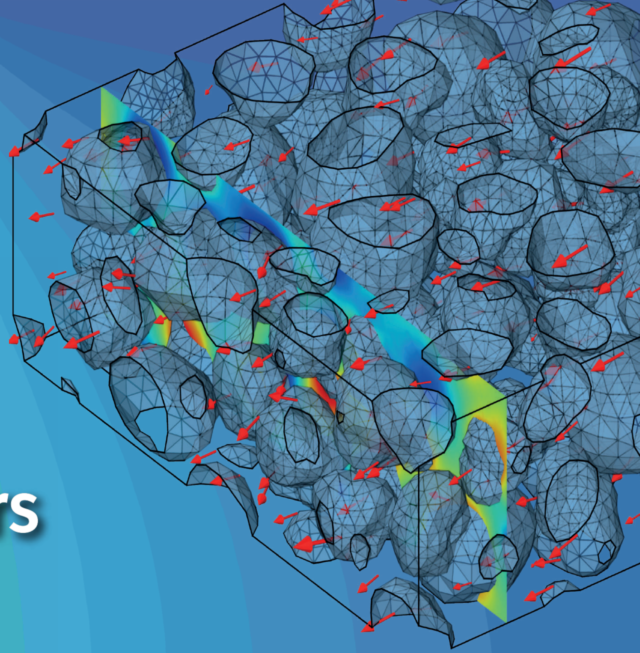

AMaSiS 2021

Applied Mathematics and Simulation for Semiconductors and Electrochemical Systems

Weierstrass Institute for Applied Analysis and Stochastics

Berlin, September 6–9, 2021

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Contents

AMaSiS 2021 is an interdisciplinary workshop dedicated to mathematical modeling of semiconductors and electrochemical systems. Due to inherent similarities between both disciplines, AMaSiS explores synergies in mathematical modeling, analysis, numerics, and simulation techniques. The conference brings together experts from applied mathematics, physics, engineering, chemistry, and material science and covers the following topics:

- electronic structure theory (density functional theory, tight-binding, effective mass models)
- non-equilibrium thermodynamics and transport theories (drift-diffusion models, heat flow, kinetics, non-equilibrium Green's functions)
- mathematical upscaling from quantum mechanics and particle systems to continuum scale (homogenization, asymptotic methods)
- semiconductor devices (light emitting diodes, transistors, etc.)
- electrochemical systems (fundamental electrochemistry, batteries, fuel cells, photo-catalysis)

Monday, 06.09.2021	
14:00 - 14:40	GET TOGETHER
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15:40	**Igor Traskunov (Ulm)** Reconsidering porous electrode theory for Lithium-Ion batteries: Rigorous up-scaling of localized fluctuations as a consequence of locally anisotropic microstructures
16:00	**Orkun Furat (Ulm)** Artificial generation of representative single Li-ion electrode particle architectures from microscopy data
16:20 - 17:00	BREAK
17:00 - 18:20	CHAIR: CLÉMENT CANCÈS
17:00	**Matthias Liero (Berlin)** Heat and carrier flow in organic semiconductor devices – modeling, analysis, and simulation
17:40	**Matthew Grayson (Evanston)** Universal relaxation equation for disordered systems
18:00	**Matthew Wolf (Bath)** Quantifying polaronic effects on the scattering and mobility of charge carriers in lead-halide perovskites
18:20 - 19:00	BREAK
19:00 - 19:40	CHAIR: ANTON VAN DER VEN
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Tuesday, 07.09.2021	
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15:40	**Clement Jourdana (Grenoble)** An interface formulation for the Poisson equation in the presence of a semiconducting single-layer material
16:00	**Petr Vágner (Berlin)** Generalized Nernst–Planck–Poisson model of solid oxide YSZ I LSM I O_2 electrode interface
16:20 - 17:00	BREAK
17:00 - 18:20	CHAIR: MICHAEL EIKERLING
17:00	**Arnulf Latz (Ulm)** Modeling of batteries from nanometer to cell scale: Beyond concentrated solution and porous electrode theory
17:40	**Mira Todorova (Düsseldorf)** Processes at solid/liquid interfaces – insights from ab initio molecular dynamics simulations with potential control
18:20 - 19:00	BREAK

Tuesday - Postersession, 07.09.2021, 19:00 – 21:00, Online

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Dilara Abdel (Berlin)
Modeling and simulation of charge transport in perovskite solar cells

Apratim Bhattacharya (Erlangen)
Homogenization of a nonlinear drift-diffusion system for multiple charged species in a porous medium

Mario Bukal (Zagreb)
Quantum transport models based on Tsallis statistics

Vito Dario Camiola (Catania)
A hydrodynamical model for charge transport in graphene nanoribbons

Benoît Gaudeul (Villeneuve d'Ascq Cedex)
Two entropic finite volume schemes for a Nernst–Planck–Poisson system with ion volume constraints

Yiannis Hadjimichael (Berlin)
Toward charge transport in bent nanowires

Alain Kangabire (Evanston)
Stochastic simulation of continuous time random walks: asymptotic rate coefficients in diffusion-limited relaxations

Boni Anisuzzaman (Berlin)
Impact of capture time on series resistance of high power diode lasers

Victor A. Kovtunenko (Graz)
Study of voltage cycling conditions on Pt oxidation and dissolution in polymer electrolyte fuel cells

Juncen Li (Evanston)
Modeling photodecay as mixed second-order relaxation in phosphorescent metal complexes

Julien Moatti (Villeneuve-d'Ascq)
Long-time behaviour of a hybrid finite volume scheme for the drift-diffusion model with magnetic field

Giovanni Nastasi (Catania)
Simulation of graphene field effect transistors

Grigor Nika (Berlin)
Derivation of an effective bulk-surface thermistor model for OLEDs

Falco Schneider (Kaiserslautern)
Improving efficiency of a numerical solver for microscopic Li-Ion battery simulation including SEI Degradation

Raphael Schoof (Karlsruhe)
Efficient parallel simulation of contact problems for chemo-mechanically modeled battery active particles

Abel Thayil (Palaiseau)
Landscape approach to quantum transport through a disordered or random potential

Wednesday, 08.09.2021	
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15:40	**Jean-Philippe Banon (Palaiseau)** Modeling of light absorption in disordered semiconductor alloys based on the Wigner–Weyl approach and the localization landscape
16:00	**Vladimir Fomin (Dresden)** Modeling of topological and geometrical effects in self-rolled micro- and nanoarchitectures
16:20 - 17:00	BREAK
17:00 - 18:20	CHAIR: MIRA TODOROVA
17:00	**Anton Van der Ven (Santa Barbara)** First-principles statistical mechanics as applied battery materials
17:40	**Claire Onsager (Evanston)** Mapping conductivity with electrical impedance tomography
18:00	**Clément Cancès (Villeneuve d'Ascq)** Towards a thermodynamically consistent model for the corrosion of iron
18:20 - 19:00	BREAK
19:00 - 19:40	CHAIR: VLADIMIR FOMIN
19:00	**Eoin O'Reilly (Cork)** Trends and challenges in semiconductor device and nanostructure modelling

Thursday, 09.09.2021	
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15:40	**Vittorio Romano (Catania)** Simulation of graphene field effect transistors by directly solving the semiclassical Boltzmann equation
16:00	**Marco Coco (Ancona)** The Pauli principle in the Monte Carlo Method for charge transport in graphene
16:20 - 17:00	Break
17:00 - 18:20	Chair: Claire Chainais-Hillairet
17:00	**Ulrike Krewer (Karlsruhe)** Reaction kinetic modeling of electrochemical (energy) cells
17:45	**Roman Schärer (Winterthur)** Towards multiscale modeling of porous electrodes: Connecting the meso- to the macroscopic scale
18:05	**Robert Eisenberg (Chicago IL)** Multiphysics of flow is important in the central nervous system: A tridomain model of optic nerve
18:20 - 19:00	Break
19:00 - 19:40	Chair:
19:00	**Michael Eikerling (Jülich)** Theory and computation of charged electrochemical interfaces
19:40 - 19:50	Closing Remarks

Invited

Homogenization of an electrokinetic model

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In this talk I will review some results on the homogenization (or upscaling) of a system of partial differential equations describing the ideal or non-ideal transport of a N-component electrolyte in a dilute Newtonian solvent through a rigid porous medium. This system describes electrokinetic effets which are important in various applications, including nuclear waste storage or Li-ion batteries. Our approach is based on a linearization argument, first proposed by O'Brien, around an equilibrium solution in the absence of external forces. Assuming that the motion is governed by a small static electric field and a small hydrodynamic force allows us to linearize the model and then to proceed to its homogenization. In particular, we prove that the effective tensor satisfies Onsager properties, namely it is symmetric positive definite. I will explain the differences with some other approaches in the homogenization of such electrokinetic equations. Eventually some numerical computations of homogenized coefficients will be discussed.

