wien, Austria)
  Drift-diffusion for memristors coupled to a network
- Stefan Portisch (Technische Universität Wien, Austria)
  Analysis of a drift-diffusion model with Fermi–Dirac statistics for memristive devices
- Josef Weinbub (Silvaco Europe Ltd., UK)
  Victory atomistic: Multi-physics simulation of materials and quantum transport

4 Abstracts (in Alphabetical Order)

4.1 Tutorials

Jesús Carrete Montaña (Universidad de Zaragoza, Spain)

Tutorial 1: Thermal conductivity calculations with the Boltzmann transport equation and machine-learning Force fields

Solutions of the Boltzmann transport equation (BTE) for phonons with inputs from density-functional-theory (DFT) calculations have been successful at providing predictive, parameter-free estimates of the thermal conductivity of many pristine and defect-laden semiconductors, albeit at very significant computational cost. Machine-learning force fields, through their ability to provide results with DFT-like quality in a small fraction of the time, can revolutionize that situation. This tutorial will first guide the audience through all the steps of a conventional DFT+BTE calculation, followed by the active learning of a descriptor-based neural-network potential. That force field will then be validated by reproducing the ab-initio results.

Michele Simoncelli (University of Cambridge, UK)

Tutorial 2: From density-functional theory to dual wave-particle transport and device simulation

Quantitative theoretical predictions for charge and heat transport phenomena in semiconductors are crucial to design devices for energy conversion or management. We present recent advances in Quantum ESPRESSO [1], an open-source density-functional-theory (DFT) software, that allows us to simulate from first principles the thermoelectric properties of semiconductors. After discussing how to compute the band structure of electrons and phonons, we introduce the framework needed to quantify their interactions. We discuss how these quantitites enter into the microscopic Wigner formulation for transport in solids [2], which enables us to predict the transport coefficients in materials ranging from crystals to glasses [2,3], and with variable level of doping [4]. Finally, we show that microscopic transport equations for electron and phonon transport can be coarse-grained into mesoscopic viscous equations useful to design devices. These are partial differential equations that generalize Ohm's [5] or Fourier's [6] laws describing not only diffusive transport but also fluid-like phenomena measured in recent, pioneering experiments [7].

[1] Giannozzi et al., J. Phys. Condens. Matter 46 (2017)
[2] Simoncelli, Marzari and Mauri, Phys. Rev. X 12 (2022)
[3] Harper, Iwanowski, Payne and Simoncelli, Physical Review Materials 8 (2024)
[4] Cepellotti, Coulter, Johansson, Fedorova and Kozinsky, J. Phys. Mater. 5 (2022)

[5] Gurzhi, Sov. Phys. Usp. 11 (1965)
[6] Simoncelli, Marzari and Cepellotti, Phys. Rev. X 10 (2020)
[7] Jaoui et al., Phys. Rev. X 12 (2022)

4.2 Invited Talks

Dilara Abdel (WIAS Berlin, Germany)

Modeling and simulation of vacancy-assisted charge transport in innovative semiconductor devices

Semiconductor technology, the backbone of the electronic industry, is omnipresent in our daily lives. Developing new semiconductor devices drives innovation and advances environmental sustainability. Promising technologies are perovskite solar cells and memristive devices based on transition metal dichalcogenide (TMDC). Perovskites and TMDCs share a common characteristic: In both materials, certain ions or atoms are not rigidly fixed in the crystalline semiconductor lattice and move around freely. This talk thoroughly investigates the impact of vacancy dynamics on device performance by deriving drift-diffusion equations using thermodynamic principles. Then, we formulate models to describe charge transport in perovskite solar cells and TMDC memristors. We discretize the transport equations via the finite volume method and establish the existence of discrete solutions. Our study concludes with simulations conducted with open-source software developed in the programming language Julia.

Urs Aeberhard (ETH Zürich, Switzerland)

Simulation of advanced solar cells - beyond the limitations of the drift-diffusion picture

In many cases, the implementation of advanced photovoltaic concepts relies on the use of nanostructure device architectures with engineered electronic structure and tailored charge carrier dynamics. In such systems, the assumptions underlying the conventional macroscopic continuum drift-diffusion-Poisson picture are not met: Charge carries are not in extended states with bulk density, and neither in thermalized quasi-equilibrium Fermi distributions, the microscopic potential landscape depends strongly on the point of operation, and transport is not diffusive, but ballistic or tunnel-assisted. On the other hand, any of these circumstances can be considered using a device simulation based on non-equilibrium Green's functions (NEGF). In my presentation, after a brief introduction of the formalism, I illustrate the application of NEGF to the simulation of advanced-concept solar cells based on three examples where straightforward application of the drift-diffusion picture fails, namely ultra-thin absorbers, hot-carrier devices, and superlattice solar cells.

