

IWCN

International Workshop on Computational Nanotechnology

May 21-23, 2025

Salt Lake City, UT

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Time	Tuesday May 20 th	Wednesday May 21 st	Thursday May 22 nd	Friday May 23 rd
9:00 – 10:30 am	IWW 1	Phonons I Invited: Laura de Sousa Oliveira	2D Materials and Devices Keynote: Eric Pop	Quantum Transport I Invited: William Frensley
10:30 – 11:00 am	Coffee Break	Coffee Break and pastries (atrium)		
11:00 am – 12:30 pm	IWW 2	Phonons II Invited: Keivan Esfarjani	Emerging Devices Invited: Wenhao Song	Quantum Transport II
12:30 pm – 2:00 pm	Lunch	Lunch (Ballroom)		Conference Adjourn
2 pm – 3:30 pm	IWW 3	Numerical Simulation Invited: Giuseppe Romano	Device Simulation Invited: Blanka Magyari-Kope	(optional: excursion to Antelope Island, no cost)
3:30 pm – 4:00 pm		Coffee Break and cookies (atrium)		
4:00 pm – 5:30 pm	IWW 4	Molecular, Organic, and Optical	Monte Carlo	
5:30 – 6:00 pm	Tutorial:	Set up posters	Conference Photo	
6:00 – 8:00 pm	Gerhard Klimeck (Amphitheater) Welcome Reception hors d'oeuvres (atrium)	Poster Session Taco bar (atrium)	Conference Dinner Plated dinner (ballroom)	

Conference Program

May 20th IWW

May 21st – 23rd IWCN

University Marriott, Salt Lake City, UT

Tuesday 5:30-8 pm: Welcome and Tutorial

Welcome Reception: hors d'oeuvres, cash bar with one ticket provided

Location: Atrium

Start time: 5:30 pm

Tutorial: *“Attracting Students to Semiconductors through Interactive Learning Experiences – a Tutorial”* by Gerhard Klimeck, Purdue University

Location: Amphitheater

Start time: 6 pm

Wed. 9-10:30 Phonons I

Time	Type	Presenter	Title
9:00-9:05 am	Conference welcome and brief opening remarks		
9:05-9:35	Invited	Laura de Sousa Oliveira	Super-suppression of Long Mean-free-path Phonons in Nanoporous Silicon
9:35-9:50	Contributed	Sandip Dhruba	Investigation of thermal transport and dislocations in lattice-matched InGaAs/InAlAs superlattices by nonequilibrium molecular dynamics simulations
9:50-10:05	Contributed	Md Mobinul Haque	Thermal Conductivity of Nanowires : Machine Learning and Monte Carlo Insights
10:05-10:20	Contributed	Oreoluwa Adesina	Evaluating Thermal Transport at The Axial Junction of Si-Ge Composite Nanowires
10:20-10:35	Contributed	Shunda Chen	Impacts of Short-range Order on Thermal Conductivity of GeSn and Si-Ge-Sn Alloys

Wed. 10:35-11:00 Coffee break

Wed. 11:00-12:30 Phonons 2

Time	Type	Presenter	Title
11:00-11:30 am	Invited	Keivan Esfarjani	Predicting Thermal Conductivity and Classifying Chemical Bonds using DFT and Machine Learning
11:30-11:45	Contributed	Shouhang Li	Phonon Thermal Transport Along the Chain Direction of Crystalline Polyethylene
11:45-12:00 pm	Contributed	Masoumeh Mahmoudi Gahrouei	Ab initio investigation of thermoelectric properties of two-dimensional MOFs
12:00-12:15	Contributed	David Mai	Applying POD-methods onto electron-phonon scattering in the Wigner equation
12:15-12:30	Contributed	Izak Baranowski	Modeling of Non-Equilibrium Phonons in Hot Carrier Solar Cells

Wed. 12:30-2:00 pm Lunch break

Wednesday 2:00-3:30 pm Simulation Methods

Time	Type	Presenter	Title
2:00-2:30 pm	Invited	Giuseppe Romano	Differentiable Hydrodynamics Simulations: From Inverse Design to Automatic Material Properties Extraction
2:30-2:45	Contributed	Anders Winka	Investigation of thermalization effects and hot carriers in ultra-scaled electronic devices
2:45-3:00	Contributed	Denis Mamaluy	Phenomenological inelastic scattering model for electron transport in mesoscopic devices
3:00-3:15	Contributed	Bernhard Pruckner	Switching of Magnetization in Strained Noncollinear Antiferromagnet Mn ₃ Sn
3:15-3:30	Contributed	Khandakar Aaditta Arnab	KROGER: An Extended Calculation Framework for Realistic Defect Modeling in Semiconductors