This is a joint work with R. Brizzi, J.-F. Dufrêche, A. Mikelic and A. Piatnitski.

Linear/nonlinear approaches for the approximation of convection-diffusion equations

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In this talk, I will introduce three numerical schemes for anisotropic convection-diffusion equations. They are hybrid finite volume schemes applicable on general meshes; two of them are linear schemes while the third one is nonlinear. I will discuss the well-posedness of the schemes and their long-time behavior. Numerical experiments will highlight the main properties of the schemes.

It is a joint work with M. Herda, S. Lemaire and J. Moatti.

Theory and computation of charged electrochemical interfaces

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The region between charged metal surface and aqueous electrolyte lies at the heart of electrochemical energy technologies. The need to understand the properties of this region, which is also known as the electrochemical double layer (EDL), continues to drive extensive research in experiment and theory [1, 2]. The fundamental challenge is to disentangle the complex interplay of electronic structure effects, potential-induced variations of double layer structure and properties, local electrochemical conditions, and kinetics of vital electrocatalytic reactions. We will present a grand-canonical model that accounts for essential components and phenomena of the EDL [3, 4]. The hybrid density-potential functional is parametrized with quantum mechanical density functional theory (DFT) calculations, compared with experimental data, and employed to study interfacial electrochemical properties. In parallel, we have adopted a computational scheme that employs the DFT/ESM-RISM method, developed by Otani and co-workers [5], and applied it to simulate the Pt (111) surface with varying number of oxygen adatoms in acidic solution [6]. With some variation to the distance of closest approach between metal and electrolyte regions being done, the hybrid solvation method reproduced the peculiar non-monotonic charging relation of the Pt-electrolyte interface, in agreement with the theoretical prediction in Ref. [3]. The presentation will conclude with a discussion of practical implications of this charging relation.

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Reaction kinetic modeling of electrochemical (energy) cells

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Our future sustainable energy systems rely on electrochemical cells, such as fuel cells, batteries and electrolysers. Only few cell technologies so far succeeded to enter mass market. This can partly be attributed to performance losses due to reaction kinetic issues at the electrodes. Processes at electrodes are highly complex: electrochemical reaction pathways may contain strongly adsorbed species that hamper fast reactant conversion and lead to high overpo-tential losses; further, unwanted side reactions, chemical reactions in the electrolyte or desorption of intermediates may cause low efficiencies and complex dynamic or hysteresis behavior. In addition, surface changes such as dissolution, restructuring, changes in oxidation state or other degradation phenomena, are frequently found in electrodes. Qualitative and especially quantitative understanding of the reactions at the electrode surface is thus an important key to improving cell performance and durability, and to identify optimal material and operating conditions. Further, models that reproduce the observed phenomena allow for a knowledge-driven design and improvement of performance of electrochemical cells.

Focus of this talk is on model-assisted analysis and identification of reaction kinetics in electrochemical cells. Besides complex multistep reactions, the role of adsorbates, local operating conditions and transport, side reactions and surface changes of electrodes will be elucidated. Examples cover established technologies like PEM electrolysis and Li-ion batteries, and electrodes of next generation cells. Kinetic-Monte-Carlo methods complement continuum-type microkinetic and microkinetic models. The combination of mechanistic modelling and dynamic electrochemical measurements is shown to yield not only a better quantitative and qualitative understanding of electrode performance, but to be the base for a knowledge-driven, model-based electrode and cell development.

Modeling of batteries from nanometer to cell scale: Beyond concentrated solution and porous electrode theory

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Improving the design of batteries to achieve higher power density, energy density, safety and longevity is a complex task, which requires not only optimizing materials but equally important optimizing function and interplay of materials as well as reducing side reactions during the operation of the battery. The function of the material during operation is determined by electrode and cell design. The interplay of the materials influences structure of double layers and emergence of interphases (e.g. the solid electrolyte interphase or SEI) which may affect dramatically reaction kinetics and overpotentials as in ionic liquids or water in salt concepts or when using multivalent ions in Post Lithium batteries. Side reactions as e.g. plating are initiated on a very local nanometer to micrometer scale and therefore strongly depends on the local overpotential distribution, which is influenced by the design of the active particle shape or morphology and local fluctuations in the SEI thickness. To capture all these phenomena within a rational design approach for batteries using modelling and simulations, it is not sufficient to rely on the traditional concentrated solution theory for electrolytes or the porous electrode theory used in the Doyle-Fuller-Newman battery models. In the presentation an overview is given about our recent theoretical developments which are extending electrolyte transport theories including double layer predictions, interface degradation modeling (SEI formation and impact on plating) and the Doyle-Fuller-Newman (DFN) upscaling paradigm for Lithium ion batteries. Our systematic Free Energy based theory for electrolytes captures complex correlated structure formation phenomena in highly concentrated electrolytes as e.g. ionic liquids or water in salt electrolytes. Our new models for SEI formation identifies thickness fluctuations on electrode scale and different growth regimes depending on the operating conditions. Finally it is shown how local overpotential fluctuations relevant for local plating conditions and for the first time observed in microstructure resolved battery simulations can be explained by local anisotropies of active particle properties which can also be captured on the macroscopic cell scale via an improved DFN approach.

Heat and carrier flow in organic semiconductor devices – Modeling, analysis, and simulation

Matthias Liero(2), **Axel Fischer**(1), **Jürgen Fuhrmann**(2), **Annegret Glitzky**(2), **Anton Kirch**(1), **and Grigor Nika**(2)

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The temperature activated hopping transport of charge carriers in organic semiconductors results in a strong interplay between electric current and heat flow. It gives rise to interesting phenomena like S-shaped current-voltage relations with regions of Negative Differential Resistance or leads to inhomogeneous luminance in large-area Organic Light Emitting Diodes (OLEDs) (see Figure 1 and [1]). Moreover, electrothermal effects influence the performance of transistors [2].

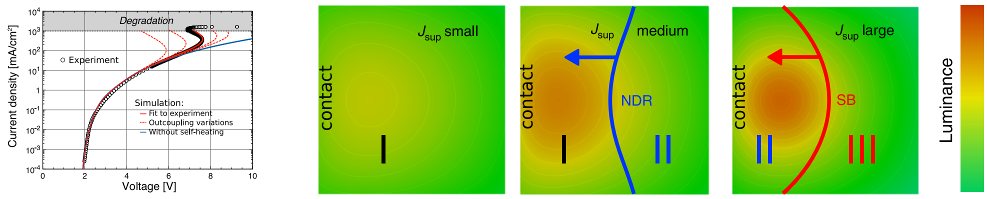

Figure 1: Left: Measured and simulated S-shaped current-voltage relations (up to thermal degradation) for OLED device, Right: Simulated luminance in OLED cross-section for increasing supplied current, I, II, III refer to different operation modes that propagate through the device: normal, local NDR, and switched-back. In the latter mode, the local currents, and hence also the luminance, decreases.

As demonstrated in [1], p-Laplace thermistor models that describe the total current and heat flow in a device, are able to capture the positive temperature feedback in OLEDs. Especially, they can reproduce experimentally observed S-shaped CV-relations and inhomogeneous current density and temperature distributions in large-area OLEDs. But, details such as separate electron and hole current flow, generation-recombination and related heat productions, as well as energy barriers at material interfaces cannot be included. Thus a description of the electrothermal behavior of organic semiconductor devices via more detailed drift-diffusion models is required. In these models the specialities of organic semiconductors have to be taken into account: On the one hand the statistical relation between chemical potentials and charge carrier densities is given by Gauss–Fermi integrals leading to bounded charge carrier densities. On the other hand the mobility functions μ_n, μ_p depend on temperature, density, and electrical field strength. The mobility laws are fitted from a numerical solution of the master equation for the hopping transport in a disordered energy landscape with a Gaussian density of states [3, 4].

In this talk, we give an overview over modeling the electrothermal behavior of organic devices with thermistor- and drift-diffusion-type models as well as hybrid concepts, summarizing [6, 5, 7, 8]. We discuss the mathematical analysis of the underlying equations, the numerical approximation via finite-volume methods based on modified Scharfetter–Gummel schemes, and present simulation results using path-following techniques for recovering the S-shaped current-voltage relations.