Zlatan Akšamija (The University of Utah, USA)

Numerical simulation of charge transport in doped conjugated polymers for organic electronics

Organic electronic materials, specifically conjugated polymers, are a cost-effective and environmentally friendly alternative to inorganics. However, they do not possess intrinsic free carriers, which means they must be doped to increase the number of free carriers and boost conductivity. Simultaneously, dopant-carrier interactions dramatically alter the energetics of the states available for transport as well as the dynamics of free carriers. In this invited talk, I will discuss our results arising from coupling a model for modification of the electronic density of states (DOS) in the presence of dopants with a phonon-assisted carrier hopping simulation through those states. We use the DOS model as input to the hopping transport simulation based on numerically solving the Pauli Master equation to analyze the transport properties of doped conjugated polymers and extract both conductivity and Seebeck coefficient at each doping concentration. In our work, we also implement carrier screening in the Debye–Hückel formalism and capture the competing roles of screening and dopant-induced disorder on transport.

Guiseppe Alì (Università della Calabria, Italy)

On the mathematical modelling of semiconductor laser diodes

A class of models for semiconductor laser diodes is discussed from a mathematical viewpoint and some existence and uniqueness results are presented.

Chris Anderson (UC Los Angeles, USA)

Computational aspects of simulations of Si based quantum devices

The task of creating simulations of Si based quantum devices useful for device design and fabrication will be discussed. A specific emphasis will be on the computational challenges that have been overcome to create useful simulations as well as a description of future computational and theoretical problems that need to be addressed in order to extend the utility of such simulations.

Félix Beaudoin (Nanoacademic Technologies Inc., Canada)

Technology computer-aided design of spin qubits in semiconductors

Spin qubits in semiconductors are a promising approach to quantum computation because of their long coherence time, small footprint, and CMOS compatibility. As spin qubits gain

industrial relevance, accurate 3D quantum TCAD simulations become essential to reduce experimental design, fabrication, and characterization costs. However, realistic 3D simulations face challenges due to cryogenic temperature and poor performance of quantum many-body solvers. This presentation introduces computationally efficient approaches for TCAD simulations of electron or hole spin-qubit systems with realistic 3D geometries. Our approach covers these key steps: 3D geometry definition, device electrostatics, single-particle Schrödinger equation, charge stability diagrams, many-body physics, and time-dependent simulations with realistic noise. Our results for practical geometries like FD-SOI quantum dots pave the way to high-throughput TCAD simulation workflows for spin-qubit quantum technologies.

Nicola Courtier (University of Oxford, UK)

Continuum-level modelling and simulation of electronic-ionic interactions in perovskite solar cells

In 10 years of development, perovskite solar cells have achieved excellent efficiencies and a gradual improvement in stability. Since perovskite materials for photovoltaics are mixed electronic-ionic conductors, it is essential to consider the density and mobility of ionic defects [1]. Defects impact both the steady-state and dynamic behaviour of perovskite cells. Studies suggest that additional Frenkel defects may form under illumination, resulting in undesirable degradation at the interfaces. Improved modelling and simulation is required to understand the relevant timescales and significance of this process on the continuum level. We extend the charge-transport model that underpins our open-source IonMonger tool [2] to investigate the impact of defect generation on device characteristics.

[1] Z. Ni, H. Jiao, C. Fei et al. Nat Energy, 7:65–73 (2022) 10.1038/s41560-021-00949-9
[2] W. Clarke, L.J. Bennett, Y. Grudeva et al. J Comput Electron 22:364–382 (2023) 10.1007/s10825-022-01988-5

Marcel Filoche (ESPCI Paris, France)

Accounting for nanoscale disorder in semiconductors with the localization landscape theory

In large bandgap compounds, the natural spatial fluctuations of the alloy composition lead to broad variations of the local band diagram, hence strong perturbations of the electronic wave functions (which are no longer Bloch states), of their density of states, and of their mutual overlaps. At a larger scale, these alterations of the fundamental assumptions affects transport, recombination, and more generally all processes involved in the device performance.

Maxime Herda (U Lille, France)

Numerical analysis of a finite volume scheme for charge transport in perovskite solar cells

In this talk, I'll consider a drift-diffusion model that describes charge transport in perovskite solar cells. In this three-species system, electrons and holes may diffuse linearly (Boltzmann approximation) or nonlinearly (e.g., due to Fermi–Dirac statistics), and volume exclusion effects are taken into account for anionic vacancies within the perovskite layer. To discretize the equations, we develop a fully-implicit in time two-point flux finite volume scheme. Utilizing a discrete entropy-dissipation relation, we perform the numerical analysis of the scheme. This is a joint work with Dilara Abdel, Claire Chainais-Hillairet and Patricio Farrell.

