NUS National University of Singapore | Department of Mathematics Faculty of Science

# Workshop on Modeling and Simulation for Semiconductor Devices

**Date:** January 20, 2026

**Venue:** S17-04-05, Department of Mathematics, NUS

**Organizing Committee:**


- Prof. Weizhu Bao (matbaowz@nus.edu.sg)
- Dr. Shuigen Liu (shuigen.liu@nus.edu.sg)


**Plenary Speaker:**

- Prof. Ansgar Jüngel, *TU Vienna*

**Invited Speaker:**

- Prof. Zhenning Cai, *NUS*
- Prof. Xiaoli Li, *Shandong University*
- Ms. Shuya Liu, *NUS*
- Dr. Wenhao Lu, *NUS*
- Dr. Maheswari Sivan, *NUS*
- Mr. Quanzhen Wan, *NUS*
- Dr. Zhe Wang, *NUS*
- Prof. Chijie Zhuang, *Tsinghua University*

| Workshop on Modeling and Simulation for Semiconductor Devices | | |
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| January 20, 2026 (S17-04-05) | | |
| Time | Title | Name |
| Chair: Weizhu Bao | | |
| 9:00–10:00 AM | **Plenary Talk:** Memristor drift-diffusion systems for brain-inspired neuromorphic computing | Ansgar Jüngel |
| 10:00–10:30 AM | **Tea Break** | |
| Chair: Shuigen Liu | | |
| 10:30–11:00 AM | Developing a power semi-conductor device simulation tool: challenge, experience and performance | Chijie Zhuang |
| 11:00–11:30 AM | Energy stable and maximum bound principle preserving schemes for the Q-tensor flow of liquid crystals | Xiaoli Li |
| 11:30–12:00 PM | The finite element method and numerical analysis for semiconductor device simulation | Wenhao Lu |
| 12:00–2:00 PM | **Lunch Break** | |
| Chair: Chijie Zhuang | | |
| 2:00–2:30 PM | Simulation of open quantum systems with frozen Gaussian approximation | Zhenning Cai |
| 2:30–3:00 PM | Electroluminescence and Light-Field Control in van der Waals Tunnel Junctions | Zhe Wang |
| 3:00–3:30 PM | A discrete duality finite volume method with harmonic average for semiconductor drift–diffusion equations | Shuya Liu |
| 3:30–4:00 PM | **Tea Break** | |
| Chair: Qingyuan Shi | | |
| 4:00–4:30 PM | Physical Insights into Vacancy-Based Memtransistors: Toward Power Efficiency, Reliable Operation, and Scalability | Maheswari Sivan |
| 4:30–5:00 PM | Dopant-enhanced polarization readout in anisotropic 2D materials | Quanzhen Wan |

# Abstracts

## Memristor drift-diffusion systems for brain-inspired neuromorphic computing

**Prof. Ansgar Jüngel**

***Institute for Analysis and Scientific Computing, TU Vienna***

More than 50 years ago, Moore predicted that the number of transistors on a microchip doubles every two years. This exponential growth is approaching its physical limit, highlighting the need for alternative computing paradigms. One promising avenue is neuromorphic computing, which aims to emulate the structure and function of the human brain. A key enabling technology is the memristor, a nonlinear resistor with memory. Memristors are capable of mimicking the dynamic conductance behavior of biological synapses, making them well-suited for implementing energy-efficient neural networks.

This talk focuses on the mathematical analysis of three-species drift-diffusion equations for memristors. We investigate the existence and boundedness of global-in-time weak solutions. The mathematical difficulties originate from the three-species setting and the different types of boundary conditions. These issues are addressed by combining free energy estimates with local and global compactness arguments. Additionally, we analyze memristor models coupled with electrical networks. One-dimensional numerical simulations capture the characteristic hysteresis behavior in the current-voltage curves, which is a fingerprint for memristive devices.

## Simulation of open quantum systems with frozen Gaussian approximation

**Prof. Zhenning Cai**

***Department of Mathematics, NUS***

In an open quantum system, the quantum mechanical object we are interested in is coupled with the environment, changing the behavior of the system by introducing quantum dissipation and non-Markovianity. Due to the system-bath interaction, even the dynamics of a single particle has to be computed using path integrals, which turns out to be a high-dimensional problem. In this talk, we will simulate such dynamics by decomposing the wave function into Gaussian wave packets and employing the frozen Gaussian approximation to evolve these wave packets. The use of frozen Gaussian approximation allows us to calculate the high-dimensional integrals analytically, and accurately compute the coupling of the system and the environment. One- and two-dimensional numerical examples are tested, showing that the wave-like structures in the density function are flattened due to the effect of the environment.

## Energy stable and maximum bound principle preserving schemes for the Q-tensor flow of liquid crystals

**Prof. Xiaoli Li**

***Department of Mathematics, Shandong University***

In this talk we present two efficient fully-discrete schemes for Q-tensor flow by using the first- and second-order stabilized exponential scalar auxiliary variable approach in time and the finite difference method for spatial discretization. The discrete energy dissipation laws are unconditionally satisfied for both two constructed schemes. A particular feature is that, for two-dimensional (2D) and a kind of three-dimensional (3D) Q-tensor flows, the unconditional maximum-bound-principle (MBP) preservation of the constructed first-order scheme is successfully established, and the proposed second-order scheme preserves the discrete MBP property with a mild restriction on the time-step sizes. Furthermore, we rigorously derive the corresponding error estimates for the fully-discrete second-order schemes by using the built-in stability results. Finally, various numerical examples validating the theoretical results, such as the orientation of liquid crystal in 2D and 3D, are presented for the constructed schemes.

