



Casa Convalescencia, Barcelona, 12-16 June 2023

Program

Monday, June 12

Special session: Quantum transport simulators

Chair: STEPHAN ROCHE

- 15:00 15:30 **TKWANT: A SOFTWARE PACKAGE FOR TIME-DEPENDENT QUANTUM TRANSPORT**
Thomas Kloss (INVITED); Neel Institute (France)
- 15:30 16:00 **NEMO: FROM ESOTERIC QUANTUM THEORY TO INDUSTRIAL TRANSISTOR DESIGNS AND GLOBAL IMPACT** Gerhard Klimeck (INVITED); Purdue University (USA)
- 16:00 16:30 **LSQUANT: LINEAR SCALING QUANTUM TRANSPORT** Jose Hugo Garcia (INVITED); ICN2 (Spain)
- 16:30 17:00 Coffee break
- 17:00 17:30 **MS-DFT: QUANTUM TRANSPORT FROM A MULTI-SPACE EXCITATION VIEWPOINT**
Yong-Hoon Kim (INVITED); KAIST (Republic of Korea)
- 17:30 18:00 **TRANSIESTA: ADVANCED APPLICATIONS IN ELECTROCHEMISTRY AND SPINTRONICS** Pablo Ordejón (INVITED); ICN2 (Spain)
- 18:00 18:30 **QUANTUM ESPRESSO: FROM DENSITY-FUNCTIONAL THEORY TO DUAL WAVE-PARTICLE TRANSPORT AND DEVICE SIMULATION** Michele Simoncelli (INVITED); University of Cambridge (UK)

19:00 Welcome reception/registration

Tuesday, June 13

8:30 Opening remarks /registration

Session: Quantum materials

Chair: GERHARD KLIMECK

- 9:00 9:30 **UNVEILING QUANTUM PHASE TRANSITION BY DISORDER AND DEFECTS IN 2D MATERIALS: JACUTINGAITE FAMILY** Adalberto Fazzio (INVITED); Brazilian Center for Research in Energy and Materials (Brazil)
- 9:30 9:45 **Haiku graphene nanoribbons with tunable topology** Rodrigo E. Menchón (1), Pedro Brandimarte (1), Daniel Sánchez-Portal (1,2) and Aran García-Lekue (1,3); (1) Donostia International Physics Center (DIPC), 20018 Donostia-San Sebastián, Spain (2) Centro de Física de Materiales CSIC-UPV/EHU, 20018 Donostia-San Sebastián, Spain (3) Ikerbasque, Basque Foundation for Science, 48013 Bilbao, Spain
- 9:45 10:00 **Hot electron dynamics in graphene –a linear scaling atomistic approach** Luis Manuel Canonico Armas, Aron W. Cummings and Stephan Roche; Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, Bellaterra, 08193 Barcelona, Spain

- 10:00 10:15 **Localized states, spin-polarisation and transport in graphene grain boundaries**
Aleksander Bach Lorentzen, Mads Brandbyge; Dept. of Physics, Technical University of Denmark (DTU) DK-2800 Kongens Lyngby, Denmark
- 10:15 10:30 **Image-Force Barrier Lowering of Contact Resistance for Two-Dimensional Materials: Direct Determination and Method of Images on a Cone Manifold** Sarah R. Evans (1) Emeric Deylgat (1,2,3), Edward Chen (4) and William G. Vandenberghe(1); (1) Department of Materials Science and Engineering, The University of Texas at Dallas. (2) Department Physics, KU Leuven, (3) Imec, Kapeldreef 75, 3001 Heverlee, Belgium, (4) Corporate Research, Taiwan Semiconductor Manufacturing Company Ltd., Taiwan.
- 10:30 10:45 **Spin-valley transport in magnetic 2D materials through multiscale simulations** D. Soriano (1), D. Marian (2), D. K. Dubey (2), E. Cannavò (2), E. G. Marin (3), and G. Fiori (2); (1) Departamento de Física Aplicada, Universidad de Alicante, 03690 Alicante, Spain (2) Dipartimento di Ingegneria dell'Informazione, Università di Pisa, Via G. Caruso 16, Pisa, 16122, Italy (3) Departamento de Electrónica, Universidad de Granada, Avenida Fuente Nueva s/n, Granada, 18071, Spain

10:45 11:15

Coffee break

Session: Quantum electron transport

Chair: WILLIAM VANDENBERGHE

- 11:15 11:45 **TREATING NON-EQUILIBRIUM GREEN'S FUNCTIONS WITH A MONTE CARLO METHOD** David K. Ferry (INVITED); Arizona State University (USA)
- 11:45 12:00 **Non-Equilibrium Green's Functions Basis in Multiband Models for Broken-Gap Antimonide-Based Tunneling Devices** T. Sato (1,2), S. Birner (1), C. Jirauschek (2), and T. Grange (3); (1) nextnano GmbH, Konrad-Zuse-Platz 8, 81829 München, Germany (2) TUM School of Computation, Information and Technology, Technical University of Munich, Hans-Piloty-Straße 1, 85748 Garching b. München, Germany (3) nextnano Lab, 12 chemin des prunelles, 38700 Corenc, France
- 12:00 12:15 **A phenomenological method to reduce NEGF simulation from 3D to 1D for lateral translation invariant systems** A. Martinez (1) and J.R. Barker (2); (1) Department of Electrical and Electronic Engineering, Swansea University, Bay Campus, UK (2) James Watt School of Engineering, University of Glasgow, Glasgow G12 8LT, UK
- 12:15 12:30 **Delta-layer tunnel junctions in semiconductors for charge sensing** J.P. Mendez and D. Mamaluy; Cognitive & Emerging Computing, Sandia National Laboratories, Albuquerque, USA
- 12:30 12:45 **A novel structure of Cooling Nano-devices: The Quantum Cascade Cooler** G. Etesse (1), C. Salhani (2,3), X. Zhu (2), N. Cavassilas (1), F. Michelini (1), K. Hirakawa (2,3), and M. Bescond (1,2); (1) Aix Marseille Université, CNRS, IM2NP UMR 7334, 13397 Marseille, France (2) Institute of Industrial Science, University of Tokyo, Japan (3) LIMMS-CNRS, IRL 2820, Tokyo, Japan
- 12:45 13:00 **Weak values: a new paradigm to characterize nanoscale systems** Xabier Oianguren-Asua, Carlos F. Destefani and Xavier Oriols; Departament d'Enginyeria Electrònica, Universitat Autònoma de Barcelona, 08193 Bellaterra, Barcelona, Spain.

