# Manasa Kaniselvan

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### Profile

- Developing atomistic simulation methods to model the motion of atoms and/or flow of electronic current in modern semiconductor devices such as transistors and emerging non-volatile memory cells
- Academic background in semiconductor and solid-state physics, and numerical methods
- Experience developing physics simulation codes from scratch in C++ and Python
- Interested in applications of Geometric Machine Learning (ML) in atomistic simulations, principles of High Performance Computing (HPC), and theory-experiment co-design of semiconductor devices

### **EDUCATION**

ETH Zurich Zurich, Switzerland Candidate for PhD, Information Technology and Electrical Engineering September 2021-present

University of Waterloo Waterloo, ON, Canada

Master of Applied Science (MASc), Electrical and Computer Engineering

September 2019–May 2021

University of Waterloo Waterloo, ON, Canada Bachelor of Applied Science (BASc), Nanotechnology Engineering. September 2014–May 2019

# EXPERIENCE

#### Scientific Assistant (PhD Candidate) - ETH Zürich

Zürich, Switzerland September 1<sup>st</sup> 2021 - 2026

Advisor: Dr. Mathieu Luisier, Professor

— Developing multi-scale atomistic models for resistive switching in emerging Non-Volatile Memories (NVM), using methods such as Density Functional Theory (DFT), ab initio quantum transport, Kinetic Monte Carlo, and Machine-learned interpolation methods. Accelerating the developed simulation codes on GPUs and multicore architectures. Working with experimental partners at ETH and IBM Zurich to realize new devices and investigate their operating mechanisms.

### PhD Intern in Device/Process Modelling - Samsung Semiconductor

San Jose, CA, USA

Supervisor: Dr. Byounghak Lee, Principle Engineer

May  $15^{th}$  2023 - August  $4^{th}$  2023

 Developed and implemented a symmetry-aware topological classification algorithm for large-scale semiconductor device and process simulations. Presented the results to partners in Samsung Korea.

#### Research Assistant (MASc Student) - University of Waterloo

Waterloo, ON, Canada

Advisor: Dr. Youngki Yoon, Associate Professor

September  $1^{st}$  2019 - September  $1^{st}$  2021

Used Density Functional Theory and Non-Equilibrium Green's Function-based transport codes to design and simulate
devices made from 2D materials. Investigated defect and strain-engineering in FET and TFET structures. Collaborated
with experimental partners at Sungkyunkwan University, South Korea, to fabricate and test devices.

#### Internship - Waterloo Institute for Nanotechnology (WIN)

Waterloo, ON, Canada

Supervisor: Dr. Dayan Ban, Professor

January  $1^{st}$  2018 - September  $1^{st}$  2018

— Wrote a MATLAB+c-mex code to simulate the operation of Resonant-Phonon Quantum Cascade Lasers, based on self-consistently solved wavefunctions and charge distributions. Implemented Markov-Chain Monte-Carlo global optimization methods to search for designs with higher-temperature lasing potential. Assisted in electro-optical characterization of fabricated devices.

#### Formulations Engineering Intern - Adaptive Surface Technologies (AST)

Cambridge, MA, USA

Supervisor: Dr. Tehila Nahum, Principle Formulations Engineer

September  $1^{st}$  2016 - April  $30^{th}$  2017

 AST develops slippery coatings on the principle of infusing a nanoporous surface with a lubricant. Worked in a team of three engineers to formulate food-safe container coatings for a customer in the consumer packaging industry.

### Internship - National Institute of Materials Science (NIMS)

Supervisor: Dr. Genki Yoshikawa, Associate Professor and Group Leader

Tsukuba, Ibaraki, Japan January  $1^{st}$  2016 - April  $1^{st}$  2016

 Optimized the coating of drop-casted polymer films on a membrane-type sensor which measures mechanical deflection upon gas absorption to perform 'olfactory' sensing. Designed and 3D printed parts to customize dispensing equipment. Used COMSOL multiphysics to model sensor performance.

### Internship - Canadian Nuclear Laboratories (CNL)

Chalk River, Ontario, Canada

Supervisor: Dr. Syed Bukhari, Research Associate, Neutron Scattering Branch

May 2015 - August 2015

 Optimized sputtering parameters to minimize the interfacial roughness between stacked metal-alloy thin films and study their nanoscale corrosion mechanisms.