Acknowledgments: This work was supported in part by the German Research Foundation (DFG) within the Cluster of Excellence Center for Advancing Electronics Dresden (cfaed), and the DFG project HEFOS (Grant No. FI 2449/1-1) and EFOD (Grant No. RE 3198/6-1). A.G., M.L., and J.F. were partly supported by the DFG under Germany's Excellence Strategy – MATH+ : The Berlin Mathematics Research Center (EXC-2046/1 – project ID: 390685689) via projects AA2-10 and AA2-6. A.K. received funding from the Cusanuswerk Foundation.

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Ion conductors, electron conductors and mixed conductors in electrochemistry

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The lecture gives an overview on thermodynamics and kinetics of electrochemical systems (batteries, fuel cells, photovoltaics). Special emphasis is laid on similarities and differences between ionic and electronic charge carriers as well as on their coupling in relevant functional materials [ ]. This provides the natural bridge to semiconductor physics. The survey concerns transport and storage, and comprises bulk properties, interfacial properties and properties of small systems. Necessity and potential of modelling are set out.

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Trends and challenges in semiconductor device and nanostructure modelling

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The use of theory and modelling for device and nanostructure design and optimisation is very well established, with many applications where the input of modelling is now routine. There still remain however many challenges in materials and device modelling, almost all related to the transition from the need for a quantum-related description at the nanoscale to classical (continuum-based) descriptions at the macroscale. We overview, with examples, some of these challenges, and routes to practical multiscale models for material and device design.

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III-Nitride light emitting diode modeling in the ultraviolet spectral range

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A multi scale transport simulation model for III-nitride light emitting diodes is presented. The simulation approach couples semiclassical transport with a $\mathbf{k}\cdot\mathbf{p}$-Schrödinger solver for the quantum wells in a self consistent way. Studies on the effect of p-side design and the inhomogeneous broadening in deep ultraviolet light emitting diodes will be presented. Deep ultraviolet (DUV) light emitting diodes (LED) made of Aluminium Gallium Nitride (AlGaN) are in high demand for medical, environmental, and technical applications. Recent research concentrates on the enhancement of the efficiency which is still below 10% [1]. One obstacle is the low free hole density in p-doped high band gap AlGaN seen through a low hole injection efficiency. Another issue is the low extraction efficiency and high re-absorption of the dominant transversal magnetic polarized emission from the quantum wells (QW) with high Al content [5]. In addition, the thin and lattice mismatched QWs are susceptible to inhomogeneous broadening (IHB) so that the spectral width of the DUV LED emission may be as large as $\sigma \approx 100$meV. We propose calibrated physical modelling of large band gap III-nitride LEDs to support the efficiency improvement because it enables an investigation of the opaque active region physics and potential bottlenecks there through the macroscopic characteristics. Our physics based transport simulator for III-nitride LEDs is based on a multi scale and multi population approach [3]. As a numerical example we analyze the impact of the acceptor doping profile, the p-side electron barrier, and the active region design on the quantum efficiency. We introduce a statistical model for the IHB [2] which enters on the microscopic level [4] and is fully integrated into the self consistent transport simulation scheme. With this model we investigate how the IHB affects the macroscopic characteristics. We demonstrate that the IHB generally increases the ideality factor and interacts with the internal quantum efficiency by mitigating electron leakage. Simulations show that the enhanced transversal electric polarized emission observed in some DUV LEDs can be related to the IHB.

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Carrier transport, radiative and non-radiative recombination in (In,Ga)N heterostructures: Insights from atomistic and multi-scale simulations

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Semiconductor nanostructures utilizing indium gallium nitride ((In,Ga)N) alloys have attracted considerable research interest due to their potential for optoelectronic device applications [1] but also recently as sources for non-classical light emission [2]. However, and in comparison to other III-V semiconductor heterostructures, (In,Ga)N-based systems exhibit very different fundamental properties. This starts with the underlying crystal structure (wurtzite vs. zincblende), ranges over to the presence of very strong electrostatic built-in fields and ultimately the observation of significant carrier localization effects in (In,Ga)N alloys [3]. In this talk, the impact of (random) alloy fluctuations on charge carrier transport, radiative and non-radiative recombination processes in (In,Ga)N-based heterostructures will be discussed.
Initially we will focus our attention on the temperature dependence of the radiative and non-radiative (Auger) recombination in (In,Ga)N quantum wells, using an atomistic tight-binding model [4]. Equipped with this knowledge, consequences for the thermal "droop" in (In,Ga)N-based light emitting diodes will be discussed [5]. In addition, we will present our approach to address the impact of random alloy fluctuations on the charge carrier transport in (In,Ga)N-based devices, employing a multi-scale simulation framework. As a test-bed, results for uni-polar (electron) transport in (In,Ga)N multi-quantum well systems will be presented [6].
In a second step, the electronic and optical properties of ultrathin, quasi-two dimensional (In,Ga)N layers embedded in GaN will be discussed [7]. These systems should *ideally* circumvent the quantum confined Stark effect and thus the spatial separation of charge carriers, which limits the efficiency of the "conventional" (In,Ga)N quantum well systems mentioned above.
Finally, consequences of random alloy fluctuations for non-classical light emission, e.g. polarization entangled or twin photons, from (In,Ga)N quantum *dots* will be discussed [8]. Here, results from a fully atomistic many-body framework, combining tight-binding electronic structure theory and a configuration interaction scheme, will be presented.

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Processes at solid/liquid interfaces – insights from ab initio molecular dynamics simulations with potential control

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Processes at the solid/liquid are at the heart of many present day technological challenges related to the improvement of battery materials, electro-catalysis, fuel cells, corrosion and others. Understanding and quantifying the underlying fundamental mechanisms will enable targeted design of desired functionalities, but is equally challenging to theoretical modelling and experimental characterisation. Recently we developed a novel potentiostat design [1] and a canonical thermopotentiostat [2] approach, in which the electrode potential of the system is controlled by tuning the excess charge of the working electrode. This enables us to study solid/liquid interfaces under realistic conditions of applied bias by ab-initio molecular dynamics simulations and obtain direct insight into key mechanisms of electrocatalysis and corrosion. The study of the H/Pt/H_2O system provides valuable insights into the role of the solvent on the work-function evolution at metal/electrolyte interfaces [3]. Applying bias to Mg/water interfaces allows us to elucidate the mechanism underlying the experimentally observed link between H-evolution under anodic conditions and Mg dissolution.

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First-principles statistical mechanics as applied battery materials

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Battery materials undergo significant chemical and dimensional changes during each charge and discharge cycle. The insertion of guest ions into electrode intercalation compounds, for example, requires cation diffusion and often leads to a variety of phase transformations that are accompanied by changes in lattice parameters. Continuum simulation approaches that rely on thermodynamic and kinetic phenomenological theories have proven invaluable in the modeling of battery behavior at the materials level. A challenge is that many of the thermodynamic and kinetic quantities that inform phenomenological theories are difficult to measure in isolation. An alternative approach is to calculate them from first principles. However, due to the importance of temperature and entropy in battery materials, it is essential that a statistical mechanics approach is used to connect the electronic structure of a battery material to its macroscopic thermodynamic and kinetic properties. In this talk I will describe how first-principles statistical mechanics approaches can be used to predict voltage curves, phase diagrams, diffusion coefficients and chemo-mechanical properties. The statistical mechanics approaches rely on effective Hamiltonians to extrapolate first-principles electronic structure methods within Monte Carlo simulations. Additional coarse graining schemes then enable a connection to be made between properties at the atomic and electronic scale to phenomenological descriptions of kinetic processes that can be modelled at the meso and continuum scales. Examples will be highlighted, including layered and spinel intercalation compounds for Li, Na, Mg and K-ion batteries as well as Wadsley-Roth intercalation compounds, which are promising anode materials.

Contributed

Modeling of light absorption in disordered semiconductor alloys based on the Wigner-Weyl approach and the localization landscape

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Light absorption and emission measurements are commonly used to study the electronic and optoelectronic properties of semiconductor alloys, and to characterize devices made of heterostructures of such alloys such as LEDs. These measurements are particularly sensitive to the band edge structure. For example, the absorption frequency threshold is in general affected by several processes: thermal processes, electric fields [1], the electron-hole Coulomb interaction [2], and alloy disorder [3] and the joint effect of the two latter [4]. Alloy disorder corresponds to the random configuration of atoms of different species on the crystal lattice, and consequently, breaks the periodic symmetry of the ion lattice potential. The common tools of solid states physics based on the Bloch theorem must then be adapted. In order to understand and predict the effect of alloy disorder on the optoelectronic properties of alloys and devices, we present a model of light absorption based on a formulation in phase space for the electronic states and on results from the localization landscape framework [5, 6, 7]. The derived model is simple, computationally efficient and yields good approximations for practical purposes. The simulated absorption coefficient is compared with eigenstates based computations in 1D and 2D, and is shown to be accurate for disorder parameters relevant for InGaN alloys. The absorption model is then applied in 3D for InGaN alloys of different compositions. The impact of the indium concentration on the Urbach tail and on the spatial distribution of the absorbed power are discussed.