13:00 15:00

Lunch and poster session I (page viii)

Session: Machine Learning

Chair: MASSIMO MACUCCI

- 15:00 15:30 **MACHINE LEARNING FOR MATERIALS AND DEVICE SIMULATIONS** Alison B. Walker (INVITED); University of Bath (UK)
- 15:30 15:45 **First-Principles Multiscale Modeling Enabled by Machine Learning Interatomic Potentials** B. Mortazavi (1,2), and X. Zhuang (1,2); (1) Department of Mathematics and Physics, Leibniz Universität Hannover, Appelstraße 11, 30167 Hannover, Germany. (2) Cluster of Excellence PhoenixD (Photonics, Optics, And Engineering-Innovation Across Disciplines), Gottfried Wilhelm Leibniz Universität Hannover, Hannover, Germany
- 15:45 16:00 **Design of Oscillatory Neural Networks by Machine Learning Algorithms** Tamas Rudner (1), Gyorgy Csaba (1), Wolfgang Porod (2); (1) Faculty of Information Technology and Bionics, Pázmány University Budapest, Hungary. (2) Department of Electrical Engineering, University of Notre Dame, USA
- 16:00 16:15 **Automatic optimization of doping profile for high performance Single-Photon Avalanche Diodes** Rémi Helleboid (1,2), Jérôme Saint-Martin (1), Marco Pala (1), Philippe Dollfus

(1), Denis Rideau (2), Gabriel Mugny (2), Isobel Nicholson (2), Jeremy Grebot (2); (1) C2N, Université Paris-Saclay – CNRS, Palaiseau, France (2) STMicroelectronics, Crolles, France – Edinburgh, United-Kingdom

16:15 16:30 **Machine learning based analysis of collective diffusion in inorganic solid-state electrolytes** Cibrán López Álvarez (1,2,3), Riccardo Rurali (3) and Claudio Cazorla (1,2); (1) Departament de Física, Universitat Politècnica de Catalunya, 08034 Barcelona, Spain, (2) Barcelona Research Center in Multiscale Science and Engineering, Universitat Politècnica de Catalunya, 08019 Barcelona, Spain (3) Institut de Ciència de Materials de Barcelona, ICMAB–CSIC, Campus UAB, 08193 Bellaterra, Spain

16:30 17:00

Coffee break

Session: Growth and interface processes

Chair: WOLFGANG POROD

17:00 17:30 **PROCESS SIMULATION IN MICRO- AND NANO-ELECTRONICS** Lado Filipovic (INVITED); Institute for Microelectronics (Austria)

17:30 17:45 **An Efficient Atomistic Method for Micro-Scale Film Growth from the Vapor Phase** E.E. Lorenz (1,2) and J. Schuster (1); (1) Fraunhofer Institute for Electronic Nanosystems, Technologie-Campus 3, 09126 Chemnitz, Germany (2) Center for Microtechnologies, Chemnitz University of Technology, 09126 Chemnitz, Germany

17:45 18:00 **Interfacial and structural characterization of polymer – electrolyte systems using classical Molecular Dynamics** M.A. Salvador (1), Elena Degoli (2), Alice Ruini (1) and Rita Magri (2); (1) Dipartimento di Scienze Fisiche, Informatiche e Matematiche, Università di Modena e Reggio Emilia, MO, Italy (2) Dipartimento di Scienze e Metodi dell'Ingegneria, Università di Modena e Reggio Emilia, RE, Italy

18:00 18:15 **3D Multi-Level-Set Simulation of Bottom Dielectric Isolation Process for Forksheet FETs** In Ki Kim and Sung-Min Hong; School of Electrical Engineering and Computer Science, Gwangju Institute of Science and Technology (GIST), Gwangju, Cheomdangwagi-ro-123, South Korea

18:15 18:30 **Theory of Electric Enthalpy of Formation in Electrified Interface** Ryong-Gyu Lee, Juho Lee, Hyeonwoo Yeo and Yong-Hoon Kim; School of Electrical Engineering, Korea Advanced Institute of Science and Technology, 291 Daehak-ro, Yuseong-gu, Daejeon 34141, Korea

Wednesday, June 14

Session: Thermal transport and dissipation

Chair: HANS KOSINA

9:00 9:30 **AB-INITIO THERMAL TRANSPORT CALCULATIONS FOR CRYSTALS AND NANOSTRUCTURES BASED ON THE BOLTZMANN TRANSPORT EQUATION** Jesus Carrete (INVITED); TU Wien (Austria)

9:30 9:45 **Full Band Monte Carlo simulation of transient and stationary thermal transport in GaAs porous nanostructures based on ab initio calculation** Junbum Park (1), Lorenzo Paulatto (2), Marco Pala (1), and Jerome Saint-Martin (1); (1) C2N, Université Paris-Saclay, CNRS, 91120, Palaiseau, France (2) IMPMC, Sorbonne Université, CNRS, 75252, Paris, France

9:45 10:00 **BTE-Barna: first-principles thermal simulation of devices based on 2D materials** M. Raya-Moreno (1), X. Cartoixà (2) and J. Carrete (3); (1) Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, 08193 Bellaterra, Spain (2) Departament d'Enginyeria Electrònica, Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain (3) Institute of Materials Chemistry, TU Wien, A-1060 Vienna, Austria