# TEACHING & SUPERVISION

#### Lectures

• Digital Electronics, Ashesi University (in collaboration with ETH Zurich)

February 2024

Primary lecturer for a 2-week block-course on Digital Electronics held as part of the ETH-Ashesi collaborative Masters program in Ghana.

### **Student Project Supervisions**

• Masters' thesis of Alexander Maeder, ETH Zurich

September 2023 - March 2024

Implementing a distributed, GPU-accelerated Kinetic Monte Carlo code for nanoionic memory device simulations. Co-supervised with Dr. Alexandros Ziogas and Vincent Maillou.

- Masters' thesis of Jente Clarysse, ETH Zurich

April 2023 - October 2023

Simulating thermally-activated switching phenomena in oxide-based resistive memory.

• Masters' semester project of Jente Clarysse, ETH Zurich

September 2022 - January 2023

Developing a graph-based model of current flow through atomistic structures.

· Masters' semester project of Zhouyang Yu, ETH Zurich

September 2022 - January 2023

Preforming quantum transport simulations on Interband Cascade Lasers (ICLs) using an in-house NEGF solver. Co-supervised with Prof. Matheiu Luisier.

• Bachelor thesis of Patrik Gjini, ETH Zurich

February 2022 - May 2022

Implemented a Fast Multipole Method algorithm to accelerate the solution of Poisson's equation on unstructured grids, written in Python. Co-supervised with Dr. Marko Mladenovic.

• Masters' semester project of Patrick Bütler, ETH Zurich

February 2022 - May 2022

Investigating phase transition-induced resistive switching in monolayer  $MoTe_2$  towards non-volatile memory applications, using ab-initio Molecular Dynamics. Co-supervised with Jonathan Backmann.

• Research projects of Patrick Kim and Raymond Chong, Deep River Science Academy

May 2015 - Aug 2015

Minimizing the interfacial roughness of sputtered metal alloy thin films to investigate nano-scale corrosion mechanisms, using X-Ray Reflectometry and X-Ray Diffraction. Counted towards the students' high-school course credit.

# **Teaching Assistant Positions**

• Quantum Transport in Nanostructures, ETH Zurich

February 2022-2024 - May 2022-2024

Taught one third of the tutorials for the course held in 2022, 2023, and 2024.

January 2021 - April 2021

• Linear Circuits (NE140), University of Waterloo Prepared and taught all remote (synchronous) tutorials.

• Nanoelectronics (NE471), University of Waterloo

September 2020 - December 2020

Held office hours for student questions, prepared assignments, and marked exams.

May 2020 - August 2020

• Electronic Circuits (NE344), University of Waterloo Prepared and taught all remote (synchronous) tutorials.

January 2020 - April 2020

• Linear Circuits (NE140), University of Waterloo Prepared and taught all tutorials.

### Team Lead - UW Nano Robotics Group (UWNRG)

Waterloo, ON, Canada January 2015 - July 2019

- UWNRG designs microbotic actuation systems to compete at the annual IEEE ICRA Microbotics Challenges.
- Led the development of a microbot called SAM (Solenoid Actuated Microbot). Managed funding applications for lab
  expenses, equipment, cleanroom usage, and conference travel costs.
- Competition Record: 3rd place (at ICRA 2015), 1st place (at ICRA 2016), 2nd place (at ICRA 2018).

### Project Funding

•	"Flexible Photovoltaics with 2I	O Material Heterostructures"	(NSERC PGSD Doctoral A	Award) - 63,000 CAD	2021
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- "Simulations of semiconductor quantum structures" (NSERC Undergraduate Student Research Award) 4,000 CAD 2018
- "Modeling of quantum cascade lasers" (NSERC Undergraduate Student Research Award) 4,000 CAD 2017

# SELECTED SCHOLARSHIPS & AWARDS

$\bullet~$ Top 10% (out of 715) Poster Commendation at the Psi-K Conference	2022
• Waterloo Faculty of Engineering Awards (x2)	2020
• Sanford Fleming Foundation (SFF) Teaching Assistant Excellence Award	2021
• Waterloo Dean's Entrance Award (Graduate)	2019
• NIMS (Japan) Internship Program Fellowship	2016
• Waterloo President's Scholarship (Undergraduate)	2014