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Towards a thermodynamically consistent model for the corrosion of iron

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The derivation of models for the corrosion of iron that are accurate in the long-time regime is a challenge of great importance in many contexts, among which the management of nuclear wastes. This motivated many previous contributions. Our starting point here is the so-called Diffusion Poisson Coupled Model (DPCM) introduced in [1, 2], which describes the evolution of a magnetite layer separating a block of metallic iron from an aqueous domain. The derivation of the DPCM proposed in [1] does not rely on energetic considerations. As a consequence, its thermodynamic stability is unclear and neither a satisfactory well-posedness result nor the assessment of the long-time behavior of the system have been established so far.

In this project, we explore some as minor as possible corrections to make the DPCM free energy diminishing. We illustrate our approach on a simplified model inspired from the one studied in [3], where only two chemical species (electrons and iron cations) are assumed to be transported in a fixed and oxide layer due to chemical and self-consistent electrostatic effects. A special attention is paid to the boundary conditions at the interfaces between the oxide and the metal and between the oxide and the solution. We propose a global existence result following the methodology introduced in the seminal contributions of Gajewski and Gröger [4]. In opposition to what was established in [3], our result does not require any compatibility condition on the physical coefficients, as a consequence of the nonlinear stability of our system inherited from thermodynamics.

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The Pauli principle in the Monte Carlo Method for charge transport in graphene

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The Monte Carlo method has become a standard toolfor the study of transport problems in electronic devices [1], together with the semiclassical Ensemble Monte Carlo method (EMC). When the Pauli principle is no longer negligible, however, the EMC suffers from some drawbacks regarding the correct reconstruction of the carrier distribution. Many attempts were made over the years to overcome this problem until a new Monte Carlo scheme which takes into account the Pauli principle correctly was developed (see [3] and references therein). Almost all of these works were based on some convenient approximations in the description of the distribution function or of the scattering terms, with no attention on the free-flight step. Earlier on [4], a novel procedure was developed for silicon, which added the Pauli principle also at the end of the free flight, and which could be used when the degeneracy effects are predominant. Here, we address the question of the correctness of representing the free flight in a quantum perspective, with the application of the Pauli principle, or if it is more appropriate to represent it in a semiclassical way with the Liouville operator. We carry out this study by performing a numerical comparison of the various approaches by looking at the effects on the electron distribution function and on the mean values of energy and velocity in the case of a suspended monolayer graphene. This problem is fundamental in the study of new materials, as graphene, where degeneracy effects are important.

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Multiphysics of flow is important in the central nervous system: A tridomain model of optic nerve

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Nerve cells in the central nervous system are packed in a glial syncytium with spaces of only 20 nm between them, but they must avoid crosstalk, just as wires in a computer must. We show that convection through the glia is the dominant mechanism preventing cross talk. Indeed, glial convection is likely to be crucial in clearing all wastes from the nervous system in health (sleep) and disease (migraine and epilepsy) using the recently discovered glymphatic system. These conclusions arise from analysis in space and time using the appropriate partial differential equations (and boundary conditions) for convection, migration, and diffusion. The flow of water and salt in optic nerve is analyzed with a multiphysics field theory derived from first physical principles, using the known anatomical structure. The results fit detailed biophysical measurements of action potentials and potassium clearance.

Modelling of topological and geometrical effects in self-rolled micro- and nanoarchitectures

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The present study is motivated by the recent progress in fabrication of high-tech 3D nanoarchitectures (e.g., open nanotubes and multishells) by using the advanced strain-driven roll-up self-organization [1]. To simulate the superconducting properties of complex superconductor nanoarchitectures, a numerical platform has been developed based on a set consisting of the time-dependent Ginzburg-Landau equation coupled with the Poisson equation and the Maxwell equation. The topological transitions between vortex-chain and phase-slip transport regimes unveiled in curved superconductor nanostructures as a function of the applied magnetic field under a strong transport current [2] open up a possibility to efficiently tailor the superconducting properties of nanostructured materials by inducing a nontrivial topology of superconductor screening currents. In particular, the non-monotonous magnetic-field-voltage and current-voltage characteristics are found in open rolled-up Nb and Sn microtubes under a strong transport current due to the occurrence of a phase-slip area followed by reentrance of the superconducting state with a chain of moving vortices when the magnetic field further increases. The effect is promising for application design of novel superconductor switching-based detectors. The phonon energy spectra in the Si/SiO_2 multishell nanotubes are obtained numerically within the atomistic lattice dynamics model [3]. Redistribution of the vibrational spectra in multishell nanotubes leads to a decrease of the phonon group velocity and the thermal conductivity as compared to homogeneous Si nanowires. Phonon scattering on the Si/SiO_2 interfaces is another key factor of strong reduction of the thermal conductivity in these structures (down to 0.2 $Wm^{-1}K^{-1}$ at room temperature). Phonon thermal transport in the multishell nanotubes can be efficiently suppressed by a proper choice of nanotube geometrical parameters: lateral cross section, thickness and number of shells. Such nanotubes have prospective applications in modern electronics, in cases when low heat conduction is required. A variety of chemical micromotors, which have attracted great attention in the last decades due to their high efficiency and thrust force, enabling several applications in the fields of environmental remediation and biomedicine. Using statistically relevant experimental data for Pt conical tubes, a holistic theoretical model is developed for bubble-propelled tubular catalytic micromotors that includes capillary forces, bubble growth, and bubble expulsion. and provides deeper insights into their propulsion physics toward optimized geometries and experimental conditions. Switching between propulsion mechanisms is unveiled at certain values of the fuel concentration, medium viscosity and surface tension [4]. This work has been partly supported by the German Research Foundation (DFG) project #FO 956/6-1 and COST Action #CA16218 of the European Cooperation in Science and Technology.

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Artificial generation of representative single Li-ion electrode particle architectures from microscopy data

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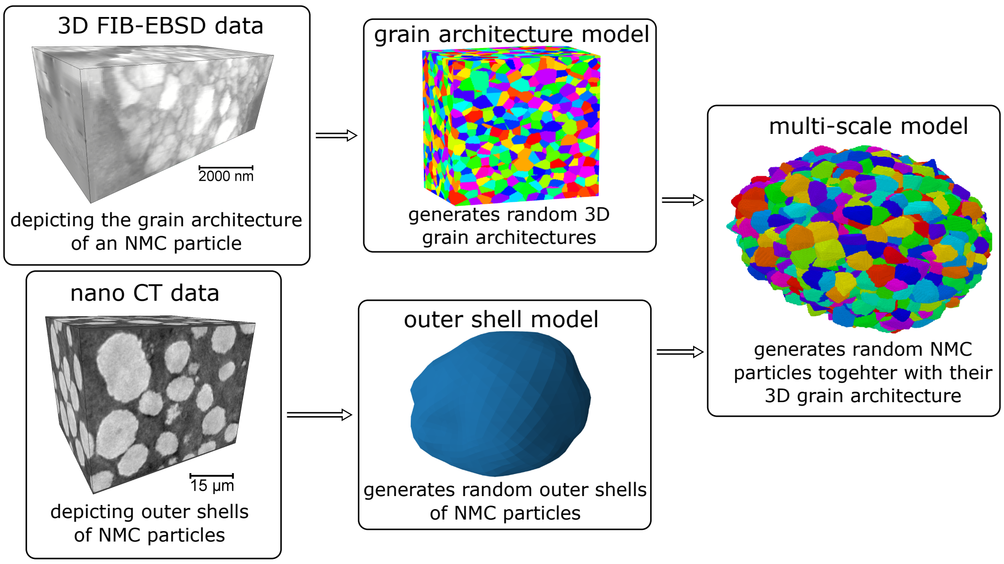
Accurately capturing both the shape and intergranular architecture of single lithium-ion electrode particles in 3D is essential for quantifying their influence on material properties, like, e.g., degradation mechanisms. Microscopy techniques like X-ray nano-computed tomography (CT) and focused ion beam (FIB) - electron backscatter diffraction (EBSD) can provide representative 3D image data of the particles' shape (outer shells) and their grain architecture, respectively. However, it can be quite time-consuming and costly to rely solely on imaging techniques for generating a sufficient amount of data for the analysis of structure-property relationships. In this talk, we present an alternative approach using stochastic geometry models. More precisely, using parametric stochastic geometry modeling, we leverage data from both nano-CT and FIB-EBSD to generate artificial but representative single particle architectures completed with grain morphological details. Therefore, a random Laguerre tessellation model is fitted to the grains depicted in FIB-EBSD data from which we can generate virtual, but statistically representative grain architectures. Analogously, we utilize nano-CT data depicting the outer shells of numerous particles to derive a random outer shell model, using mixtures of Gaussian random fields on the sphere. By combining both models, we can generate a large number of virtual particles with statistically representative shapes and grain morphologies. Moreover, by systematic variation of model parameters, even further virtual particles covering a broad range of structural scenarios can be generated. Then, such virtual particles can be used as input for numerical simulations, i.e., for virtual materials testing to study the influence of a material's geometry on its physical properties in the search for improved particle architectures of high energy- or power-density cells.