10:00 10:15 **Dynamics of Long-Wavelength Phonons Near Boundaries and Interfaces in Nanomaterials** L. Avazpour, M.K. Eryilmaz, and I. Knezevic; Department of Electrical and Computer Engineering, University of Wisconsin – Madison Madison, WI 53706 USA

10:15 10:30 **Strong anharmonicity at the origin of anomalous thermal conductivity in Cs₂NaYbCl₆** Antonio Cappai, Claudio Meli, Francesco Quochi, Michele Saba, Daniela Marongiu and Luciano Colombo; Dipartimento di Fisica, Università di Cagliari, Italy

10:30 10:45 **Temperature-induced boomerang effect of electron flow in semiconductor heterostructures** C. Belabbas (1), A. Crépieux (2), N. Cavassilas (1), F. Michelini1, X. Zhu (3), C. Salhani (3,4), G. Etesse (1), K. Hirakawa (3, 4, 5) and M. Bescond (1,3); (1) IM2NP UMR-CNRS, Aix Marseille Université, Université de Toulon, Marseille, France. (2) Aix Marseille Univ, Université de Toulon, CNRS, CPT, Marseille, France (3) Institute of Industrial Science, University of Tokyo, Japan, (4) LIMMS-CNRS, IRL 2820, Tokyo, Japan

10:45 11:15

Coffee break

Session: Semiclassical electron transport

Chair: DRAGICA VASILESKA

- 11:15 11:45 **IMPACTS OF BAND STRUCTURES AND SCATTERING PROCESSES ON HIGH-FIELD CARRIER TRANSPORT IN WIDE BANDGAP SEMICONDUCTORS** Nobuya Mori (INVITED); Osaka University (Japan)
- 11:45 12:00 **Effect of Electron-Electron Scattering on the Energy Distribution in Semiconductor Devices** Hans Kosina and Josef Gull; Institute for Microelectronics, TU Wien, Gußhausstraße 27–29, 1040 Wien, Austria
- 12:00 12:15 **Efficient ab initio electronic transport methods** Z. Li, P. Graziosi (2) and N. Neophytou (1); (2) School of Engineering, University of Warwick, Coventry, CV4 7AL, UK (2) CNR-Bologna, Italy
- 12:15 12:30 **Modelling of Schottky-Barrier Diodes Operating under Strong Reverse-Bias Conditions** B. Orfao, B. G. Vasallo, S. Pérez, J. Mateos, and T. González; Dpto. De Física Aplicada and USAL-NANOLAB, Universidad de Salamanca, 37008 Salamanca, Spain
- 12:30 12:45 **Influence of Deformation Potential Scattering on Impact Ionization in Ultra-Wide Bandgap Materials** J. Shoemaker, R. Vatan, T. Biswas, A. Singh, M. Saraniti, S.M. Goodnick; Arizona State University, Tempe, AZ, USA
- 12:45 13:00 **Upper Valley and Degeneracy Interplay on the Mobility of Transition Metal Dichalcogenides: Insights from Monte Carlo Simulation** José M. Iglesias (1), Karol Kalna (2), Raúl Rengel (3) and Elena Pascual (3); (1) Department of Applied Mathematics, University of Salamanca, 37008 Salamanca, Spain (2) Nanoelectronic Devices Computational Group, Faculty of Science & Engineering, Swansea University, Swansea SA1 8EN, Wales, United Kingdom (3) Department of Applied Physics, University of Salamanca, 37008 Salamanca, Spain

13:00 15:00

Lunch and poster session II (page ix)

Session: Advanced nanoelectronics

Chair: TOMÁS GONZÁLEZ

- 15:00 15:30 **WHERE IS SEMICONDUCTOR TECHNOLOGY HEADING? A VIEW FROM THE INDUSTRY AND IMPLICATIONS ON COMPUTATIONAL NANOTECHNOLOGY** Carlos H. Diaz (INVITED); Senior Director in R&D (TSMC)
- 15:30 15:45 **Nanowire transport and edge passivation** P. Blaise (1), T. Kubis (2), E. Guichard (1); (1) Silvaco Inc., Santa Clara, CA 95054, USA and Montbonnot-Saint-Martin, 38330, FRANCE (2) School of Electrical and Computer Engineering, Purdue University, West Lafayette, IN 47907, USA
- 15:45:16:00 **Modeling Self-Heating Effects in 28 nm Technology Node Fully-Depleted SOI Devices** Z. Wang (1), D. Vasileska (1), C.S. Soares (2), G.I. Wirth (2), M.A. Pavanello (3) and M. Povolotskyi (4); (1) Arizona State University, Tempe, AZ, USA (2) UFRGS, Porto Alegre, Brazil (3) Centro Universitario FEI, Sao Bernardo do Campo, Brazil (4) Jacobs, Hanover, MD, USA
- 16:00 16:15 **Closing the “10-100 eV Gap” for Electron Thermalization in GaN Devices from First Principles** Dallin O. Nielsen (1), Chris G. Van de Walle (2), Sokrates T. Pantelides (3,4), Ronald D. Schrimpf (4), Daniel M. Fleetwood (4), and Massimo V. Fischetti (1); (1) Department of Materials Science and Engineering, University of Texas at Dallas (2) Materials Department, University of California, Santa Barbara (3) Department of Physics and Astronomy, Vanderbilt University (4) Department of Electrical and Computer Engineering, Vanderbilt University

16:15 16:30 **3D Quantum Corrected Monte Carlo Simulation of n-FinFETs** C. S. Soares (1), G. F. Furtado (2), A. C. J. Rossetto (3), G. I. Wirth, D. Vasileska (4); (1) Programa de Pós-Graduação em Microeletrônica Universidade Federal do Rio Grande do Sul Porto Alegre, Brazil. (2) Silvacó, Porto Alegre, RS, Brazil. (3) Centro de Desenvolvimento Tecnológico Universidade Federal de Pelotas Pelotas, Brazil (4) Department of Electrical Engineering Arizona State University Tempe, USA