Ansgar Jüngel (Technische Universität Wien, Austria)

Memristor drift-diffusion systems for brain-inspired neuromorphic computing

More than 50 years ago, Moore predicted that the number of transistors on a microchip doubles every two years. This exponential growth is ending today because of physical limits, and new technologies are needed. Neuromorphic computing seems to be a promising avenue. An encouraging device as technology enabler of neuromorphic computing is the memristor. Memristors can be seen as nonlinear resistors with memory, mimicking the conductance response of biological synapses. This talk is concerned with the mathematical analysis of three-species drift-diffusion equations for memristors. We prove the global existence of weak solutions in any space dimension and global bounded solutions in two dimensions. Allowing for degenerate diffusion, the boundedness of solutions can be shown in three dimensions as well. The mathematical difficulties originate from the three-species situation and the mixed boundary conditions. Our idea is to exploit carefully the estimates from the free energy and to combine local and global compactness results. Numerical experiments in one dimension reproduce hysteresis effects in the current-voltage characteristics, which are a fingerprint for memristive devices.

Christoph Jungemann (RWTH Aachen, Germany)

Simulation of nanowire NMOSFETs based on the Boltzmann equation with Godunov-type stabilization

Stabilization of the Boltzmann equation for quasi-ballistic and diffusive transport in nanowire transistors can be challenging. Godunov's method is a reliable stabilization scheme, which results in a system matrix which is positive definite and guarantees a positive distribution

function. The numerical damping due to Godunov's method enables the use of explicit time integration methods which can be CPU-efficiently processed in parallel. On the other hand, the inherent asymmetry of the stabilization scheme can lead to problems in the case of strong scattering and coarse grids in real space. The versatility of the approach will be demonstrated for a nanowire transistor, for which stationary and transient simulation results are presented. This is joint work with T. Linn, M. Noei, and P. Luckner.

Evelyne Knapp (ZHAW Winterthur, Switzerland)

Parameter extraction for large-area semiconductor devices

The extraction of material parameters from (large-area) semiconductor devices is a crucial aspect of studying phenomena such as degradation in perovskite solar cells. This process involves the precise determination of key parameters like carrier mobility, ionic conductivity, trap states, etc., all of which are essential for understanding device performance and long-term reliability. To achieve this, we employ advanced techniques including spatially resolved measurements alongside traditional current-voltage (IV) measurements to accurately identify the underlying model parameters. Emphasis is placed on integrating machine learning algorithms, particularly physics-informed neural networks (PINNs), to enhance the accuracy and efficiency of parameter extraction. PINNs offer a novel framework by incorporating physical laws directly into the neural network training process, thereby improving the reliability of the extracted parameters compared to pure neural networks. Additionally, we compare the performance of PINNs with traditional methods.

Mathieu Luisier (ETH Zürich, Switzerland)

Theory and algorithms for extreme-scale nano-device simulations

Modern nano-device simulations require tools that capture quantum mechanical effects from first-principles and that account for non-ideal effects such electron-phonon or electron-electron interactions. In this presentation, a modelling framework that fulfils these criteria will be presented, focusing on its numerical algorithms, implementation strategy, and parallelisation scheme. Concrete examples demonstrating the benefit of the chosen approach will be discussed.

Constanza Lucia Manganelli (Leibniz-Institut für innovative Mikroelektronik, Germany)

Strain engineering in CMOS micro-electronics. How to tailor.

The significance of strain engineering in CMOS microelectronics extends across diverse applications, encompassing opto-electronics, sensing, and quantum technologies, and in materials such as heterostructures, and perovskites. Experimental analyses (Photoluminescence, Raman, X-Ray Spectroscopy) and simulation platforms enable the prediction and optimization of material processes and device designs. In this context, we present a systematic study elucidating how the temperature-dependent distribution of strain can significantly impact the optical and transport performance of semiconductor devices. Our investigation focuses on strained Ge microdisks, crucial components for developing guidelines for integrated light emitters. Additionally, we explore the role of metal electrodes in quantum buses within CMOS-compatible devices. The research provides valuable insights into strain effects on semiconductor devices, laying a foundation for developing and optimizing future microelectronic technologies.

Cristina Medina Bailón (Universidad de Granada, Spain)

Quantum corrections in EMC: From multi-subband to quantum transport

As the scaling of electronic devices approaches to the end of the roadmap, their performance is degraded due to the appearance of the short-channel effects (SCEs). Classicaly, the loss of gate terminal control over the channel and the increase of the influence of source and drain regions have been the reasons of the degradation of threshold voltage and the subthreshold characteristics. In this way, device architecture optimizations are mainly focused on the reduction of SCEs. However, at such small dimensions different transport quantum phenomena start to play an important role in the behavior of the transistors. In particular, direct Source-to-Drain tunneling (S/D tunneling) through the narrow potential barrier, gate leakage mechanisms (GLM) in ultrathin insulators and band-to-band tunneling (BTBT) at high drain bias conditions and for TFET applications must be included in device simulators. The inclusion of these phenomena in Multi-Subband Ensemble Monte Carlo simulators (MS-EMC) is shown to extend the validity of such tools. In particular, an effective computational scheme of tunneling mechanisms (including S/D tunneling, GLM and BTBT) is shown for a better understanding of the physical limitations and required optimizations of future devices.