Wed. 3:30-4:00 pm Coffee break

Wednesday 4:00-5:30 pm

Molecular, Organic, and Optical

Time	Type	Presenter	Title
4:00-4:15 pm	Contributed	Patrizio Graziosi	Electron-phonon coupling and mobility modeling in organic semiconductors: a new and efficient methodology
4:15-4:30	Contributed	Zdenek Futera	Electron Transport in Biomolecular Junctions Studied by DFT and Tight Binding Approaches
4:30-4:45	Contributed	Muhamed Duhandžić	Charge carrier transport mechanisms in doped conjugated polymers
4:45-5:00	Contributed	Minsu Jeong	First-principles study of the quasi-Fermi level splitting in ferrocene-based molecular junctions
5:00-5:15	Contributed	Abdelilah Benali	Modeling strong light-matter interaction in polaritonic semiconductors as open systems
5:15-5:30	Contributed	Marcin Makowiec	NEGF computation of optical absorption in InAs/GaSb type-II superlattices

Wednesday 6:00-8:00 pm Poster Session

	Presenter	Title
1	Gerhard Klimeck	Changing the Typical Simulation Flow through Interactive Data Viewers and Drivers
2	Shuva Mitra	Theoretical modeling of twist-angle-dependent plasmon resonances in moire 2D materials
3	Mike Scarpulla	How Excess Carriers Change Steady State Concentrations of Point Defects
4	C.S. Soares	Design Considerations for a 5 nm n-FinFET using a Full-band Monte Carlo Simulator
5	Yeongjun Lim	Robust Mode Space Method for Heterostructure Transport Enabled by Machine Learning Approach
6	Min-Hui Chuang	A Calibrated Mobility Model for Monolayer Molybdenum Disulfide Device Simulation
7	Alan Carlos Junior Rossetto	Self-Heating and Hot Carrier Degradation Interaction in 28-nm FD-SOI pFETs
8	Dalton Zirbel	Theoretical modeling of quantum-well structures in dilute bismide optoelectronics
9	Nikiphoros Vlastos	Probing Light-Induced Isomerization Dynamics of Azobenzene Confined within Metal-Organic Frameworks: A Time-Dependent Density Functional Theory Investigation
10	Luca Gnoli	A computational approach to polymorphism in BDT organic semiconductors
11	Alathea Davies	Honeycomb-Kagome Band Structures of Highly Tunable Graphene-Like Covalent Organic Frameworks
12	Ali Jalali	Two-dimensional Magnetic Metal Organic Frameworks: Computational Study of Electron and Phonon Transport
13	Gowtham Nirmal Jonnalagadda	Electron Transport Mechanisms in Cytochrome b562 Junctions
14	David Mai	Importance of the Wigner equation for the analysis of the ballistic phonon transport
15	Aidan Belanger	Phonon Monte Carlo Investigation of Hydrodynamic Transport in Graphene Micro Ribbons
16	Alison Jensen	Atomistic Modeling Insights of Thermal Boundary Transport Between a Surrogate Fuel (CeO ₂) and a Fission Product (Pd)
17	Md Mobinul Haque	Elastic-Wave Modeling of Long-Wavelength Phonon Dynamics in Superlattice Nanowires With Rough Interfaces
18	Lucky K. Antonopoulos	A generalised framework for defining discrete Wigner functions via the Gottesman-Kitaev-Preskill code
19	V. Ganiu	Impact of Slope Limiters on DG Methods Solving Quantum-Liouville Type Equations
20	Xiaoyin Li	Topological Nodal-Point Superconductivity in Two-Dimensional Ferroelectric Hybrid Perovskites
21	Dongming Li	Nonlinear Eigenvalue Algorithms with Applications

Thursday 9-10:30 2D Materials

Time	Type	Presenter	Title
9:00-9:30	Keynote	Eric Pop	Electro-Thermal Transport in 2D Materials, Devices, and Applications
9:30-9:45	Contributed	Anass Sebbar	Coherent thermal transport in isotopic graphene superlattices: a NEGF study
9:45-10:00	Contributed	Dongming Li	A New Method for Bandstructure Calculation and Its Application to Edge Termination Effects in Graphene
10:00-10:15	Contributed	Shoaib Mansoori	Theoretical Study of Carrier Transport in Bilayer Transition Metal Dichalcogenides
10:15-10:30	Contributed	Emeric Deylgat and William Vandenberghe	Electrostatic Model of Metal-Induced Gap States in Metal Edge, Top and Hybrid Contacts to MoS ₂ transistors

