

Tuesday 26th

16:30 - 18:30 Round Table on the Perspectives of Modeling
(Working Group 5 of Nano-ICT)

There will be a panel presentation, followed by discussion with all participants. All IWCE 2010 attendees are invited to join.

18:30-20:00 Welcome Reception and Registration

Wednesday 27th

8:00-9:00 Registration

9:00-9:15 Workshop Opening

9:15-10:45 Nanowires I

Chairman: Christoph Jungemann

Si nanowires: the future of nanoelectronics? (Invited)

R. Rurali

Band Structure and Ballistic Conductance of Strained Si Nanowires

J. Kim, M. V. Fischetti

Electronic Band Structure Modeling in Strained Si-Nanowires: Two Band $\vec{k} \cdot \vec{p}$ vs. Tight Binding

Z. Stanojević, O. Baumgartner, V. Sverdlov, H. Kosina

Point-defect Scattering in Silicon Nanowires

A. Pecchia, G. Penazzi, A. Di Carlo

Impurity and phonon-limited electron mobilities in 110-oriented silicon nanowires

Y. M. Niquet, M. Persson, H. Mera, W. Zhang, C. Delerue, G. Allan, E. Wang

10:45-11:15 Coffee Break

11:15-12:45 Semiclassical Methods

Chairman: Andreas Schenk

High-order spherical harmonics solution of the Boltzmann equation and noise modeling (Invited)

C. Jungemann, S.-M. Hong, G. Matz

A Percolative Approach to Transport and Excess Noise in Polyacene Semiconductors

C. Pennetta, A. Carbone, L. Reggiani

Brownian Noise in FET Based Nano-Pore Sensors

I. Moore, C. Millar, S. Roy and A. Asenov

A deterministic Boltzmann solver for GaAs devices based on the spherical harmonics expansion

J. Bieder, S.-M. Hong, C. Jungemann

A Monte Carlo Simulation of Reproducible Hysteresis in RRAM

A. Makarov, V. Sverdlov, S. Selberherr

12:45-14:15 Lunch

14:15-15:45 Graphene Devices

Chairman: Gianluca Fiori

Quantum transport of Dirac fermions in graphene nanostructures (Invited)

P. Dollfus

On the Role of Line-Edge Roughness on the Diffusion and Localization in GNRs

M. Pourfath, A. Yazdanpanah, M. Fathipour, H. Kosina

Phonon and Electron Transport in Graphene Nanoribbons

F. Mazzamuto, V. Hung Nguyen, C. Caër, V. N. Do, C. Chassat, J. Saint-Martin, P. Dollfus

Numerical solution of the Dirac equation for an armchair graphene nanoribbon in the presence of a transversally variable potential

P. Marconcini, D. Logoteta, M. Macucci

The Effect of Disorder in Superfluid Graphene Bilayers

B. Dellabetta, M. J. Gilbert

15:45-16:15 Coffee Break

16:15-18:30 Poster Session I

Model-Comparison Study of Quasi-Ballistic Electron Transport in Nanoscale Semiconductor Devices

T. Tang, I. Yoon, N. Sano, S. Jin, M. Fischetti, Y. J. Park

A reduced-order technique for the acceleration of electronic structure calculations

M. Penna, F. Bertazzi, M. Goano

Handshaking multiscale thermal model of nanostructured devices

G. Romano, M. Auf der Maur, A. Pecchia, A. Di Carlo

Development of a Highly Parallelized Micromagnetic Simulator for Graphics Processors

A. A. Khan, P. Lugli, W. Porod, G. Csaba

Transport properties of curved nanostructures in magnetic field

B. Novakovic, I. Knezevic

Simulations of Complex Nuclear Events from High Energy Ion Tracks in Integrated Circuits with 3D NanoTCAD

A. Fedoseyev, R. Arslanbekov, M. Turowski

Channel Length Dependence of Discrete Dopant effects in narrow Si Nanowire Transistors: A full 3D NEGF study

A. Martinez, M. Aldegunde, A. Asenov

Dissipative quantum transport and terahertz gain in nanowire superlattices

T. Grange, P. Vogl

2-D rotational invariant multi subband Schrödinger-Poisson solver to model nanowire o transistors

D. Sels, B. Sorée, G. Groeseneken

Three-dimensional $k \cdot p$ quantum simulations of p-type nanowire MOS transistors: influence of ionized impurity