Modeling approach: FIB-EBSD data is used to calibrate a grain architecture model (top). From nano-CT data an outer shell model is fitted (bottom). By combining both models, we can generate representative particle architectures (right).

Universal relaxation equation for disordered systems

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Slower-than-exponential relaxations often occur in disordered systems and, lacking a microscopic theory, are commonly fit to the empirical Kohlrausch-Williams-Watts (KWW) stretched exponential or the Curie-von Schweidler (CvS) power-law algebraic decay. In this work an anomalous-diffusion limited, mixed second-order reaction equation is used to unify the above relaxation laws as different limits of the same overall behavior. Here, relaxation is modeled as a mixed second-order reaction between a concentration of reactants that undergo anomalous diffusion, and a concentration of stationary reactants. The resulting general expression is able to unify transients for a broad class of physical systems. The fit equation uses four parameters: the minority-to-majority reactant ratio $0 \leq m \leq 1$, the anomalous power-law exponent $0 \leq \beta \leq 1$, the characteristic relaxation time τ, and the relaxation amplitude f_δ. With the power-law $\beta < 1$, the $m = 0$ and $m = 1$ limits, respectively, of the minority reactant ratio are shown to correspond to the KWW and CvS expressions, respectively, and the intermediate m values represent a new class of previously unrecognized relaxation functions. A fitting algorithm is introduced that identifies confidence intervals for each of the four experimental parameters. Three parameters are observed to have quadratic variance around the best fit values, allowing a Wronskian formulation to yield confidence intervals. The mixing parameter m, on the other hand, has a variance which is non-quadratic, making the confidence interval highly asymmetric. This analysis unifies two empirical laws that were previously considered distinct and provides new physical insight to prominent previously published experimental transients. Prominent examples of disordered systems from biomechanics, energy storage, and dielectric relaxation show excellent fits to the proposed relaxation expression.

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An interface formulation for the Poisson equation in the presence of a semiconducting single-layer material

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Single-layer materials such as graphene are promising for various applications, in particular to optimize electronic devices. For instance, 2D semiconductor materials allow to design transistors with channel thickness on the atomic scale. In this context, we are interested in performing self-consistent computations to study the transport of electrons in devices such as a graphene field-effect transistor. In this work, we concentrate on the numerical resolution of the Poisson equation proposing to model the single-layer structure as an interface. More precisely, we consider a device with an active zone made of a single-layer material sandwiched between two thick insulator regions (oxide). The associated Poisson equation is characterized by both a surface particle density and an out-of-plane dielectric permittivity exhibited in a region of effective dielectric thickness surrounding the single-layer material, as emphasized in [1]. To avoid mesh refinements, we derive an interface problem based on the natural domain decomposition suggested by the physical device, averaging the potential across the dielectric effective region. It is inspired by [2] where this approach is used to model fractures in porous media. We obtain two Laplace equations in the oxide subdomains coupled with an effective Poisson equation on the interface with an extra source term that represents the contribution of the surrounding environment to the channel material. After a presentation of the interface model, we discuss its discretization with a finite element method, using the so-called three-fields formulation, where the weak continuity between the oxide subdomains and the interface is imposed by means of Lagrange multipliers following [3]. Interestingly, the interface discretization does not need to match with the one of the subdomains and we take advantage of this flexibility in the numerical experiments we are performing to illustrate the approach.

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Mapping conductivity with electrical impedance tomography

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In semiconductor fabrication, the conductivity distribution provides essential information about inhomogeneities, such as variations in deposition layer thickness, dopant concentration gradients, and local defects that affect electronic device performance. Electrical impedance tomography (EIT) is a fast characterization method whereby applied current and voltage measurements on the periphery of a semiconductor map its internal conductivity [1]. In this so-called inverse problem, a model space is created to span all possible conductivity distributions while a data space spans all possible boundary measurements, and the mapping problem is equivalent to transforming a vector from data space to model space. Present day EIT methods are constrained by resolution limitations of their contact configurations, as well as by the construction of the inverse mapping problem. But by increasing the number of contacts one can expand the data space for significant improvements in resolution and accuracy. And by defining a reduced model space of orthonormal basis functions, computation speeds can be significantly enhanced.

In this work, we include more contacts than standard methods to expand the data space and fewer basis functions to reduce the model space. In standard EIT, the Sheffield measurement protocol is used to define the data space, whereby two adjacent current contacts are paired with two adjacent voltage contacts which are themselves cyclically permuted around the sample. However, the Sheffield protocol produces a data space whose measurements contain a significant amount of redundant information, and our method uses a Monte Carlo search of the expanded data space to identify optimal measurement configurations for signal-to-noise improvement. Simultaneously, we reduce the model space by defining a smaller set of continuous orthonormal basis functions over the volume to eliminate the underdetermined nature of the EIT problem. In standard EIT, a finite element mesh forms the model space thereby requiring regularization to converge to a solution. This reduced set of basis functions, on the other hand, results in a well-defined problem while minimizing the computational time.

With the above improvements to the data space and model space, the Jacobian relating the two can be deconstructed using singular value decomposition (SVD). The comparison of vector properties and singular values provides metrics to select measurement protocols that provide new information with high signal to noise. The method above is observed to enhance the signal to noise ratio by over 600% compared to the standard EIT method employing the Sheffield protocol for the same resolution and same number of measurements. Phantom models representing different inhomogeneity scenarios will be presented along with the improvements in mapping resolution and accuracy.

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Simulation of graphene field effect transistors by directly solving the semiclassical Boltzmann equation

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In the last years an increasing interest has been devoted to graphene field effect transistors (GFETs) as potential candidates for high-speed analog electronics, where transistor current gain is more important than ratio current ON/current OFF. Several types of GFETs have been considered in the literature [1]: top-gated graphene based transistors, obtained synthesizing graphene on silicon dioxide wafer, and double gate GFETs. The current-voltage curves present a behaviour different from that of devices made of semi-conductors, like Si or GaAs, because of the zero gap in monolayer graphene. The current is no longer a monotone function of the gate voltage but there exists an inversion gate voltage [1]. As a consequence, there is a certain degree of uncertainty in the determination of the current-off regime which requires a rather well tuning of the gate-source voltage.

Lately, some attempts to simulate Graphene Field Effects transistors (GFETs) have been performed (see for example [2, 3, 4, 5]) with simplified models like drift-diffusion. The latter contains several functions to be fitted by experimental data such as mobilities and generation-recombination terms. Often adaptations of the expressions used for standard semiconductors are adopted and a reduced 1D Poisson equation is coupled to the equations for the charge transport. It is therefore warranted to have a confirmation of the obtained results by a direct solution of the semiclassical Boltzmann equation for charge transport in graphene. Here a discontinuous Galerkin method, already developed in ([6, 7]), is used to simulate some challenging geometry for future GFETs by numerically solving the Boltzamnn equations for electrons and holes in graphene.

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Towards multiscale modeling of porous electrodes: Connecting the meso- to the macroscopic scale

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Redox flow batteries are an emerging technology for grid energy storage applications thanks to their promising properties, such as long cycle life and safety. Porous electrodes are a core component of flow batteries that facilitate the electron transfer between the liquid electrolyte and solid electrode by providing high specific surface areas. We are interested in macroscopic homogenized descriptions of the coupled processes of mass transport and heterogeneous reactions in porous electrodes, allowing for efficient simulations over macroscopic domains. The effective macroscopic properties, such as the dispersion tensor or the effective reaction rate depend on the pore-scale properties of the porous electrode, such as the morphology and surface properties of the electrode.