16:30 17:00

Coffee break

Session: Quantum electron transport II

Chair: MARC BESCOND

- 17:00 17:15 **Edge-states interferometers in graphene nanoribbons: a time-dependent modelling** G. Forghieri (1), P. Bordone (1), and A. Bertoni (2); (1) Università di Modena e Reggio Emilia, via Campi, 213/A, Modena, Italy (2) Istituto Nanoscienze – CNR, Modena, Italy
- 17:15 17:30 **A Coupled Electrostatic – Quantum Transport Framework for Exascale Systems** S. S. Sawant (1), F. Léonard (2), J. Yao (1), and A. Nonaka (1); (1) Lawrence Berkeley National Laboratory, Berkeley, California, 94720, USA (2) Sandia National Laboratories, Livermore, California, 94550, USA
- 17:30 17:45 **Acoustic phonon modulation of terahertz quantum cascade lasers** A. Demic (1), A. Valavanis (1), J. Bailey (2), P. Dean (1), L. H. Li (1), A. G. Davies (1), E. H. Linfield (1), P. Harrison (3), J. E. Cunningham (1), A. Kent (2); (1) School of Electronic and Electrical Engineering, University of Leeds, Leeds LS2 9JT, UK (2) School of Physics and Astronomy, University of Nottingham, Nottingham NG7 2RD, UK (3) School of Computing and Engineering, University of Huddersfield, Huddersfield HD1 3DH, UK
- 17:45 18:00 **Simulation of Single-Electron Shuttling for Spin-Qubit Transport in a SiGe Quantum Bus** L. Ermoneit (1), B. Schmidt (1), J. Fuhrmann(1), T. Koprucki (1), L. R. Schreiber (2), and M. Kantner (2); (1) Weierstrass Institute for Applied Analysis and Stochastics, Mohrenstr. 39, 10117 Berlin, Germany (2) ARA-FIT Institute for Quantum Information, Forschungszentrum Jülich GmbH and Institute of Physics, RWTH Aachen University, Otto-Blumenthal-Str., 52074 Aachen, Germany
- 18:00 18:15 **Coherent Wigner Dynamics of a Superposition State in a Tunable Barrier Quantum Dot** M. Ballicchia, M. Nedjalkov, and J. Weinbub; Institute for Microelectronics, TU Wien, Gußhausstraße 27–29, 1040 Wien, Austria
- 18:15 18:30 **Incorporation of the Tight Binding Hamiltonian into Quantum Liouville-type Equations** A. Abdi, M. Pech, and D. Schulz; Chair for High Frequency Techniques, TU Dortmund, Friedrich-Wöhler-Weg 4, 44227 Dortmund, Germany

Thursday, June 15

Session: Engineered nanomaterials and nanostructures

Chair: TILLMANN KUBIS

- 9:00 9:30 **MULTISCALE MODELLING AND COMPUTATIONAL SPECTROSCOPY** Kersti Hermansson (INVITED); Uppsala University (Sweden)
- 9:30 9:45 **Solving Kohn-Sham Equations of Heterobilayer Systems Beyond 1000 Atoms: Twist Angle-dependent Piezoelectricity** Han-Wei Hsiao, Namita Narendra, and Tillmann Kubis; Elmore Family School of Electrical and Computer Engineering, Purdue University, West Lafayette, IN, USA
- 9:45 10:00 **Anomalous transient blue-shift in the internal stretch mode of CO on Pd(111)** Raul Bombín (1,2,3), Alberto S. Muzas (2), Dino Novko (4), J. Iñaki Juaristi (1,2,5) and Maite Alducin (1,5); (1) Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), Donostia-San Sebastián, Spain (2) Departamento de Polímeros y Materiales Avanzados: Física, Química y Tecnología, Facultad de Químicas (UPV/EHU), Donostia-San Sebastián, Spain (3) Departament de Física, Universitat Politècnica de Catalunya, Barcelona, Spain (4) Institute of Physics, Zagreb, Croatia (5) Donostia International Physics Center (DIPC), Donostia-San Sebastián, Spain
- 10:00 10:15 **Ab initio calculation of mobility degradation caused by Si-vacancies in SiC/SiO₂ channels** Colin Kälin, Mathieu Luisier; Integrated Systems Laboratory, ETH Zürich, Switzerland
- 10:15 10:30 **Modelling the electrical conductivity of carbon nanotube films** T.R. Durrant (1,2), D.Z. Gao (2), Y. Giret (2) and A.L. Shluger (1); (1) Department of Physics and Astronomy, University College

London. Gower Street, London WC1E 6BT, UK (2) Nanolayers Research Computing Ltd.1 Granville Court, Granville Road, London N12 0HL, UK

10:30 10:45 **Electric fields for tuning molecular orientation in TPD-modified glasses** [Marta Rodríguez-López](#) (1), Antonio, Cappai (2), Claudio Melis (2), Luciano Colombo (2), Javier Rodríguez-Viejo (1), Marta Gonzalez-Silveira (1); (1) Group of Thermal properties of Nanoscale Materials (GTNaM), Universitat Autònoma de Barcelona (UAB) & Catalan Institute of Nanoscience and Nanotechnology (ICN2), Barcelona, Spain. (2) Dipartimento di Fisica, Università di Cagliari, Cittadella Universitaria, Monserrato (Ca), Italy.