N. Pons, N. Cavassilas, M. Bescond, F. Michelini, L. Raymond, M. Lannoo

A Comprehensive Atomistic Analysis of Bandstructure Velocities in Si Nanowires

N. Neophytou, G. Klimeck, H. Kosina

Effects of deviations in the cross-section of square Nanowires

I. M. Tienda-Luna, F. G. Ruiz, A. Godoy, L. Donetti, F. Gámiz

Evaluation of threshold voltage dispersion in 45 nm CMOS technology with TCAD-based sensitivity analysis

V. Bonfiglio, G. Iannaccone

Cellular Monte Carlo study of RF and DC Short-Channel effects in terms of minimum Aspect Ratio in GaN and InGaAs HEMTs

D. Guerra, F. A. Marino, R. Akis, D. K. Ferry, S. Goodnick, M. Saraniti

Cellular Monte Carlo Investigation of InAs and InGaAs Quantum Well Field Effect Transistors

D. Guerra, R. Akis, D. K. Ferry, S. M. Goodnick, M. Saraniti, F. A. Marino

Effect of the Channel Thickness on the Performance of the Implant-Free Quantum-Well MOSFET

A. Martinez, B. Benbakhti, A. Asenov

Advanced T-matrix method for quantum simulation of nanoscale field-effect transistors

I. Semenikhin, V. Vyurkov, A. Orlikovsky

Impact of scattering on the performance of Si nanowire FETs: from diffusive to ballistic regime

M. Aldegunde, A. Martinez, A. Asenov

Simplified Calculation Method of Electron Subband Profile in Ballistic Nanowire MOSFET

T. Numata, S. Uno, A. Sawicka, K. Nakazato, G. Mil'nikov, Y. Kamakura, N. Mori

Numerical simulation of a subband model based on the Maximum Entropy Principle

D. Camiola, G. Mascali, V. Romano

Capacitance-Voltage Calculations for Si, Ge, and III-V MOS Structures: DOS Bottleneck

T. P. O'Regan, P. K. Hurley, M. V. Fischetti

Catalytic Surfaces of Silicon Nanopores, a Brownian Dynamics Study

P. Ramaprasad, S. Goodnick, M. Saraniti

Equivalent-circuit Model for Electrostatic Micro-torsion Mirror

K. Matsuda

Thursday 28th

8:45-10:15 Quantum Methods and Spintronics

Chairman: Stephen Goodnick

The nonequilibrium Green's functions method and descendants: ways to avoid and to go (Invited)

P. Vogl, T. Kubis, P. Greck

Spin-orbital strain effects in semiconductors

F. Micheli, N. Pons, N. Cavassilas, M. Bescond, M. Szczap

Fully self-consistent simulation of silicon nanocrystal-based single-electron transistor

V. Talbo, A. Valentin, S. Galdin-Retailleau, P. Dollfus

Simulation of spin transport, magnetization dynamics in FNF structures within a drift-diffusion model

M. Wenin, W. Pötz

Self-Consistent Study of Transport in MnDoped Semiconductor Heterostructures

C. Ertler, P. Senekowitsch, J. Fabian, W. Pötz

10:15-10:45 Coffee Break

10:45-11:45 Atomistic and ab initio Techniques

Chairman: Manjeri Anantram

Electron-Phonon Scattering in Atomistically Resolved Nanoelectronic Devices (Invited)
M. Luisier

Ab initio calculation of the vibrational influence on hole-trapping

F. Schanovsky, W. Goes, T. Grasser

“Ab initio” Surface Roughness Scattering in 3D Monte Carlo

C. Alexander, A. Asenov

11:45-13:00 Numerical Simulation of Semiconductor Properties

Chairman: Marco Saraniti

Theory of High Field Transport and Impact Ionization in III-Nitride Semiconductors
(Invited)

E. Bellotti, M. Moresco, F. Bertazzi

EMC/FDTD/MD for Multiphysics Characterization of Semiconductors at THz Frequencies

K. J. Willis, S. C. Hagness, I. Knezevic

Ionized donor reordering in typical heterostructures

M. Totaro, P. Marconcini, M. Macucci

Auger lifetime in narrow gap semiconductors

F. Bertazzi, M. Goano, E. Bellotti

13:00-14:30 Lunch

14:30-16:15 Optoelectronics

Chairman: Peter Vogl

Rough interfaces in THz quantum cascade lasers (Invited)

T. Kubis, G. Klimeck

Computational modeling of light emission properties of nanowires in the presence of strain (Invited)

P. Anantram

Efficient Implementation of the Fourier Modal Method (RCWA) for the Optical Simulation of Optoelectronic Devices