Nella Rotundo (Università degli Studi di Firenze, Italy)

Perturbation approach and existence and uniqueness analysis for the forward lateral photovoltage scanning problem

Estimating crystal inhomogeneities in semiconductors noninvasively is crucial for various

industrial applications, especially for maintaining high-purity crystals. Doping fluctuations create local electric fields, detectable by generating electron-hole pairs through electromagnetic radiation and measuring the resulting current. Lateral Photovoltage Scanning (LPS) method uses this principle with laser beams. We focus on a nonlinear drift-diffusion model for LPS, addressing the coupling between charge transport and the external circuit. By deriving a scaled unipolar model and using a perturbation approach, we simplify the system while retaining essential physics. This yields four different problems for which we can prove the existence and uniqueness of solutions.

Alberto Tibaldi (Politecnico di Torino, Italy)

Small-signal and noise analysis of nanodevices based on a quantum transport model

The talk will focus on the multiscale modeling of nanostructured optoelectronic devices. Our approach, based on the nonequilibrium Green's function framework, allows to describe the complex interplay between coherent transport, intraband dephasing processes, and interband transitions originated by defects, photons, and carrier-carrier interactions. The resulting model provides a genuine quantum-kinetic description of tunneling, miniband transport, hopping, and carrier extraction in terms of quasi-Fermi levels and electric fields, germane to the drift-diffusion framework. Focus will be placed on the latest developments of our simulation framework. First, we will discuss novel strategies for the acceleration of the method convergence through the formulation of exact Newton–Raphson methods for the achievement of the self-consistent Born approximation. Then, we will move to the study of small-signal and noise properties in nanostructured devices. This is joint work with Jesus Alberto Gonzalez Montoya and Francesco Bertazzi (both Politecnico di Torino).

William Vandenberghe (UT Dallas, USA)

Dielectric, magnetic, and contact properties of two-dimensional materials

Over the past decades, electronic devices have become ubiquitous appearing in computers, cell phones, displays, lighting, internet, household appliances, and cars. New and improved (cheaper and faster) electronic devices have become an indispensable component of economic growth. To address the unrelenting demand for new devices, our research focuses on the theoretical modeling of future electronic devices that realize superior performance. One of the most promising avenues to realize a big improvement in electronic devices is the introduction of Two-Dimensional (2D) Materials. We present an overview of our recent progress in modeling dielectric, magnetic, and contact properties of 2D materials. We first highlight how the dielectric properties can be calculated in a robust way. We show how leveraging materials databases, 32 novel candidate 2D dielectrics with a large band gap can be identified. Calculating the

electron affinity and bandgap of all 32 materials, we estimate the leakage current and identify oxyhalides like LaOBr and LaOCl as promising 2D "high-k" future dielectrics. Next, we show how magnetic properties can be determined from first principles while accounting for long-range interactions and the anisotropy of the exchange interaction. We apply our method on known 2D ferromagnets like CrI3, and CrGeTe3 to verify good agreement with experiments. We subsequently study the magnetic order of doped transition-metal dichalcogenides (TMDs) and identify V-doped MoSe2 as the most promising doped TMD-based 2D ferromagnet. Finally, we show our progress in understanding electrical contacts to semiconducting 2D materials like TMDs. Calculating the current flowing from the metal to the semiconductor, we show that when the 2D material is surrounded by a "low-k" dielectric, the contact resistance is dramatically improved. The recipe we identify for making low-resistance contacts is: low Schottky barrier, high doping concentration, and low dielectric constant of the surrounding dielectric.

Bernd Witzigmann (FAU Erlangen-Nürnberg, Germany)

Numerical simulation of carrier injection effciency in ultraviolet light-emitting diodes

We study the carrier injection effciency (CIE) in multiple-quantum well UV-LEDs using a microscopic model. We show that for a 265 nm LED, the CIE a major factor that limits the external quantum effciency.

4.3 Contributed Talks

Balázs Bámer (Technische Universität Wien, Austria)

Cluster-based multivariate spline model for dopant activation in SiC

Ion implantation in SiC damages its crystallinity, resulting in the clustering of inactive dopants. Subsequent annealing repairs the crystal structure and activates the implant. Current models for this process are fully empirical, and a physical understanding is unavailable. To generate a physical model of dopant activation, we study the time-dependent reaction between the as-implanted species, such as dopants, defects, and clusters, described using a set of ODEs. Combining known post-annealing activation ratios and implant conditions (temperature and dose), a global optimizer is applied to find the initial dopant, defect, and cluster concentrations as free parameters. The optimizer systematically tunes these parameters and evaluates the ODEs in each step to get the simulated activation ratio. Its deviation from the empirical model is used as feedback to the optimizer to tune the parameters. The optimizer's initial concentrations are approximated using multi-variate B-splines.
This is joint work with Sabine Leroch [1], Andreas Hössinger [2], and Lado Filipovic [1].