Here we consider periodic porous media with simplified geometries, allowing the pore-scale transport problem to be formulated over periodic unit cells.. The electrolyte is modelled as a dilute, multicomponent mixture occupying the pore-space Ω_β. Assuming an incompressible Newtonian fluid, the steady-state pore-scale flow can be described by

$$\mathrm{Re}\left((\mathbf{v}\cdot\nabla)\mathbf{v}\right) = \Delta\mathbf{v} - \nabla p, \quad \mathbf{x}\in\Omega_\beta \tag{1}$$

and the dimensionless mass transport problem of species α is given by

$$\begin{aligned} \mathrm{Pe}(\mathbf{v}\cdot\nabla c_\alpha) &= \Delta c_\alpha, \quad \mathbf{x}\in\Omega_\beta, \\ -\mathbf{n}\cdot\nabla c_\alpha &= \mathrm{Ki}\cdot r_\alpha, \quad \mathbf{x}\in A_{\beta\sigma}, \end{aligned} \tag{2}$$

where $A_{\beta\sigma}$ is the interfacial area, Pe is the Peclet number and Ki denotes a kinetic number. The source term r_α accounts for interfacial mass fluxes resulting from electrochemical reactions or adsorption of species at the electrode surface.

We use the method of volume averaging [5] for up-scaling the pore-scale problem to derive effective macroscopic descriptions and study their dependence on the pore-scale properties.

In future work we intend to consider the problem of up-scaling of more complex electrochemical interface descriptions based on the framework of non-equilibrium thermodynamics [2, 3, 1], which allow the incorporation of additional interface properties that could be provided by lower-scale descriptions, such as kinetic Monte Carlo simulations.

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Reconsidering porous electrode theory for Lithium-Ion batteries: Rigorous upscaling of localized fluctuations as a consequence of locally anisotropic microstructures

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A class of numerical models known under different names (Newman model, DFN, P2D, porous electrode theory)[1,2] has been widely used in the modeling of electrochemical systems with porous electrodes, in particular to predict the behaviour of lithium-ion cells. The models treat the composite materials as effective homogeneous media. Detailed phenomena on the pore and particle scale have to be treated within microstructure-resolving models which distinguish the transport and reaction processes on the scale of the individual phases[3].
The DFN-type models are relatively inexpensive computationally and intuitive, and thus help get simulation results and their interpretations faster. The problem of their relation to the microscopic transport-reaction equations was addressed in the literature by applying formal volume averaging rules to the latter; the mathematical correctness of the volume averaging was investigated with the help of the asymptotic homogenization ansatz for partial differential equations (PDEs)[4,5]. Due to the lack of strict time scale separation in lithium-ion cells some phenomena can not however be mathematically rigorously homogenized. Even in the simplest basic DFN model the lithium mass transport in the active material does not satisfy the necessary homogenization criteria and is treated heuristically as transport in some “effective” spherical particle per volume element of the homogenized models.
One important deviation between the DFN-based and the microstructure-resolving simulations has been found in the form of spatially localized fluctuations of the overpotential on the active material interface. In this talk we will present a mathematical analysis that demonstrates that these fluctuations are closely related to the homogenization application bottlenecks in the DFN derivation, which cannot be accounted for by the basic DFN assumptions. The analysis strongly relies on the theory of PDEs and on the asymptotic properties of their solutions. The properties of the fluctuation dynamics are derived in a semi-analytical manner, an agreement with the numerical results is demonstrated [6].
As a next step, building on this analysis, a new reduced-order lithium-ion cell model is proposed that can be considered as a DFN modification and that can reproduce the local fluctuations at the same time [7]. In conclusion, we will comment on the possible role of our findings in the future applications and cover the following questions: when and why the original DFN model’s predictions agree well with the microscopic simulations, despite the lack of mathematical rigour, and when not; how our theory can assist in developing mathematically rigorous upscaled DFN-like models to include more phenomena (like side reaction, binder influence, mechanics, anisotropic transport), both in lithium-ion context and generally for similar transport-reaction systems.

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Generalized Nernst-Planck-Poisson model of solid oxide YSZ|LSM|O_2 electrode interface

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A nanoscale-continuum generalized Nernst-Planck-Poisson model describing transport of oxide ions O^{2-} in the face-centered cubic yttria-stabilized zirconia (YSZ) was formulated in the framework of non- equilibrium thermodynamics [1] and investigated in [6]. The model was resolved numerically in the 1D half cell geometry and it accounted for the experimentally observed capacitance of a blocking YSZ|Au|O_2 electrode [5]. The nanoscale-continuum model of bulk YSZ was further endowed with triple phase boundary (TPB) reaction mechanism of lanthanum strontium manganite (LSM), oxygen; i.e. YSZ(s)|LSM(s)|O_2(g), electrode. The generalized mass action law kinetics [3] was employed to model the TPB reaction mechanism which included adsorption of the bulk O^2- ions, electron-transfer reaction, adsorption of gaseous oxygen and drift-diffusional equilibrium of the LSM electrons. We found that the scaling of the reactions rates w.r.t. mass densities was necessary to qualitatively match the dependencies on the O_2 partial pressure observed in the experiments. Moreover, the robust formulation of the reaction kinetics [4] allowed to show that assumption of the shared TPB lattice sites unlike the separate sites model rendered the oxygen adsorption in accordance with the measurements in the low frequency region of the impedance spectra. Finally, the drift-diffusion equilibrium of electrons introduced the jump of the electrochemical potential of electrons between the surface and the LSM bulk in to the chemical affinity. Since the jump which was realized outside the simulation domain, it was assumed to be proportional to the difference of the electrostatic potential due to the space-charge layer in the YSZ. This resulted into a non-local boundary condition and was instrumental in the fitting of cyclic voltammetry measurements. The fitted dataset spans temperatures from 700°C to 850°C. The numerical solution of the coupled drift-diffusion system with the non-local boundary condition was provided by the finite volume solve based one the Voronoi cells [2].

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Quantifying polaronic effects on the scattering and mobility of charge carriers in lead-halide perovskites

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The formation of polarons due to the interaction between charge carriers and lattice ions has been proposed to have wide-ranging effects on charge carrier dynamics in lead–halide perovskites. The hypothesis underlying many of those proposals is that charge carriers are 'protected' from scattering by their incorporation into large polarons. Following the approach of Kadanoff for scattering due to polar optical phonons, we derive expressions for the rates of scattering of polarons by acoustic phonons and ionised impurities, and compute the energy and angular dependent rates for electrons and holes in $MAPbI_3$, $MAPbBr_3$ and $CsPbI_3$. We then use the ensemble Monte Carlo method to compute polaron distribution functions that satisfy a Boltzmann transport equation incorporating the same three scattering mechanisms, from which we extract mobilities for temperatures in the range 50–500 K. A comparison of the results with those of analogous calculations for bare band carriers indicates that polaronic effects on the scattering and mobilities of charge carriers in lead–halide perovskites are more limited than has been suggested in some parts of the recent literature.

Poster

Modeling and simulation of charge transport in perovskite solar cells

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Perovskite solar cells have become one of the fastest growing photovoltaic technologies within the last few years. However, their commercialization is still in its early stages. Furthermore, which exact physical operation mechanisms play a fundamental role within such devices is not fully understood yet, but it is shown in experiments that besides the movement of electric carriers, ion movement within the perovskite needs to be taken into account. For this reason it is paramount to understand the electronic-ionic charge transport in perovskites better via improved modelling and simulation.

In our contribution, we present a new drift-diffusion model for the charge transport in perovskite solar cells based on fundamental principles of thermodynamics and statistical physics. Unlike other models in the literature, our model is formulated in terms of quasi Fermi potentials instead of densities. This allows to easily include nonlinear diffusion (based on Fermi-Dirac, Gauss-Fermi or Blakemore statistics for example) as well as limit the ion depletion (via the Fermi-Dirac integral of order -1). Finally, we present a finite volume based solver and corresponding simulations to underline the importance of our modelling approach.

Theoretical and experimental study of capture time effects on the series resistance of quantum-well diode lasers

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Series resistance is one of the main factors limiting conversion efficiency in GaAs based broad area lasers, especially at high bias. Experimental results for GaAs-based single quantum well structures differing in the Al content of the optical confinement and cladding layers show an unexpected increase of the series resistance with decreasing heat sink temperature. We developed a theoretical model combining a one dimensional drift-diffusion model (solved under the condition of local charge neutrality, as appropriate to diode lasers), to describe the current flow outside of the quantum well, with a model describing the quantum well capture-escape process and a laser model. We show that the finite capture time is responsible for an additional contribution to the measured series resistance and that the simulation results reproduce well the experimental findings.