10:45 11:15

Coffee break

Session: 2D materials and devices

Chair: KAROL KALNA

11:15 11:30 **Shot noise in disordered graphene samples** P. Marconcini (1), D. Logoteta (2) and [M. Macucci](#) (1); (1) Dipartimento di Ingegneria dell'Informazione, Università di Pisa, Via Caruso 16, 56122 Pisa, Italy (2) Dipartimento di Ingegneria dell'Informazione, Elettronica e Telecomunicazioni (DIET), Università di Roma La Sapienza, via Eudossiana 18, 00184 Roma

11:30 11:45 **Engineering of Charge Current Flow in Nanoporous Graphenes** [I. Alcón](#) (1), A. Cummings (1) and S. Roche (1,2); (1) Catalan Institute of Nanoscience and Nanotechnology (ICN2), Campus UAB, Bellaterra, 08193 Barcelona, Spain (2) ICREA, Institutió Catalana de Recerca I Estudis Avançats, 08070 Barcelona, Spain

11:45 12:00 **Recombination Time in Drift-Diffusion Models of Graphene Field-Effect Transistors** [Pedro C. Feijoo](#) (1,2), Ferney A. Chaves (2) and David Jiménez (2); (1) Departamento de Matemática Aplicada a la Ingeniería Industrial, C/José Gutiérrez Abascal 2, 28006 Madrid, Universidad Politécnica de Madrid (2) Departament d'Enginyeria Electrònica, C/ de les Sitges s/n, 08193 Cerdanyola del Vallès (Barcelona), Universitat Autònoma de Barcelona, Spain

12:00 12:15 **Numerical simulation of terahertz carrier dynamics in monolayer MoS₂** [Shuva Mitra](#), Laleh Avazpour, and Irena Knezevic; Department of Electrical and Computer Engineering University of Wisconsin-Madison, Madison, WI 53706, USA

12:15 12:30 **Quantum Transport Study of Metal-TMD Contacts: Role of the Dielectric Environment** [Pranay Kumar Reddy Baikadi](#) (1), Peter Reyntjens (1,2), Maarten L. Van de Put (2) and William G. Vandenberghe (1); Department of Materials Science and Engineering, The University of Texas, Dallas, TX, USA (2) Department of Material Engineering, KU Leuven, Belgium

12:30 12:45 **Electrothermal Properties of 2D Materials** S. Klein (1), [Z. Aksamija](#) (2); (1) University of Massachusetts, Amherst, MA, USA, (2) University of Utah, Salt Lake City, UT, USA

12:45 13:00 **First-principles study of water molecules at the electrified graphene surface** [Hyeonwoo Yeo](#), Juho Lee, Ryong Gyu Lee, Seunghyun Yu, and Yong-Hoon Kim; School of Electrical Engineering, Korea Advanced Institute of Science and Technology (KAIST), 291 Daehak-ro, Yuseong-gu, Daejeon 34141, Korea

13:00 15:00

Lunch and poster session III (page x)

Session: Special session in honor of David K. Ferry

Chair: STEPHEN GOODNICK

15:00 15:15 **Wigner Transport in Magnetic Fields** M. Ballicchia, C. Etl, [M. Nedjalkov](#), and J. Weinbub; Institute for Microelectronics, TU Wien, Gußhausstraße 27–29, 1040 Wien, Austria

15:15 15:30 **Kirchhoff Coupling Generates ATP, the Chemical Energy of Life** [Robert Eisenberg](#); Illinois Institute of Technology, Rush University, University of Illinois, Chicago IL USA

15:30 16:15 **50 Years in the Semiconductor Underground: A Retrospective** [Stephen Goodnick](#) (1), [Paolo Lugli](#) (2) [Dragica Vasileska](#) (3) [Irena Knezevic](#) (4) and [Wolfgang Porod](#) (5); (1)Arizona State University (USA), (2)University of Bolzano (Italy), (3) Arizona State University (USA), (4) University of Wisconsin-Madison (USA) and (5) Notre Dame University (USA)

18:00 20:00

Visit to Barcelona

20:00

Gala dinner

Friday, June 16

Session: Neuromorphic computing

Chair: CARLO JACOBONI

- 9:00 9:30 **MEMRISTORS WITH THOUSANDS OF CONDUCTANCE LEVELS FOR ANALOG COMPUTING** J. Joshua Yang (INVITED); Future of Computing Institute University of Southern California (USA)
- 9:30 9:45 **Probabilistic viiodelling of resistive switching in emerging ReRAM cells** Y. V. Pershin (1) and V. A. Slipko (2); (1) Department of Physics and Astronomy, University of South Carolina, Columbia, SC 29208, USA (2) Institute of Physics, Opole University, Opole 45-052
- 9:45:10:00 **Compact modelling of memristors for neuromorphic circuit simulation** F. Aguirre, J. Suñé and E. Miranda; Departament d'Enginyeria Electrònica. Universitat Autònoma de Barcelona Campus de Bellaterra, 08193-Bellaterra (SPAIN)
- 10:00 10:15 **Molecular dynamics simulation of the full operation cycle of a HfO₂-based RRAM cell** X. Cartoixà (1), M. L. Urquiza (1,2), Md M. Islam (3), A. C. T. van Duin (4), and A. Strachan (5); (1) Departament d'Enginyeria Electrònica, Universitat Autònoma de Barcelona, 08193 Bellaterra (Barcelona), Spain, (2) Laboratoire des Solides Irradiés, École Polytechnique, Institut Polytechnique de Paris, Paris, France (3) Department of Mechanical Engineering, Wayne State University, Detroit, Michigan 48202, USA (4) Department of Mechanical Engineering, Pennsylvania State University, 240 Research East Building, University Park Pennsylvania 16802, USA (5) School of Materials Engineering, Purdue University, West Lafayette, Indiana 47907 USA
- 10:15 10:30 **Multiscale Modelling of Dielectric Breakdown in Amorphous HfO₂** Jack Strand (1,2) and Alexander Shluger (1); (1) Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK (2) Nanolayers Research Computing Ltd, 1 Granville Court, Granville Road, London, England, N12 0HL
- 10:30 10:45 **Termination-Dependence of Resistive Switching in SrTiO₃-based Valence Change Memory** M. Mladenovic, M. Kaniselman, C. Weilenmann, A. Emboras, and M. Luisier; Integrated Systems Laboratory, ETH Zürich, Gloriastrasse 35, 8092, Zürich, Switzerland
- 10:45 11:00 **Temperature-Dependent Electric Switching of Chalcogenide Memories Below the ns Limit** R. Brunetti, M. Rudan, and C. Jacoboni; FIM Department, University of Modena and Reggio Emilia, Modena, Italy, DEI Department, University of Bologna, Bologna, Italy
- 11:00 11:30 Coffee break