[1] Christian Doppler Laboratory for Multi-Scale Process Modeling of Semiconductor Devices and Sensors, Institute for Microelectronics, TU Wien, 1040 Vienna, Austria
[2] Silvaco Europe Ltd., St Ives, Cambridgeshire, PE27 5JL, United Kingdom

Vito Dario Camiola (Università di Catania, Italy)

Quantum MEP hydrodynamical model for charge transport

A well known procedure to get quantum hydrodynamical models for charge transport is to resort to the Wigner equations and deduce the hierarchy of the moment equations as in the semiclassical approach. If one truncates the moment hierarchy to a finite order, the resulting set of balance equations requires some closure assumption because the number of unknowns exceed the number of equations. In the classical and semiclassical kinetic theory a sound approach to get the desired closure relations is that based on the Maximum Entropy Principle (MEP). Here I am going to present a quantum hydrodynamical model which is valid for a general energy band (case not present in literature) considering a closure of the moment system deduced by the Wigner equation resorting to a quantum version of MEP. Explicit formulas for quantum correction at order are obtained with the aid of the Moyal calculus for silicon and graphene removing the limitation that the quantum corrections are based on the equilibrium Wigner function as in the cases already discussed in literature. As an application, quantum correction to the mobilities are deduced.

Claire Chainais-Hillairet (Université de Lille, France)

A drift-diffusion-Poisson system on a moving domain: Some theoretical and numerical results

The drift-diffusion-Poisson system is well known and widely used in the modelling of semiconductor devices. The description of charge transport in some oxide layers also leads to drift-diffusion-Poisson systems. But in this framework chemical reactions at the interfaces lead to Robin boundary conditions for the flux densities and to moving interfaces. In this talk I will present a thermodynamically consistent drift-diffusion-Poisson model describing the evolution of an oxide layer, and I will review the mathematical results we have recently obtained for this model from both a theoretical and a numerical point of view. This is a joint work with Clément Cancès, Federica Raimondi and Juliette Venel.

Clément Jourdana (Université Grenoble Alpes, France)

Uniform accuracy towards numerical approximations for a Bloch model

To describe light-matter interactions in quantum optics, a Maxwell–Bloch model can be used. It leads to the time evolution of the density matrix associated to a quantum system coupled to that of the classical electromagnetic field. Here, we consider a given electromagnetic field varying on a fast scale and we are interested in the long time evolution of the Bloch solution. In that regime, it has been proved, introducing successive approximations and using averaging techniques, that the diagonal part of the density matrix is asymptotically solution to a Master equation with averaged transition rates. With B. Bidégaray-Fesquet and L. Trémant, we have used the information given by these successive approximations to build a numerical scheme for the diagonal part of the density matrix that is uniformly accurate, i.e. whose accuracy does not depend on the asymptotic parameter. The idea is to capture the asymptotic behaviour and the rest in a “macro" and a “micro" variable respectively.

Julien Moatti (Technische Universität Wien, Austria)

High-efficiency and reliable schemes for drift-diffusion systems

We are interested in the numerical approximation of drift-diffusion systems, used for e.g. to model semiconductor devices. Among the various existing numerical methods for simulating such devices, the finite-volume Scharfetter-Gummel scheme is well known to offer a reliable approximation, but its use is limited to orthogonal meshes, and the approximation is simply low-order. We present here a new approach based on the Hybrid High-Order method, devised to preserve 1) the decay of a physically motivated free energy; 2) the positivity of computed densities; while being high-order (in space) and allowing general polytopic meshes for easy

local refinement. Emphasis will be given to computational efficiency compared to the classical Scharfetter–Gummel scheme.

Orazio Muscato (Università di Catania, Italy)

Wigner–Boltzmann Monte Carlo simulation of thermionic cooling devices based on resonant-tunneling AlGaAs/GaAs heterostructure

Temperature stabilization by means of electronic refrigerators has attracted much interest, as a scalable, reliable and green option. Research in this field has mainly focused on two approaches, which rely either on thermoelectricity (based on the Peltier effect) or thermionic emission of hot carriers. Thermionic devices were proposed as an alternative to thermoelectric devices, able to reduce the effects of carrier scattering and lattice thermal conduction. We study by means of full quantum simulations the operating principle and performance of a semiconductor heterostructure refrigerator combining resonant tunneling filtering and thermionic emission. Our model takes into account the coupling between the electric and thermal currents by self-consistently solving the Wigner–Boltzmann transport equation using the signed Monte Carlo method and the heat equation. We show that the device can achieve relatively high cooling power values, while in the considered implementation, the maximum lattice temperature drop is severely limited by the thermal conductivity of the constituting materials. Quantum simulations demonstrate that cooling properties of such tilted barrier devices are significantly improved in the out-of-equilibrium regime, where the thermionic cooling concept offers its best efficiency.