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Homogenization of a nonlinear drift-diffusion system for multiple charged species in a porous medium

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We consider a nonlinear drift-diffusion system for multiple charged species in a porous medium in 2D and 3D with periodic microstructure. The system consists of the transport equation for the concentration of the species and the Poisson equation for the electric potential. The diffusion terms depend nonlinearly on the concentrations. We consider zero flux boundary conditions for the species concentrations and non-homogeneous Neumann boundary condition for the electric potential. The aim is the rigorous derivation of an effective (homogenized) model in the limit when the scale parameter ϵ tends to zero. This is based on uniform a priori estimates for the solutions of the microscopic model. The crucial result is the uniform L^∞-estimate for the concentration in space and time. This result is based on a maximum principle, and exploits the fact that there exists a nonnegative free energy functional which is monotonically decreasing along the solutions of the system. By using weak and strong two-scale convergence properties of the microscopic solutions, effective models are derived in the limit $\epsilon \to 0$ for different scalings of the microscopic model.

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Quantum transport models based on Tsallis statistics

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In early 2000's, Degond and Ringhofer developed a comprehensive approach for the derivation of quantum hydrodynamic models from first principles [2, 3]. Starting from the collisional quantum Liouville equation they derive a whole hierarchy of moment models, where the moment model is closed by the constrained entropy minimization principle. The entropy is von Neumann (quantum Boltzmann) entropy and constraints are moments given in terms of local quantities (density, energy, etc.). As a consequence of the quantum nature, the resulting models are nonlocal. Our work extends this approach to the constrained minimization of quantum Tsallis entropies in the context of Tsallis statistics [1], where the moments are calculated by nonlinear means. In particular we derive the corresponding drift-diffusion and energy transport models. Furthermore, thanks to expansions in terms of the scaled Planck constant, analogously to [3], we also derive localized models given in terms of fourth-order evolution equations.

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A hydrodynamical model for charge transport in graphene nanoribbons

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Since its first isolation as a single layer of carbon atoms graphene has appeared as one of the most promising material for the new era of electronic devices [1]. It presents high electronic mobility at room temperature and high current density, nevertheless the absence of a band gap in its band structure does not make it a good solution for controlling the current flux. For solving the drawback the pristine graphene can be substituted by graphene nano-ribbons, narrow strips of graphene that exhibit a band gap depending on the width of the strip [2, 3].
Here we propose a hydrodynamical model for the charge transport in graphene nano-ribbons that takes into account the gap in band structure and the electron scattering with the lattice structure and with the edge [4].

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Two entropic finite volume schemes for a Nernst-Planck-Poisson system with ion volume constraints

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In this poster, we consider a drift-diffusion system with cross-coupling through the chemical potentials comprising a model for the motion of finite size ions in liquid electrolytes. The drift term is due to the self-consistent electric field maintained by the ions and described by a Poisson equation. This poster summarizes the results obtained in the eponymous preprint [5], with additions from the simpler model studied in [1], and motivated by the model presended in [4] from [2, 3].

The poster revolves around three columns. The first column is dedicated to the origin of the model, the different formulation of the fluxes and a proposition of two schemes. The second column concerns an existence result of the numerical schemes, emphasis could be made on the coercivity formulation or the jump-propagation approach to derive bounds from this coercivity using a simple 4-cells toy mesh example. The last column provides details on how the entropy-dissipation distance relates to the euclidean metric, and thus a compactness estimate. Convergence properties -some of them assuming non-degenerate solutions- are provided.

Finally as a virtual footer, numerical experiments show the behavior of these schemes.

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Toward charge transport in bent nanowires

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Nanowires are of great interest for their potential applications in optoelectronics, solar cells, and sensors, to name a few. In this talk, we study the elastic and electric properties of bent nanowires. We consider nanowires consisting of asymmetrically lattice-mismatched materials, which by construction induces strain across the heterostructure's interface. This inherent strain is sufficient to bend the nanowires up to 180 degrees, as shown in experiments. This mechanical property opens new possibilities in the design and use of bent nano heterostructures.

We propose a non-linear model that captures the finite-strain elastic deformation in the material frame of reference. The continuous mechanics model is combined with the polarization potential equation to study the piezoelectric behavior of the mechanical deformations. Using the finite element method, we calculate the strain field and polarization potential. With these calculations, we can derive the band energy profiles on a cross-section of the nanowire. Finally, we aim to study the charge carrier transport in bent nanowires based on a drift-diffusion van Roosbroeck type of model.

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Stochastic simulation of continuous time random walks: Asymptotic rate coefficients in diffusion-limited relaxations

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In amorphous semiconductors, polymers, and composites, relaxation rates are known to relax according to a slower-than-exponential decay rate which can be explained through the microscopic theory of continuous time random walks (CTRW) [1]. However, simulations of such systems are currently restricted to analytical wait-time distribution functions, and it is necessary to develop a computational CTRW formalism that can handle more generic wait time distributions that represent real physical systems. Here, a reaction limited by standard diffusion is simulated stochastically following the wait-time distribution formalism from CTRW theory. A step-by-step simulation of the diffusive random walk reveals the fraction of surviving reactants $P(t)$ as a function of time, and the time-dependent unimolecular reaction rate coefficient $K(t)$. The accuracy of the simulation is confirmed by comparing to analytical expressions from the continuum limit and to the asymptotic solution from Fickian diffusion. A transient feature observed at the start of the reaction is shown to be related to the initial separation of the walkers from the reaction sites and can be used to calibrate this separation distance. Shot noise is shown to be the dominant noise source in the simulation, and its amplitude is calibrated. Within the uncertainty of the noise, the simulated reaction rate coefficient is within 1 % of the known analytical value using 10^7 walkers. The stochastic simulations presented here can be generalized to model anomalous diffusion-limited reactions in regimes where the governing wait-time distributions yield no analytical solution.

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Study of voltage cycling conditions on Pt oxidation and dissolution in polymer electrolyte fuel cells

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Our study is devoted to the electrochemical behavior of platinum (Pt) catalyst layer (CL) in a polymer electrolyte fuel cell membrane (PEM) at various operating conditions and at different voltage (electric potential difference versus a reference of 0 V) cycling applied in accelerated stress tests. The degradation of platinum is described in a spatially one-dimensional model between CL-gas diffusion layer and CL-PEM interfaces. The Holby's model for unknown Pt ion concentration, Pt particle diameter, and PtO coverage ratio is considered with respect to two electro-chemical reactions: (i) the Pt ion dissolution, and (ii) the Pt oxide coverage of catalyst, with reaction rates presented by Butler–Volmer functions of exponential type.

The theoretical study of the underlying diffusion system with the nonlinear reactions is presented by analytical methods and gives explicit solutions through a first integral of the ODE system when omitting the diffusion. Numerical tests are obtained using a second order implicit-explicit IMEX scheme. The computer simulation shows a linear decay of the mean Pt mass loss ratio. The lifetime of the catalyst depends on the voltage profile and the upper potential level. By this, the degradation phenomenon would be impossible without the diffusion.

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Modeling photodecay as mixed second-order relaxation in phosphorescent metal complexes

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Several metal complex compounds are interesting as triplet emitters and have application as dopants in optoelectronic devices, such as organic light-emmitting diodes (OLEDS) and light-emitting electrochemical cells (LEECs). A series of tridentate $\mathrm{Pt^{II}}$ complexes with tunable emission wavelength was designed, synthesized and recently characterized [1]. However, proper understanding of the phosphorescent process is required for optimizing performance, and to date the phosphorescent decay has only been fit with empirical double-exponential fits to yield an approximate average lifetime τ. Such heuristic bi-exponentials require *four* fit parameters (two amplitudes and two decay times) without an obvious microscopic justification for these *two* time scales.

Here, a generalized differential equation is used to describe a mixed 2^{nd} order relaxation process which requires only *three* fit parameters and *one* time scale, as follows:

$$f'(t) = -\frac{1}{\tau}\left[(1-m)f(t)m\frac{f^2(t)}{f_\Delta}\right], \tag{1}$$

where the initial ratio of minority-to-majority reactant is m, which also describes the weighting factors for first-order $(1-m)$ and second order m relaxation terms in Eq. (1), respectively. For example, $m = 0$ corresponds to a pure uni-molecular reaction, $m = 1$ corresponds to a pure bi-molecular reaction and $0 < m < 1$ indicates mixed behaviour. By integrating this differential equation, we solve an expression for $f(t)$, where molecularity m, time constant τ, and decay amplitude f_Δ can be fitted to the relaxation data.