Session: Electrons under electromagnetic fields

Chair: IRENA KNEZEVIC

- 11:30 12:00 **QUANTUM PHOTODETECTORS** Francois Léonard (INVITED); Sandia National Laboratories (USA)
- 12:00 12:15 **Impact of hBN-encapsulation on light absorption in 2D-TMD-based photodetectors** A. A. Díaz-Burgos, A. Toral-López, J. Cuesta, E.G. Marín, F. Pasadas, F.G. Ruiz, A. Godoy; Departamento de Electrónica y Tecnología de Computadores, Universidad de Granada, Granada, Spain
- 12:15 12:30 **Dual-Potential Finite-Difference Method for Electrodynamics Within Multiphysics Solvers** S. W. Belling, L. Avazpour and I. Knezevic; Department of Electrical and Computer Engineering, University of Wisconsin – Madison Madison, WI 53706 USA
- 12:30 12:45 **Polaritonic features in the THz displacement current through RTDs in microcavities** C. F. Destefani (1), M. Villani (1), X. Cartoixà (1), M. Feiginov (2), and X. Oriols (1); (1) Department of Electronic Engineering, Universitat Autònoma de Barcelona, Spain (2) Department of Electrical Engineering and Information Technology, Technische Universität Wien, Austria
- 12:45 13:00 **Switching Performance of Mo-based pMTJ and dsMTJ structures** B. Pruckner (1) S. Fiorentini (1), N. Jorstad (2), T. Hadamek (1), S. Selberherr (2), W. Goes (3), and V. Sverdlov (1,2); (1) Christian Doppler Laboratory for Nonvolatile Magnetoresistive Memory and Logic at the (2) Institute for Microelectronics, TU Wien, Gußhausstraße 27–29, A-1040 Wien, Austria (3) Silvaco Europe, Cambridge, United Kingdom
- 13:00 13:15 **Deterministic Approach for Skyrmionic Dynamics at Non-zero Temperatures** C. Navau, J. Castell-Queralt, L. Gonzalez-Gómez, N. Del-Valle; Departament de Física, Universitat Autònoma de Barcelona, 08193 Bellaterra, Barcelona, Catalonia, Spain
- 13:15 Closing remarks

Poster session I Tuesday June 13 13:00 15:00

Mach-Zehnder-like interferometry with graphene nanoribbon networks [Sofia Sanz](#) (1), Nick Papior (2), Geza Giedke (3,4), Daniel Sanchez-Portal (5), Mads Brandbyge (1), Thomas Frederiksen (3,4); (1) Department of Physics, DTU, DK-2800 Kgs. Lyngby, Denmark, (2) DTU Computing Center DK-2800 Kgs. Lyngby, Denmark, (3) Donostia International Physics Center (DIPC), E-20018, Donostia-San Sebastian, Spain, (4) IKERBASQUE, Basque Foundation for Science, E-48013, Bilbao, Spain (5) Centro de Fisica de Materiales CSIC-UPV/EHU, E-20018, Donostia-San Sebastian, Spain

Two conductivity regimes in semiconductor δ -layer tunnel junctions [D. Mamaluy](#) and J.P. Mendez; Cognitive & Emerging Computing, Sandia National Laboratories, Albuquerque, USA

Charge Transport Properties of Cytochrome b562 on Gold Interfaces [G.N. Jonnalagadda](#), Z. Futera; Faculty of Science, University of South Bohemia, Branisovska 1760, 370 05 Ceske Budejovice, Czech Republic

Coherent and Incoherent Electron Transport through Protein Junctions Investigated by DFT-based Approaches [Z. Futera](#); Faculty of Science, University of South Bohemia, Branisovska 1760, 370 05 Ceske Budejovice, Czech Republic

Schrödinger Equation Solver Based on Data-Driven Physics-Informed Generic Building Blocks [Martin Veresko](#), Ming-Cheng Cheng; Department of ECE, Clarkson University, 8 Clarkson Ave, Potsdam NT, United States

Considerations on Treating Polar-Optical Phonon Scattering in Real Space [D.K. Ferry](#); School of Electrical, Computer, and Energy Engineering, Arizona State University, Tempe, AZ 25287-6206 USA

Spin-selective transport phenomena in helical molecular wires [R. Korytá](#) (1), Š. Marek (1), J. van Ruitenbeekz (2) and F. Eversy (3); (1) Charles University, Czech Republic, (2) Institute of Theoretical Physics, University of Regensburg, Germany (3) Huygens-Kamerlingh Onnes Laboratory, Leiden University, Netherlands

Efficient Method to Obtain Target Bias Solutions of 6F2 DRAM Cells with Geometric

Fluctuations [Geonho Park](#), Seung-Cheol Han, and Sung-Min Hong; School of Electrical Engineering and Computer Science, Gwangju Institute of Science and Technology

First-principles Study on As Antisites in InGaAs Alloys, GaAs and InAs [Yucheol Cho](#), Gyeongdo Ham and Daeshik Kim*; School of Electrical Engineering, Korea Advanced Institute of Science and Technology, Daejeon, 34141, South Korea

First-Principles investigation of polytypic defects in InP [Christian Dam Vedel](#) (1,2), Søren Smidstrup (2), Vihar P. Georgiev (1); (1) Device Modelling Group, School of Engineering, University of Glasgow, United Kingdom (2) Synopsys Denmark ApS, Copenhagen, Denmark

Multiscale simulations of ink-jet printed devices [D. Marian](#) (1), P. K. Dubey (1), M. Perucchini (1), E. G. Marin (2), and G. Fiori (1); (1) Dipartimento di Ingegneria dell'Informazione, Università di Pisa, Via G. Caruso 16, Pisa, 16122, Italy (2) Departamento de Electrónica, Universidad de Granada, Avenida Fuente Nueva s/n, Granada, 18071, Spain