Michael O'Donovan (WIAS Berlin, Germany)

Multi-scale simulation of electronic and transport properties in (Al,Ga)N quantum well systems for UV-C emission

The semiconductor material Aluminium Gallium Nitride has recently attracted attention for use in UV-C optoelectronic devices [1]. Understanding the electronic structure of these devices is important when aiming to improve efficiency. Carrier localization and band ordering should be considered to accurately describe electronic and optical properties. We use a tight-binding (TB) model to study the electronic structure of (Al,Ga)N quantum wells. Our calculations show that the density of states and degree of optical polarization depend on alloy composition, disorder and well size. The obtained electronic structure provides input for drift-diffusion (DD) calculations, including the extraction of an energy landscape from TB. This procedure allows us to establish a multi-scale DD framework [2]. Quantum corrections are included via localization landscape theory [3].

[1] J. Phys. D: Appl. Phys. 53 503001 (2020)
[2] J. Appl. Phys. 130, 065702 (2021)
[3] Phys. Rev. B 95 144204 (2017)

Vittorio Romano (Università di Catania, Italy)

Optimal control of a semiclassical Boltzmann equation for charge transport in graphene

The construction of semiconductor nanostructures requires efficient and accurate methodologies that accommodate physical and engineering details as well as the required functionality of the resulting device. Within this framework, we developed a model for controlling charge transport in graphene for the design of new devices. The semiclassical Boltzmann equation [1] represents an accurate model for graphene simulation that accommodates microscopic effects. In this model, a natural control mechanism is an external electric field due to an applied voltage at the metallic contacts. With this control, we can manipulate the momentum and current through the graphene. In our work, these tasks are formulated with ensemble cost functionals [2,3,4]. This choice appears natural since ensemble cost functionals can be interpreted as ensemble averages of potential functions determining the desired mean trajectory and final target. We focus on a space-homogeneous time-dependent electric control field whose cost in the cost functional is given by a quadratic H^1 term that guarantees continuous control functions. Well-posedness of the control problem is proved, and the characterization of optimal controls by an optimality system is discussed. The latter is approximated by a discontinuous Galerkin scheme and the optimization is performed by using a nonlinear conjugate gradient method. Results of numerical experiments are presented that demonstrate the ability of the proposed control framework to design control fields.

[1] A. Majorana, G. Nastasi, V. Romano, Simulation of bipolar charge transport in graphene by using a discontinuous Galerkin method, Comm. Comp. Phys. 26, 454-482 (2021).
[2] J. Bartsch, A. Borzì, F. Fanelli, S. Roy, A theoretical investigation of Brockett's ensemble optimal control problems, Calc. Var. Partial Differ. Equ. 58 (2019).
[3] J. Bartsch, G. Nastasi, A. Borzì, Optimal control of the Keilson–Storer master equation in a Monte Carlo framework, J. Comput. Theor. Transp. 50, 454-482 (2021).
[4] G. Nastasi, A. Borzì, V. Romano, Optimal control of a semiclassical Boltzmann equation for charge transport in graphene, Commun. Nonlinear Sci. Numer. Simul. 132, 107933 (2024).

Abel Thayil (WIAS Berlin, Germany)

Optimization of valley splitting in Si/SiGe spin qubits

Silicon-germanium (SiGe) based heterostructures are a major candidate for realizing fully scalable quantum computers due to their inherently long spin coherence times and compatibility with existing semiconductor fabrication techniques. A critical challenge in strained Si/SiGe quantum wells is the existence of two nearly degenerate conduction band minima that can lead to leakage of quantum information. In the literature, several strategies have been proposed to enhance the energy splitting between the two valleys such as sharp interfaces, oscillating Ge-concentrations (wiggle well) and shear strain engineering. In this work, we formulate the design of the epitaxial profile in the quantum well as an optimization problem and seek for an optimized alloy composition profile that maximizes the valley splitting while respecting several manufacturing limitations. Our theory is based on a recently proposed extended virtual crystal approximation to properly account for the disorder in SiGe alloys. We demonstrate that our approach reproduces existing heuristics such as the wiggle well and the Germanium spike as limiting cases but also finds enhanced epitaxial profiles. Our work thus presents an interesting design tool to tailor the valley splitting in Si/SiGe heterostructures.