We implemented a fitting algorithm to this function with a simulated annealing Monte Carlo algorithm which automatically identifies confidence intervals for each parameter. This algorithm was used to analyze the luminescence decay of $\mathrm{Pt^{II}}$ complex triplet emitters at different temperatures (77 K and room temperature), ambient gases (air and Ar) and different excitation powers. The m, τ, and f_Δ are observed to fit the experimental relaxation curve with high confidence, offering a microscopic model for the relaxation. The resulting fits are as good as, or better than, the bi-exponential fits with one less fit parameter, strongly suggesting that we have identified the proper underlying origin of this behavior. In the low-temperature Ar-ambient data, $m = 0.13$ was observed with error less than 0.01, indicating that a considerable component of second order relaxation was present. We report data on power dependent experiments to investigate the possible physical nature of the majority and minority components in the mixed second order reaction described by Eq. (1).

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Long-time behaviour of a hybrid finite volume scheme for the drift-diffusion model with magnetic field

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In this talk, we introduce a Hybrid Finite Volume (HFV) scheme to discretise the isothermal drift-diffusion system for semiconductors.
The HFV schemes [1] - generalisations of classical two-point finite volume schemes - are devised to handle general polygonal/polyhedral meshes, alongside with anisotropic diffusion tensors. Especially, the scheme introduced here can be used in situations where the semiconductor is immersed in a magnetic field [2].
The scheme is based on the nonlinear discretisation introduced in [3]. Its analysis relies on the preservation of a discrete entropy structure, which mimics the continuous behaviour of the system. Using these properties, we show the existence of solutions to the scheme, and ensure the positivity of the carrier densities. Moreover, we establish the convergence of the discrete solution towards a discrete thermal equilibrium as time tends to infinity.
We will give some numerical illustration of our theoretical results.

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Simulation of graphene field effect transistors

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Metal Oxide Semiconductor Field Effect Transistor (MOSFET) is the backbone of the modern integrated circuits. In the case the active area is made of traditional semiconductor materials such as, for example, silicon or gallium arsenide, a lot of analysis and simulations have been performed in order to optimize the design.
Lately, a great attention has been devoted to graphene [1] on account of its peculiar features and, in particular, from the point of view of nano-electronics, for the high electrical conductivity. It is highly tempting to try to replace the traditional semiconductors with graphene in the active area of electron devices like the MOSFETs (cfr. [2, 3, 4, 5]).
Here, graphene field effect transistors, where the active area is made of monolayer large-area graphene, are simulated including a full 2D Poisson equation and a drift-diffusion model with mobilities deduced by a direct numerical solution of the semiclassical Boltzmann equations for charge transport by a suitable discontinuous Galerkin approach (cfr. [6, 7, 8]).
The critical issue in a graphene field effect transistor is the difficulty of fixing the off state which requires an accurate calibration of the gate voltages. We propose and simulate a graphene field effect transistor structure which has well-behaved characteristic curves similar to those of conventional (with gap) semiconductor materials. The introduced device has a clear off region and can be the prototype of devices suited for post-silicon nanoscale electron technology. We compare numerical results with the simulation of standard GFET structures.

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Derivation of an effective bulk-surface thermistor model for OLEDs

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We derive an effective electrothermal model for a thin-film OLED from a recently introduced fully three-dimensional $p(x)$-Laplace thermistor model describing the heat and current flow through the thin OLED [1, 2]. The OLED is mounted on a glass substrate and consists of several thin layers that scale differently with respect to the multiscale parameter $\epsilon > 0$, which is the ratio between the total thickness and the lateral extent of the OLED. Assuming physically motivated scalings in the electrical flux functions, uniform a priori bounds are derived for the solutions of the three-dimensional system which facilitates the extraction of converging subsequences with limits that are identified as solutions of a dimension reduced system [3]. In the latter, the effective current-flow equation is given by two semilinear equations in the two-dimensional cross-sections of the electrodes and algebraic equations for the continuity of the electrical fluxes through the organic layers. The effective heat equation is formulated only in the glass substrate with Joule heat term on the part of the boundary where the OLED is mounted.

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Improving efficiency of a numerical solver for microscopic Li-Ion battery simulation including SEI degradation

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With the ongoing electrification of the transport sector as well as the shift of the energy sector to renewable energies, Lithium-ion batteries have gained significant attention as electrical power sources and storage devices, in particular due to their high energy density. To further optimize cell design and cell life time, it is crucial to understand and minimize degradation processes inside the battery. The overall designing process can be supported by developing suitable mathematical models and solvers.

In this talk we focus on a numerical solver for a microscopic electrochemical model for Lithium-ion batteries [1] including a model for the Solid Electrolyte Interphase (SEI) [2], one of the major degradation processes leading to capacity fade of the battery. In the isothermal setting of the original model [1] we solve for two quantities, the lithium ion concentration c and the electro-(chemical) potential ϕ. This results in a coupled system of parabolic and elliptic PDEs of the form

$$\begin{pmatrix} \partial_t c \\ 0 \end{pmatrix} = \begin{pmatrix} G^c(c,\phi) \\ G^\phi(c,\phi) \end{pmatrix}. \tag{1}$$

Introducing the SEI model, the Butler Volmer reaction kinetics at the anode interface are mostly replaced by an expression describing the total current density i_{tot} flowing across the interface, which can no longer be directly eliminated, as it is given by an implicit nonlinear equation. The SEI layer itself is not spatially resolved, but the local thickness of the layer is stored in corresponding variables L. Adding the set of nonlinear algebraic constraints for the total current density and a set of ODEs capturing the SEI layer growth, we obtain a system

$$\begin{pmatrix} \partial_t c \\ 0 \\ 0 \\ \partial_t L \end{pmatrix} = \begin{pmatrix} G^c(c,\phi,i_{\text{tot}},L) \\ G^\phi(c,\phi,i_{\text{tot}}) \\ G^{i_{\text{tot}}}(c,\phi,i_{\text{tot}},L) \\ G^L(\phi,i_{\text{tot}},L) \end{pmatrix}, \tag{2}$$

containing additional types of equations and physical processes compared to (1). Using a fully implicit monolithic solver, we notice a significant performance degradation comparing simulations with and without SEI.

Thus, we propose an alternative solver combining operator splitting and preconditioning of the resulting linear systems in order to separate the newly introduced equations step by step. The obtained linear systems exhibit a similar structure compared to the ones of the basic battery model. First numerical results suggest that the new solver can improve the performance for SEI simulations, yielding performance results in line with the ones observed for non SEI simulations.

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Efficient parallel simulation of contact problems for chemo-mechanically modeled battery active particles

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Lithium ion batteries (LIBs) are one of the key technologies in terms of future energy storage to meet the challenges posed by climate change. During battery operation, mechanical degradation is a crucial aging mechanism of LIBs. An inhomogeneous lithium concentration profile during charging and discharging can lead to large mechanical stresses, which can finally induce particle fracture. This behavior is particularly crucial for phase separating electrode materials, where large concentration gradients evolve. However, the increase in mechanical stress must not be neglected if the swelling of the particle is restricted to a limited surrounding area, e.g., due to the material structure or the current collector.

The used particle model couples lithium diffusion, large deformations and phase separation based on a thermodynamically consistent transport theory, see [2]. A solid solution model describes the diffusion and a finite strain theory models the deformations. A phase-field model is used to deal with the phase separation. In the end, a common free energy density connects all different phenomena. To incorporate the restricted swelling, the model is extended by an obstacle contact, compare [4].

The resulting Cahn–Hilliard-type phase-field model approach is computationally expensive to solve. To overcome the current limited applications, the highly efficient adaptive numerical solution algorithm in space and time from [1, 3] is used. The particle contact is treated with the concept of the primal-dual active set algorithm. Additionally, a parallel distributed memory implementation leads to a larger range of electrode particle shapes examined. Finally, physical and numerical aspects of the model and the solver for an electrode particle of lithium iron phosphate are investigated and discussed. The influence and interrelation of phase separation and mechanics as well as different shaped obstacles are pointed out. The efficiency and the large computational savings due to the adaptive solution algorithm as well as the parallel distributed memory implementation allow the further analysis of computationally demanding parameter regimes and also three-dimensional particle geometries.

Keywords: Lithium ion battery, phase-field model, mechanics, contact problem, numerical simulation, finite element method.

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Landscape approach to quantum transport through a disordered or random potential

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Accounting for the effects of disorder in semiconductor devices, especially carrier localization, is a real challenge as it requires to compute quantum effects at the nanoscale in devices where the overall dimensions are typically of the order of 100 nm or more. The localization landscape theory, introduced first in 2012 and later applied to nitride-based alloys, enables us to account for such effects. In this theory, an effective potential (the reciprocal of the landscape) predicts the regions of localization of the eigenstates, their corresponding energies, and more globally the local density of states without having to explicitly solve the Schrodinger equation. We present here a model for electronic transport based on that theory. We detail the mathematical structure of this model which incorporates hopping between the localized states, and then analyze numerical simulations of transport in disordered semiconductor alloys.

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