An extended Hueckel theory parameterization of Germanium for doped SiGe alloys [D. Dick](#) (1,3), F. Fuchs (2,3), S. Gemming (3,4) and J. Schuster (1,2,3); (1) Center for Microtechnologies, Chemnitz University of Technology, Chemnitz, Germany (2) Fraunhofer IISIT institute for Electronic Nano Systems (ENAS), Chemnitz, Germany (3) Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Chemnitz, Germany (4) Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany

Time-Domain Computation of the Linewidth Enhancement Factor in Multi-Quantum-Well

Semiconductor Optical Amplifiers [Ö.E. Aşırım](#), C. Jirauschek; TUM School of Computation, Information and Technology, Technical University of Munich, Hans-Piloty Straße 1, 85748 Garching, Germany

Multiscale simulation of high harmonic generation using artificial intelligence [Javier Serrano](#), José Miguel Pablos-Marín and Carlos Hernández-García; Grupo de Investigación en Aplicaciones del Láser y Fotónica, Departamento de Física Aplicada Universidad de Salamanca, Pl. Merced s/n, E-37008 Salamanca, Spain

Application of Discontinuous Galerkin Methods onto Quantum-Liouville type Equations [V. Ganiu](#), D. Schulz; Chair for High Frequency Techniques, TU Dortmund, Friedrich-Woehler-Weg 4, 44227 Dortmund, Germany

Poster session II Wednesday, June 14 13:00 15:00

Full-Band Device Simulator with Real-Space Treatment of the Short-Range Coulomb

Interactions for Modeling 4H-SiC VDMOS Devices [Dragica Vasileska](#) and Chi-Yin Cheng; School of Electrical, Computer and Energy Engineering Arizona State University, Tempe, AZ 85287-5706

Schottky barriers in one-dimensional field-effect transistors: a model-based Characterization

[Anibal Pacheco-Sanchez](#), David Jiménez; Departament d'Enginyeria Electrònica, Escola d'Enginyeria, Universitat Autònoma de Barcelona, Bellaterra 08193, Spain.

Silicon passivation of zigzag graphene edge enabling robust spin-polarized nanogap quantum transport

Juho Lee, [Seunghyun Yu](#) and Yong-Hoon Kim; School of Electrical Engineering, Korea Advanced Institute of Science and Technology (KAIST), 291 Daehak-ro, Yuseong-gu, Daejeon 34141, Korea

Monte Carlo Simulations of Electrons in Al₄SiC₄ Ternary Carbide

[K. Kalna](#) (1) and D. Chaussende (2); (1) NanoDeCo Group, Dept. Electronic & Electrical Engineering, Faculty of Science & Engineering, Swansea University, Swansea, SA1 8EN, Wales, United Kingdom (2) Université Grenoble Alpes, CNRS, Grenoble INP, SIMaP, 38000 Grenoble, France

Ab initio heat dynamics in phonon-based dark matter detectors

[M. Raya-Moreno](#) (1), B. J. Kavanagh (2), E. Vilanova (1), L. Fàbrega (1) and R. Rurali (1); (1) Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, 08193 Bellaterra, Spain (2) Instituto de Física de Cantabria (IFCA, UC-CSIC), Av. De los Castros, 39005 Santander, Spain

Revealing the Thermal and Mechanical Properties of Amorphous Boron Nitride

[Onurcan Kaya](#), Ivan Cole and Stephan Roche; Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, Bellaterra, 08193 Barcelona, Spain

Phonon transport across Ge/GaAs heterojunctions by nonequilibrium molecular dynamics

[T. Albrigi](#) and R. Rurali; Institut de Ciència de Materials de Barcelona (ICMAB-CSIC) Campus UAB, 08193 Bellaterra, Spain

Electrothermal simulations of a thermal sensor integrated with a 4H-SiC JFET

D. Monaghan, [A. Martinez](#) and M. Jennings; Department of Electrical and Electronic Engineering, Swansea University, UK Swansea, UK

Effects of structural arrangements on thermoelectric properties of SiX (X=N,P,As,Sb,Bi)

monolayers [Subhradip Ghosh](#), and Himanshu Murari; Department of Physics, Indian Institute of Technology Guwahati, Guwahati-781039, India

Analysis of Wave speed in magneto-thermoelastic nonlocal micropolar orthotropic medium

[Anand Kumar Yadav](#) (1) and Sangeeta Kumari (2); (1) Shishu Niketan Model Senior Secondary School, Sector 22-D, Chandigarh, India (2) Department of mathematics, Chandigarh University, Gharuan, Punjab, India

Towards a semi-classical simulator for the energy distribution functions in optically

excited hot carrier semiconductor devices J. R. Barker (1) and [A. M. Martinez](#) (2); (1) James Watt School of Engineering, University of Glasgow, Glasgow G12 8LT, UK (2) Department of Electrical and Electronic Engineering, Swansea University, Bay Campus, UK

Breakdown of GaN-based Planar Gunn Diodes investigated through a Combined Deep

Learning-Monte Carlo Model [S. García-Sánchez](#), R. Rengel, S. Pérez, T. González and J. Mateos; Applied Physics Department and NANOLAB, Universidad de Salamanca, Salamanca 37008, Spain

DECaNT Numerical Tool for Exciton Dynamics in Carbon Nanotube Films

S. S. Sanders, [S. W. Belling](#) and I. Knezevic; Department of Electrical and Computer Engineering, University of Wisconsin – Madison Madison, WI 53706, USA

Efficient Monte Carlo Electron Transport Formalism for Highly Nanostructured Materials

[Pankaj Priyadarshi](#) and Neophytos Neophytou; School of Engineering, University of Warwick, Coventry, CV4 7AL, United Kingdom

Thermal and electrical properties of nanocrystalline superionic Na_xCu_{1.75S} (x=0.1, 0.15, 0.2, 0.25) compounds

[M.M. Kubenova](#), K.A. Kuterbekov, M.Kh. Balapanov, A.M. Kabyshev, K.Zh. Bekmyrza, Zh.A. Mukhan and A.K. Kulanov; L.N. Gumilyov Eurasian National University, 010008 Astana, Kazakhstan

Extending the small-signal modelling of GFETs to ambipolarity regime

Nikolaos Mavredakis, [Anibal Pacheco-Sanchez](#), David Jiménez; N. Mavredakis, A. Pacheco and D. Jiménez are with the Departament d'Enginyeria Electrònica, Escola d'Enginyeria, Universitat Autònoma de Barcelona, Bellaterra 08193, Spain.