4.4 Posters

Lasse Ermoneit (WIAS Berlin, Germany)

Simulation and optimal control of single-electron shuttling in a SiGe quantum bus

Spin qubits in Si/SiGe heterostructures are leading candidates for fault-tolerant, universal quantum computing, requiring a bus shuttle for coherent electron transport to interlink different functional units of the quantum processor. These quantum bus shuttle are an essential element in developing a scalable quantum computer. The shuttling fidelity is typically constrained by unavoidable material defects and fabrication imperfections, which can cause spin-dephasing. In this work, we present a numerical simulation framework for conveyor-mode spin-qubit shuttling within a realistic Si/SiGe quantum bus, focusing on the influence of charged defects on the orbital dynamics of the transported electron. We apply quantum optimal control theory to design control pulses that minimize the accumulation of energy uncertainty and therefore enable a nearly deterministic transfer of the electron through the channel. The optimization is carried out using a quasi-Newton method. The resulting control protocol facilitates quasi-adiabatic driving without compromising shuttling speed.

Jürgen Fuhrmann (WIAS Berlin, Germany)

Development of numerical methods and tools for drift-diffusion simulations

The implicit Euler Voronoi box-based finite volume method with modified Scharfetter–Gummel fluxes provides a framework for thermodynamically consistent discretizations of drift diffusion systems in electronics, electrochemistry, and biology. For semiconductors, this approach has been implemented in the C /Python based simulator WIAS/ddfermi. The new Julia package VoronoiFVM.jl solves nonlinear coupled PDE systems of diffusion-reaction-convection type in one, two, and three space dimensions. It uses automatic differentiation to obtain the Jacobi matrices for the nonlinear solve and provides the solver kernel for the semiconductor simulator ChargeTransport.jl and the Nernst–Planck–Poisson solver LiquidElectrolytes.jl. The poster discusses the discretization approach and developments towards larger scale simulations based on algebraic multigrid preconditioning using the AMGCL library.
This is joint work with D. Abdel, M. O'Donovan, P. Farrell, P. Jaap, Th. Koprucki, and T. Streckenbach (all of them WIAS Berlin).

Annegret Glitzky (WIAS Berlin, Germany)

Electrothermal models for organic semiconductor devices

The temperature activated hopping transport of charge carriers in organic semiconductor materials leads to a strong interplay between electrical current and heat flow. As a consequence, interesting phenomena like S-shaped current-voltage relations with regions of negative differential resistance occur or the luminance as well as the temperature distribution in large-area organic light emitting diodes become strongly inhomogeneous. To model the electrothermal behavior of organic devices by means of coupled systems of partial differential equations, we discuss p(x)-Laplace thermistor models, energy-drift-diffusion-type models as well as hybrid concepts. In drift-diffusion-type models the specialities of organic semiconductors have to be taken into account: the statistical relation between chemical potentials and charge carrier densities is given by Gauss–Fermi integrals leading to bounded charge carrier densities. Moreover, the mobility functions depend on temperature, density, and electrical field strength. We summarize the mathematical analysis of the underlying equations, the numerical approximation via finite-volume methods based on generalized Scharfetter–Gummel schemes, and present simulation results where path-following techniques are used to recover the S-shaped current-voltage relations. This is joint work with Matthias Liero and Jürgen Fuhrmann (both WIAS Berlin) and is based on a close cooperation with the Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and the Institute of Applied Physics of the TU Dresden, Germany.

Yiannis Hadjimichael (WIAS Berlin, Germany)

Strain distribution in zincblende and wurtzite GaAs nanowires bent by a one-sided (In, Al)As shell

We present a mathematical model to accurately describe how 3D heterostructures respond to strain caused by lattice mismatch. Our model incorporates non-linear elasticity and takes into account local prestrain within each material region. We applied this model to hexagonal heteronanowires and conducted numerical simulations using finite element methods analyzing how the structures bend with varying material compositions and cross-sectional geometries. Moreover, we compared the calculated curvature with analytically derived formulations to ensure the reliability of our model. The findings of our study provide valuable insights into the behavior of strained bent heterostructures. By comparing the strain profiles of wurtzite and zincblende crystal structures we have revealed distinct characteristics and a previously unnoticed torsion effect for zincblende crystals. Finally, we show the significant potential of strain to influence piezoelectricity and the electronic band structure.

Christine Keller (WIAS Berlin, Germany)

A drift-diffusion model to describe ion channel dynamics

We present a model for ion channels in cell membranes based on non-equilibrium thermodynamics, which accounts for finite ion size effects, solvation phenomena and charges on the membrane and channel proteins. We place particular emphasis on consistent modeling of the selectivity filter and treat it as an additional embedded domain in which the constituents can change their chemical properties. The diffusion process through the filter is determined by an independent diffusion coefficient, and de- and resolvation reactions are introduced as interface conditions. The resulting system of drift-diffusion equations is solved in Julia using the generalized Nernst–Planck–Poisson solver LiquidElectrolytes.jl implemented on top of the solver kernel VoronoiFVM.jl for coupled nonlinear PDE systems. A comparison with experimental results for calcium-selective ion channels demonstrates the validity of our approach.
This is joint work with J. Fuhrmann, B. Wagner, and M. Landstorfer (all of them WIAS Berlin).