I. Semenikhin, M. Zanucoli, V. Vyurkov, E. Sangiorgi, C. Fiegna

Coupled Carrier-Field Monte-Carlo Analysis of Mid-IR Quantum Cascade Lasers

A. Mátyás, S. Katz, S. Söntges, A. Vizbaras, P. Lugli, M. C. Amann, C. Jirauschek

Simulation of the Buxton-Clarke Model for Organic Photovoltaic Cells

J.W. Jerome, M.A. Ratner, J.D. Servaites, C.-W. Shu, S. Tan

16:15-16:45 Coffee Break

16:45-19:00 Poster Session II

Transient-regime quantum transport in two-terminal nanostructures

B. Novakovic, I. Knezevic

Design Optimization of GNR Tunneling-FETs for Low Voltage Operation Using EHT-Based NEGF Simulation

X. Guan, S. Huang, J. Kang, J. Zhang, Z. Yu

Quantum phase-space approach to the transport simulation in graphene devices.

O. Morandi, F. Schuerrer

Phonon Bottleneck Effects in Rectangular Graphene Quantum Dots

J. Qian, M. Dutta, M. A. Strosio

Schred V2.0, Tool to model MOS capacitors

G. Kannan, D. Vasileska

Interface Optical Phonon Modes in Wurtzite Quantum Heterostructures

S. Liao, M. Dutta, M. A. Strosio

The BITLLES simulator for nanoscale devices

F. L. Traversa, G. Albareda, A. Alarcón, A. Benali, A. Padró, X. Cartoixà, R. Rurali, and X. Oriols

Computational Study of InAs/GaAs Quantum Dot Arrays

F. M. Gómez-Campos, S. Rodríguez-Bolívar, A. Luque-Rodríguez, J. A. López-Villanueva, J. E. Carceller

Performance of Discontinuous Galerkin Solver for Semiconductor Boltzmann Equations

Y. Cheng, I. M. Gamba, A. Majorana, C.-W. Shu

3D Ensemble Monte Carlo Device Simulations of Random Trap Induced Degradation in Drain Current and in Threshold Voltage in the Presence of Random Dopant Distributions for 45 nm Gate Length MOSFETs

N. Ashraf, D. Vasileska

Statistical Estimation of Electrostatic and Transport Contributions to Device Parameter Variation

U. Kovac, C. Alexander, A. Asenov

Monte Carlo Simulation Study of Hole Mobility in Germanium MOS Inversion Layers

C. Riddet, J. R. Watling, K. H. Chan, A. Asenov

Monte Carlo study of transport properties in junctionless transistors

W. Vitale, M. Mohamed, U. Ravaioli

Self-Consistent Electrothermal Monte Carlo Modeling of Nanowire MISFETs

T. Sadi, J.-L. Thobel, F. Dessenne

Stackable devices based on chaotic conduction

G. Pennelli

Novel artificial molecules: Optoelectronic properties of two quantum dots coupled by a quantum wire

F. Michelini, M.-A. Dupertuis, E. Kapon

Thirty-band $\vec{k} \cdot \vec{p}$ model for Si-based optoelectronics

M. Szczap, F. Michelini, N. Cavassilas

Simulation of Raman Enhancement in SERS- Active Substrates with Au Layer Considering Different Geometry of Nanoparticles

H.-W. Cheng, Y. Li

Multi-Color Photodetector based on Quantum Dots and Resonant-Tunneling Diodes Coupled with Conductive Polymers

S. Liao, M. Dutta, M. A. Strosio

Valley Degeneracy in (110) Si Quantum Wells: Strain and Misorientation Effects

Z. Jiang, N. Kharche, G. Klimeck

Electronic properties of nanosize GNRs: the role of the anchoring groups

L. Á. de Cienfuegos, S. Rodríguez-Bolívar, F. M. Gómez Campos, T. García, J.A. López-Villanueva, J.E. Carceller, E. Buñuel, D. J. Cárdenas, A. Martín-Lasanta, J. M. Cuerva

Subband Representation in Atomistic Transport Simulation of Nanowire Transistors

G.V. Mil'nikov, N. Mori, Y. Kamakura, H. Minari

Atomistic modeling of the phonon dispersion in free-standing $\langle 100 \rangle$ Si nanowires

A. Paul, M. Luisier, G. Klimeck

Ab initio Calibration of the Empirical Pseudopotential Method for Strained Silicon