Poster session III Thursday, June 15 13:00 15:00

Simulation-based Optimization of a Sensor-Indenter System for Thin Layer Crack Detection F.

[Tremmel](#) (1), O. Nagler (1), C. Kutter (2), and R. Holmer (3); (1) Infineon Technologies AG, Am Campeon 1-15, 85579 Neubiberg, Germany (2) Polytronic Systems (EMFT) Institute of Physics, UniBw München, Germany (3) Faculty of Electrical Engineering and Information Technology, OTH Regensburg, Germany

Functionalized TaS₂ for thermoelectric applications: an ab-initio investigation [Francesco Siddi](#),

Antonio Cappai, Luciano Colombo and Claudio Melis; Department of Physics, University of Cagliari, Italy

Monte Carlo Solution to Excess Noise and Spatial Blur in Amorphous Selenium Thin-films

[Dragica Vasileska](#) (1), Atreyo Mukherjee (2), and Amir H. Goldan (3); (1) School of Electrical, Computer and Energy Engineering, Arizona State University, AZ, US (2) Department of Electrical Engineering, Stony Brook University, NY, US (3) Department of Radiology, Weill Cornell Medical College, Cornell University, New York, NY, USA

Impurity- and remote-phonon-limited mobility in TMD monolayers [Shoaib Mansoori](#), Sanjay

Gopalan, and Massimo V. Fischetti; Department of Materials Science and Engineering, The University of Texas at Dallas, 800 W. Campbell Rd., Richardson, TX 75080

Self-consistent k.p band structure in doped core-shell nanowires with type-I, type-II and

broken-gap radial heterointerfaces A. Vezzosi (1), [A. Bertoni](#) (2), and G. Goldoni(1, 2); (1) Università di

Modena e Reggio Emilia, via Campi, 213/A, Modena, Italy (2) Istituto Nanoscienze – CNR, Modena, Italy

A Sunlight Cooling Device Based on a 2D van der Waals Heterojunction [P. Dalla Valle](#), M. Bescond,

F. Michelini, and N. Cavassilas; Aix Marseille Université, CNRS, Université de Toulon, IM2NP UMR 7334, 13397, Marseille, France

Ab initio effective dragged thermoelectric properties in Si nanowires [M. Raya-Moreno](#) (1), R. Rurali

(1) and X. Cartoixà (2); (1) Institut de Ciència de Materials de Barcelona (ICMABCSIC), Campus UAB, 08193 Bellaterra, Spain (2) Departament d'Enginyeria Electrònica, Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain

Resistance calculation in metal-2D contacts: Accuracy of numerical integration Peter Reyntjens

(1,2,3), Pranay Baikadi (2), Raseong Kim (4), Maarten Van de Put (3), Bart Sorée (1,3,5) and [William G. Vandenberghe](#) (2); (1) Department of Electrical Engineering, KULeuven (2) Department of Materials Science, UT Dallas (3) Imec (4) Components Research, Intel Corporation, Hillsboro, OR 97124 USA (5) Department of Physics, Universiteit Antwerpen

FiPo FDTD Algorithm: Modeling Electric and Magnetic Fields with Potentials A and ϕ for

Quantum Transport Solvers L. Avazpour, M.L. King, S.W. Belling, and [I. Knezevic](#); Department of Electrical and

Computer Engineering University of Wisconsin-Madison, Madison, WI 53706, USA

Noise impact on memristor performance: improvement of neuromorphic binary STDP [E.](#)

[Salvador](#) (1), R. Rodriguez (1), E. Miranda (1), J. Martin-Martinez (1), A. Rubio (2), V. Ntinis (2), G. Ch. Sirakoulis (3), A. Crespo-Yepes (1), M. Nafria (1); (1) Electronic Engineering Department, Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain (2) Electronic Engineering Department, Universitat Politècnica de Catalunya, 08034, Barcelona, Spain (3) Dept. of Electrical & Computer Engineering, Democritus University of Thrace, 67100, Xanthi, Greece

Control of the local magnetic states in graphene with voltage and gating [Fei Gao](#) (1,2), Yu Zhang

(3), Lin He (3), Shiwu Gao (4) and Mads Brandbyge (1); (1) Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark (2) Donostia International Physics Center (DIPC), 20018 Donostia-San Sebastián, Spain (3) Center for Advanced Quantum Studies, Department of Physics, Beijing Normal University, 100875 Beijing, China (4) Beijing Computational Science Research Center, 100193 Beijing, China

General Maxwell-Bloch modelling of self-induced transparency in N-level atom [A. Demic](#) (1), T.B

Gill (1), M.A. Talukder (2), D. Indjin (1), P. Dean (1); (1) School of Electronic and Electrical Engineering, University of Leeds, Leeds LS2 9JT, UK (2) Electrical and Electronic Engineering, Bangladesh University of Engineering and Technology, Dhaka-1205, Bangladesh

Electronic and Magnetic Properties of Eu doped GaN nanowires: An Ab-initio study for spin-

optoelectronic applications [V. K. Gudelli](#) and I. S. Roqan; Physical Sciences and Engineering Division, King Abdullah

University of Science and Technology, Thuwal-23955-6900, Saudi Arabia

From radiofrequency to infrared antennas: downscaling a rectangular loop geometry [D.K.](#)

[Maram](#), J. Garcia, R. Ruiz, X. Cartoixà, G. Abadal; Dept. Enginyeria Electrònica, Campus UAB, 08193-Bellaterra, Spain;