

# AMaSiS 2024 Schedule

## September 11 (Wednesday)

08:15 - 9:00 | **Registration**  
*Leibniz Headquarters*

09:00 - 9:20 | **Opening**  
*Lecture Hall "Hannover"*

### Numerical Methods A

09:20 - 9:55 | **Mathieu Luisier**  
Theory and algorithms for extreme-scale nano-device simulations

09:55 - 10:30 | **Christoph Jungemann**  
Simulation of nanowire NMOSFETs based on the Boltzmann equation with Godunov-type stabilization

10:30 - 11:00 | **Coffee Break**

### Drift-Diffusion A

11:00 - 11:35 | **Ansgar Jünger**  
Memristor drift-diffusion systems for brain-inspired neuromorphic computing

11:35 - 12:10 | **Dilara Abdel**  
Modeling and simulation of vacancy-assisted charge transport in innovative semiconductor devices

12:10 - 12:30 | **Claire Chainais-Hillairet**  
A drift-diffusion-Poisson system on a moving domain: Some theoretical and numerical results

12:30 - 14:00 | **Lunch Break**

### UV Light and Alloy Disorder

14:00 - 14:35 | **Bernd Witzigmann**  
Numerical simulation of carrier injection efficiency in ultraviolet light-emitting diodes

14:35 - 15:10 | **Marcel Filoche**  
Accounting for nanoscale disorder in semiconductors with the localization landscape theory

15:10 - 15:30 | **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**

### 2D Materials

16:00 - 16:35 | **William Vandenberghe**  
Dielectric, magnetic, and contact properties of two-dimensional materials

16:35 - 16:55 | **Vittorio Romano**  
Optimal control of a semiclassical Boltzmann equation for charge transport in graphene

16:55 - 17:15 | **Poster Pitching**  
*Lecture Hall "Hannover"*

### Poster Session

17:30 - 19:00 | **Poster Session**  
*Atrium*

## September 12 (Thursday)

### Numerical Methods B

09:00 - 9:35 | **Zlatan Akšamija**  
Numerical simulation of charge transport in doped conjugated polymers for organic electronics

09:35 - 10:10 | **Evelyne Knapp**  
Parameter extraction for large-area semiconductor devices

10:10 - 10:30 | **Clément Jourdana**  
Uniform accuracy towards numerical approximations for a Bloch model

10:30 - 11:00 | **Coffee Break**

### Spin-Qubit Devices

11:00 - 11:35 | **Chris Anderson**  
Computational aspects of simulations of Si based quantum devices

11:35 - 12:10 | **Félix Beaudoin**  
Technology computer-aided design of spin qubits in semiconductors

12:10 - 12:30 | **Abel Thayil**  
Optimization of valley splitting in Si/SiGe spin qubits

12:30 - 14:00 | **Lunch Break**

### Quantum Transport

14:00 - 14:35 | **Alberto Tibaldi**  
Small-signal and noise analysis of nanodevices based on a quantum transport model

14:35 - 15:10 | **Cristina Medina Bailón**  
Quantum corrections in EMC: From multisubband to quantum transport

15:10 - 15:30 | **Vito Dario Camiola**  
Quantum MEP hydrodynamical model for charge transport

15:30 - 15:50 | **Orazio Muscato**  
Wigner-Boltzmann Monte Carlo simulation of thermionic cooling devices based on resonant-tunneling AlGaAs/GaAs heterostructure

15:50 - 16:20 | **Coffee Break**

### Photovoltaics

16:20 - 16:55 | **Nicola Courtier**  
Continuum-level modelling and simulation of electronic-ionic interactions in perovskite solar cells

16:55 - 17:30 | **Urs Aeberhard**  
Simulation of advanced solar cells – beyond the limitations of the drift-diffusion picture

from 18:30 | **Workshop Dinner**  
*Restaurant Tapas y Más*  
*Neue Grünstraße 17-18, 10179 Berlin*

## September 13 (Friday)

### Drift-Diffusion B

09:00 - 9:35 | **Giuseppe Ali**  
On the mathematical modelling of semiconductor laser diodes

09:35 - 10:10 | **Maxime Herda**  
Numerical analysis of a finite volume scheme for charge transport in perovskite solar cells

10:10 - 10:30 | **Julien Moatti**  
High-efficiency and reliable schemes for drift-diffusion systems

10:30 - 11:00 | **Coffee Break**

### Materials Modeling

11:00 - 11:35 | **Costanza Lucia Manganeli**  
Strain engineering in CMOS micro-electronics. How to tailor.

11:35 - 12:10 | **Nella Rotundo**  
Perturbation approach and existence and uniqueness analysis for the forward lateral photovoltage scanning problem

12:10 - 12:30 | **Balázs Bámer**  
Cluster-based multivariate spline model for dopant activation in SiC



# AMaSiS 2024 Tutorials

September 10 (Tuesday)

08:15 – 9:10 | **Registration**  
Humboldt University, Hausvogteiplatz 5-7

09:10 – 9:15 | **Welcome**  
Lecture Hall 007

## Tutorial 1

09:15 – 10:45 | **Jesús Carrete Montaña**  
Thermal conductivity calculations with the Boltzmann transport equation and machine-learning force fields

10:45 – 11:15 | **Coffee Break**

11:15 – 12:45 | **Jesús Carrete Montaña**  
*continuation*

12:45 – 14:00 | **Lunch Break**

## Tutorial 2

14:00 – 15:30 | **Michele Simoncelli**  
From density-functional theory to dual wave-particle transport and device simulation

15:30 – 16:00 | **Coffee Break**

16:00 – 17:30 | **Michele Simoncelli**  
*continuation*

# AMaSiS 2024 List of Posters

P1 | **Lasse Ermoneit** (WIAS Berlin, Germany)

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

P2 | **Annegret Glitzky** (WIAS Berlin, Germany)

Electrothermal models for organic semiconductor devices

P3 | **Yiannis Hadjimichael** (WIAS Berlin, Germany)

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

P4 | **Hendrik Leenders** (RWTH Aachen, Germany)

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

P5 | **Tuan Tung Nguyen** (Technische Universität Wien, Austria)

Drift-diffusion for memristors coupled to a network

P6 | **Stefan Portisch** (Technische Universität Wien, Austria)

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

P7 | **Josef Weinbub** (Silvaco, Inc.)

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

P8 | **Steffen Maaß** (Technical University Berlin, Germany)

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

P9 | **Christine Keller** (WIAS Berlin, Germany)

A drift-diffusion model to describe ion channel dynamics

P10 | **Jürgen Fuhrmann** (WIAS Berlin, Germany)

Development of numerical methods and tools for drift-diffusion simulations