F. O. Heinz, L. Smith

19:15 - Buses to the dinner location (in Lucca) leave from the workshop venue

20:30 - Conference Dinner

Friday 29th

8:45-9:45 Carbon Electronics

Chairman: Hans Kosina

Self-Consistent Simulation of Array-Based CNFETs: Impact of Tube Pitch on RF Performance

K. Holland, N. Paydavosi, M. Vaidyanathan

Spectral modeling and propagation schemes for time-dependent quantum systems

Z. Chen, E. Polizzi

A multi-scale approach for the performance assessment of hydrogenated graphene Field-Effect Transistors

G. Fiori, S. Lebègue, A. Betti, P. Michetti, M. Klintenberg, O. Eriksson, G. Iannaccone

Enhanced Shot Noise in Carbon Nanotube FET due to electron-hole interaction

A. Betti, G. Fiori, G. Iannaccone

9:45-10:45 Novel Computational Architectures

Chairman: Philippe Dollfus

Nanomagnetic Logic (Invited)

W. Porod

Computational Model of Partially Irradiated Nanodots for Field-coupled Computing Devices

X. Ju, S. Wartenburg, M. Becherer, J. Kiermaier, S. Breitzkreutz, P. Lugli, G. Csaba

Behavior of Nanomagnet Logic in the Presence of Thermal Noise

G. Csaba, W. Porod

10:45-11:15 Coffee Break

11:15-13:00 MOS Devices

Chairman: Steve Laux

Phonon-induced transverse-mode coupling in double-gate transistor

N. Cavassilas, M. Bescond, F. Michelini

Comparison of Semiclassical Transport Formulations Including Quantum Corrections for Advanced Devices with High-k Gate Stacks

F. M. Bufler, V. Aubry-Fortuna, A. Bournel, M. Braccioli, P. Dollfus, D. Esseni, C. Fiegna, F. Gamiz, M. De Michielis, P. Palestri, J. Saint-Martin, C. Sampedro, E. Sangiorgi, L. Selmi, P. Toniutti

Programming Efficiency and Drain Disturb Trade- off in Embedded Non Volatile Memories

A. Zaka, P. Palestri, D. Rideau, M. Iellina, E. Dornel, Q. Rafhay, C. Tavernier, H. Jaouen

Small signal analysis of electrically-stressed oxides with Poisson-Schroedinger based multiphonon capture model

D. Garetto, Y. M. Randriamihaja, D. Rideau, E. Dornel, W. F. Clark, A. Schmid, V. Huard, H. Jaouen, Y. Leblebici

Random Work Function Variation Induced Threshold Voltage Fluctuation in 16-nm Bulk FinFET Devices with High-k-Metal-Gate Material

H.-W. Cheng and Y. Li

Simulation of Landau quantization effects due to strong magnetic fields in (110) Si hole inversion layers

A. T. Pham, C. Jungemann, B. Meinerzhagen

Quantum Transport in Nanowire p-type Schottky Barrier MOSFETs with the $k \cdot p$ Method

M. Shin

13:00-14:30 Lunch

14:30-15:30 Advanced Computational Techniques

Chairman: Joseph Jerome

FEAST for Nanoelectronic Modeling and Simulations (Invited)

E. Polizzi

Effective mass versus tight-binding: Where is the discord?

H. Mera, M. Persson, Y. M. Niquet, M. Bescond

Supersolid in Thermal Phase Diagram of Symmetric Electron-Hole Semiconductor Bilayer

M. Y. Alaoui Lamrani(bouadani), M. J. Gilbert

15:30-16:30 Nanowires II

Chairman: Michael Stroscio

Emission and absorption of optical phonons in multigate silicon nanowire MOSFETs

N. Dehdashti, A. Kranati, I. Ferain, CW Lee, R. Yan, P. Razavi, R. Yu, JP Colinge

Silicon Nanowire Thermoelectrics: Myth or Reality?

E. B. Ramayya, J. Chen, I. Knezevic

Thermal Modeling of Nanodevices

D. Vasileska, K. Raleva, A. Hossain, S. M. Goodnick, Z. Aksamija, and I. Knezevic

Phonon transport and thermoelectric properties of silicon nanomembranes and nanoribbons

Z. Aksamija, I. Knezevic

16:30-16:50 Coffee Break

Special Session on Computational Hubs (rescheduled)

16:50-17:20 “nanoHUB: more than a web-app”

17:20-17:50 “NanoICT hub: development and perspectives”

17:50-18:20 Questions from the audience and discussion

18:20-18:30 Workshop Closure