## A discrete duality finite volume method with harmonic average for semiconductor drift–diffusion equations

**Ms. Shuya Liu**

***Department of Mathematics, NUS***

Obtaining reliable numerical solutions for the classical drift–diffusion (DD) model, which constitutes a standard macroscopic description in semiconductor device simulation, remains challenging in regimes dominated by strong drift, sharp doping variations, and complex device geometries.

In this talk, I will present a hybrid numerical approach that combines the discrete duality finite volume (DDFV) framework with harmonic averaging techniques for the discretization of the DD model. The proposed scheme achieves robust and accurate approximations on general unstructured meshes, without relying on restrictive mesh admissibility conditions. Numerical experiments demonstrate that the method remains stable and free of spurious oscillations, even in the presence of heavy doping profiles and sharp PN junctions.

## The finite element method and numerical analysis for semiconductor device simulation

**Dr. Wenhao Lu**

***Department of Mathematics, NUS***

his talk studies finite element methods and numerical analysis for semiconductor device simulation. In Part I, we develop a unified a priori error-analysis framework for the Schrödinger–Poisson system, and introduce a two-grid inexact-Newton strategy to mitigate the computational bottleneck caused by full Jacobian matrices in nonlinear iterations. In Part II, we incorporate the quantum-corrected drift–diffusion model into the same framework. Our main contribution is an existence theory for the discrete problem that does not rely on the classical discrete maximum principle, thereby removing the conventional mesh-geometry restrictions (Delaunay meshes in 2D or acute meshes in 3D) and substantially weakening the required geometric assumptions on the mesh. In Part III, we present ongoing work on electro-thermal drift–diffusion models, including the coupled modeling ingredients and our current progress on discretization and analysis.

## Physical Insights into Vacancy-Based Memtransistors: Toward Power Efficiency, Reliable Operation, and Scalability

**Dr. Maheswari Sivan**

***Department of Electrical and Computer Engineering, NUS***

The rapidly growing energy demand of AI-driven computing systems has created an urgent need for more power-efficient microelectronic technologies. A major contributor to this energy cost is the memory wall, where frequent data transfer between physically separated processing and memory units dominates system power consumption. Memtransistors which are devices that merge transistors with memristive behavior offer a promising route toward overcoming this bottleneck by enabling in-situ computation within the memory itself. In this talk, I will present how novel materials beyond silicon, particularly two-dimensional semiconductors, can be engineered to realize vacancy based memtransistors with enhanced energy efficiency and scalability. I will introduce an advanced physics-based model that captures the coupled dynamics of lattice temperature, ionic vacancies, and channel electrostatics, allowing accurate prediction of how gate potential, mobile ions, and charge carriers collectively govern memristive switching. Using this framework, I will show how careful control of threshold-voltage shifts, read-bias polarity, and contact work functions can be used to achieve low-power operation and high read reliability. Finally, I will discuss how the strong correlations among switching mechanisms, material systems, and device architectures provide clear guidelines for optimizing operating modes and device designs, paving the way for robust, scalable memtransistor-based computing platforms.

## Dopant-enhanced polarization readout in anisotropic 2D materials

**Mr. Quanzhen Wan**

***College of Design and Engineering, NUS***

Polarization offers an additional information channel for data transfer, yet most on-chip decoding approaches rely on nanostructured optics that incur insertion loss and strict fabrication tolerances. Here we demonstrate that Pt doping in ReS2 provides a direct route to polarization-resolved photodetection. DFT identifies Pt as the most effective among 19 screened dopants, inducing directional orbital hybridization and band reshaping. Devices with 1% Pt exhibit an anisotropy ratio that increases from 1.45 to an average of 10.5, with maxima exceeding 16. Concomitantly, at the source-drain contact region, both the thermionic and tunneling barrier reduces, lowering the

contact resistance to 0.62 kΩ·μm and enabling microsecond response. Simulations show that the enhanced anisotropy supports polarization-multiplexed image transmission with signal-to-noise ratio rising from 12 to over 37 dB as the resolvable polarization states increases. These results establish chemical doping as an effective pathway toward compact, high-contrast polarization-resolved optoelectronics for imaging and high-density data transmission.

## Electroluminescence and Light-Field Control in van der Waals Tunnel Junctions

**Dr. Zhe Wang**

***Department of Electrical and Computer Engineering, NUS***

Electroluminescence in plasmonic metal-insulator-metal (MIM) tunnel junctions arises from inelastic electron tunnelling and provides a compact electrical source of optical excitation. A modeling framework is adopted to connect experimentally measured transport characteristics to optical emission through an effective source description and a local density of optical states (LDOS) picture, enabling a unified treatment of radiative, guided, and non-radiative channels. This perspective motivates a transition from conventional MIM junctions to van der Waals (vdW) tunnel junctions. By incorporating two-dimensional (2D) materials as electrodes and tunnel barriers, vdW junctions reduce dissipative losses and offer improved compatibility with engineered photonic environments. Using electromagnetic simulations, structures are developed that support efficient free-space radiation, low-loss waveguide coupling, and the reuse of near-field energy typically regarded as non-radiative loss. Building on this platform, coupling vdW tunnel junctions with metacavities provides additional degrees of freedom for controlling emission directionality, polarization, and phase, thereby enabling electrically driven structured-light sources.

## Developing a power semi-conductor device simulation tool: challenge, experience and performance

**Prof. Chijie Zhuang**

***Department of Electrical Engineering, Tsinghua University***

[TBD]