Hendrik Leenders (RWTH Aachen, Germany)

Numerical methods for solving the Boltzmann transport equation in 2D material devices

2D materials as transport layers for field-effect transistors are intensively investigated due to their superior properties at nm dimensions compared to silicon that might help not only to extend Moore's law, but also to push the performance of transistors. Since the approximations of the drift-diffusion model are questionable at small length scales, the Boltzmann transport equation (BTE) is solved deterministically for the 2D material channel region and takes into account the Pauli exclusion principle, scattering by acoustic and polar-optical phonons, and the band structure over the entire Brillouin zone. A recently developed Godnov-type stabilization scheme is adapted for an arbitrary band structure, ensuring the nonnegativity of distribution function regardless of the scattering rates. The arising Riemann problem at the interfaces between the spatial Voronoi boxes is solved exactly with Godunov's scheme under conservation of the flux and the transversal k-vector.

Steffen Maass (Technische Universität Berlin, Germany)

Monolithic coupling of a CatMAP based microkinetic model for heterogeneous electrocatalysis and ion transport with finite ion sizes

CatMAP is a Python package for expressing and solving microkinetic models parametrized by the relative energies of the intermediate states obtained from ab-initio calculations within the framework of density-functional theory. Ringe et al. used a CatMAP model iteratively coupled

to a generalized Nernst-Planck-Poisson system realized in COMSOL multiphysics to simulate CO2 electroreduction on gold surfaces. As a more robust approach, we develop the Julia package CatmapInterface.jl which uses Julia's symbolic manipulation capabilities to translate a CatMAP specification of a microkinetic model into Julia code which realises a reaction boundary condition to the generalized Nernst–Planck–Poisson solver LiquidElectrolytes.jl implemented on top of the solver kernel VoronoiFVM.jl for coupled nonlinear PDE systems.
This is joint work with J. Fuhrmann (WIAS Berlin) and S. Ringe.

Tuan Tung Nguyen (Technische Universität Wien, Austria)

Drift-diffusion for memristors coupled to a network

The memristor is a novel semiconductor device equipped with a memory due to the change of its electrical resistance. In this way, it may mimic the behavior of a synapse in the human brain. We analyze a model of memristors that are coupled with an electric network consisting of various electronic devices. While nonlinear drift-diffusion equations describe the motion of charged particles within the memristor, the node potentials in the network follow Kirchhoff's laws, i.e. ordinary differential equations and algebraic constraints. The coupling between them results in a system of partial differential-algebraic equations. The existence analysis employs entropy methods crucially.

Stefan Portisch (Technische Universität Wien, Austria)

Analysis of a drift-diffusion model with Fermi–Dirac statistics for memristive devices

Memristors can be seen as nonlinear resistors with memory. This makes them a promising device in neuromorphic computing, as they show a resistive switching behaviour, thus being ideal candidates to build artificial neurons or synapses. Perovskite solar cells have emerged as a groundbreaking technology, due to the perovskite materials' outstanding optical and electronical properties. These perovskite materials exhibit a memristive behaviour, which naturally leads to their use in memristors. We analyze a drift-diffusion model for memristors including Fermi–Dirac statistics for the electrons and holes and Blakemore statistics for the oxygen vacancies, coupled to a Poisson equation for the electric potential. Using a-priori estimates obtained from the related free energy functional we prove the existence of weak solutions to the system. Additionally we show the uniform-in-time boundedness of solutions in three space dimensions.

Josef Weinbub (Silvaco Europe Ltd., UK)

Victory atomistic: Multi-physics simulation of materials and quantum transport

Designing next generation nanoelectronic devices, such as nanowire/nanosheet/2D FETs, requires to consider highly confined transport channels, feature sizes in low single-digit nanometer regime, electron wave nature, material-specific band structures, and extreme temperatures. These demand a multi-physics modeling and simulation approach, linking atomistic electronic structure calculations with quantum transport simulations. The Victory Atomistic simulator, inherited from Nemo5, provides such capabilities by using a combination of a tight-binding approach for the first, and a non-equilibrium Green?s function approach for the latter. Victory Atomistic can be integrated into technology computer-aided design (TCAD) and design technology co-optimization (DTCO) workflows. Software capabilities are introduced as well as some examples are shown. Among the key messages is the need for atomistic simulations and a discussion of collaboration ideas. This is joint work with Philippe Blaise (Silvaco Europe Ltd.).