Thursday 10:30-11:00 Coffee break

Thursday 11:00-12:30 Emerging Devices

Time	Type	Presenter	Title
11:00-11:30	Invited	Wenhao Song	Advancing Analog Precision: Memristor Technology for Scientific Computing
11:30-11:45	Contributed	Sylvester Wambua Makumi	Impact of Electrostatic Pressure on the TBC of 2D-Substrate Interfaces
11:45-12:00	Contributed	A. Alleysson	Quantum transport of excitons in lateral TMDs heterostructures
12:00-12:15	Contributed	Mauro Dossena	Influence of disordered oxides on the mobility of monolayer WS ₂ : an ab initio study
12:15-12:30	Contributed	Chieh-Yang Chen and Yiming Li	Effect of Random Nanosized Titanium Nitride Grains on Monolayer MoS ₂ Field-Effect Transistors

Thursday 12:30-2:00 pm Lunch break

Thursday 2:00-3:30 pm Device Simulation

Time	Type	Presenter	Title
2:00-2:30 pm	Invited	Blanka Magyari-Kope	Innovating Tomorrow's Semiconductor Technology: Computational Strategies for Material Optimization
2:30-2:45	Contributed	Ashwin Tunga	A full 3D TCAD framework for nanosheet transistors including quantum-confined channels
2:45-3:00	Contributed	Min-Hui Chuang	Performance Boost of GAA Si NS CFET via Tungsten Source/Drain Sidewalls
3:00-3:15	Contributed	Dallin Nielsen	Thermalization and Effects of Radiation-Induced Charge-Carriers in Semiconductors and GaN/Al _{0.25} Ga _{0.75} N HEMTs
3:15-3:30	Contributed	Jianshi Sun	Unlocking high hole mobility in diamond over a wide temperature range via efficient shear strain

Thursday 3:30-4:00 pm Coffee break

Thursday 4:00-5:30 pm Monte Carlo

Time	Type	Presenter	Title
4:00-4:15 pm	Contributed	Josef Gull and Hans Kosina	Electron-Electron Scattering in Monte Carlo-based Device Simulations
4:15-4:30	Contributed	Tobias Reiter	GPU-based Monte Carlo Ray Tracing for Flux Calculation in Process Simulation
4:30-4:45	Contributed	Caroline dos Santos Soares	The impact of oxide-traps on n-NWFET using a quantum-corrected Monte Carlo simulator
4:45-5:00	Contributed	Orazio Muscato	Signed particle Monte Carlo quantum simulation of thermionic cooling devices based on resonant tunneling heterostructure
5:00-5:15	Contributed	Rémi Helleboid	Self-Consistent Advection-Diffusion Monte Carlo Simulation of Quenching in Single-Photon Avalanche Diodes
5:15-5:30	Contributed	Siddhant Gangwal	Hierarchical Framework for Modeling Electrostatics and Mobility in $\text{Ge}_{1-x}\text{Sn}_x/\text{Ge}$ Heterostructures

Thursday 6:00-8:00 pm Conference Dinner

Friday 9-10:30 Quantum Transport I

Time	Type	Presenter	Title
9:00-9:30	Invited	William Frensley	Design Principles for Discrete Models of Nanoelectronic Systems
9:30-9:45	Contributed	M. Pech	Time-resolved Quantum Transport in Open Systems: Phase Versus Real-Space Methods
9:45-10:00	Contributed	Filippo Passeri	Implementation of quantum transmitting boundary method in a 1D electron transport code
10:00-10:15	Contributed	A. Martinez	Scaled 1D NEGF model for 3D Oxide Barriers and Resonant Tunneling Diodes
10:15-10:30	Contributed	Jeongwon Lee, Ryong-Gyu Lee, Hyeonwoo Yeo, and Yong-Hoon Kim	Effects of the internal dipole alignment on the quantum transport properties of two-dimensional halide perovskite devices

Friday 10:30-11:00 Coffee break

Friday 11:00-12:30 Quantum Transport II

Time	Type	Presenter	Title
11:00-11:15	Contributed	Massimo Macucci	Phase noise model for qubit control
11:15-11:30	Contributed	Andrzej Kolek	Interband tunneling in a superlattice absorber
11:30-11:45	Contributed	Juan Pedro Mendez Granado	Predictive quantum transport simulations for advanced nano-scale FET-based sensors
11:45-12:00	Contributed	Juan José Seoane	Exploring quantum technologies through THz polaritonic semiconductor devices
12:00-12:30	Closing Remarks and announcement of the next IWCN in 2027		

Friday 12:30 Conference Adjourn

- Optional: excursion to Antelope Island, no cost