### Peer-Reviewed Journal Articles & Conference Papers

- '\*' = equal contribution, '+' = supervised masters students
- 1. M. Kaniselvan, M. Mladenović, J. Clarysse+, and M. Luisier, "Insights behind multi-level conductance transitions in HfO<sub>x</sub> memristors". Device Research Conference (DRC), June 2024.
- M. Sritharan, R.K.A Bennett, M. Kaniselvan, and Y. Yoon, "A Comparative Study on 2D Materials with Native High-Oxides for Ultrascaled Transistors", Materials Today Electronics, March 2024. doi:10.1016/j.mtelec.2024.100096
- 3. Alexander Maeder+, **Manasa Kaniselvan**, Marko Mladenovic, Mathieu Luisier and Alexandros Nikoloas Ziogas, "Scalable Simulations of Resistive Memory Devices: A Dynamical Monte Carlo Approach." *Platform for Advanced Scientific Computing (PASC24)*, Zurich, Switzerland, June 2024.
- 4. M. Kaniselvan, M. Luisier, and M. Mladenovic, "Atomistic Modelling of Field-Induced Resistive Switching in Valence Change Memory," ACS Nano, April 2023. doi: 10.1021/acsnano.2c12575 (\*Journal Cover Article)
  - In the media: [Covered by ETH] [Covered by the Werner Siemens Foundation]
- 5. Marko Mladenovic, **Manasa Kaniselvan**, Christoph Weilenmann, Alexandros Emboras, and Mathieu Luisier *Termination-Dependence of Resistive Switching in SrTiO*<sub>3</sub>-based Valence Change Memory. International Workshop on Computational Nanotechnology (IWCN), Barcelona, Spain, June 2023. Talk.
- 6. H. Park\*, A. Sen\*, M. Kaniselvan, A.AlMutairi, A. Bal, L. Lee, Y.Yoon, and S. Kim, "Wafer-scale Nanoporous 2D Active Pixel Image Sensor Matrix with Highly Uniformity, High Sensitivity, and Rapid Switching," *Advanced Materials*, February 2023. doi: 10.1002/adma.202210715 (\*Journal Cover Article)
- M. Kaniselvan, M. Luisier, and M. Mladenovic, "An Atomistic Modelling Framework for Valence Change Memory Cells," Solid State Electronics: LETTERS from the International Conference on Simulation of Semiconductor Processes and Devices 2022, October 2022 doi: 10.10632F5.0053789
- 8. M. Kaniselvan, M. Sritharan, and Y. Yoon, "Mitigating Tunneling Leakage in Ultrascaled HfS<sub>2</sub> pMOS Devices with Uniaxial Strain," *IEEE Electron Device Letters*, June 2022 doi:10.1109/LED.2022.3179228 (\*Editor's Pick)

- 9. M. Kaniselvan and Y. Yoon, "Strain-tuning PtSe<sub>2</sub> for high ON-current lateral tunnel field-effect transistors," Applied Physics Letters, vol. 119, no. 7, p. 073102, Aug. 2021. doi:10.1063%2F5.0053789
- 10. G. Han, M. Kaniselvan, and Y. Yoon, "Photoresponse of MoSe<sub>2</sub> Transistors: A Fully Numerical Quantum Transport Simulation Study," ACS Applied Electronic Materials, vol. 2, no. 11, pp. 3765–3772, Nov. 2020. doi:10.1021/acsaelm.0c00795
- 11. M. Naqi\*, **M. Kaniselvan\***, S. Choo\*, G. Han, S. Kang, J. Kim, Y. Yoon, and S. Kim, "Ultrasensitive Multilayer MoS<sub>2</sub>-Based Photodetector with Permanently Grounded Gate Effect," *Advanced Electronic Materials*, vol. 6, no. 4, p. 1901256, Feb. 2020. doi: 10.1002/aelm.201901256.

#### Submitted manuscripts:

- 12. M. Kaniselvan\*, A. Maeder\*+, M. Mladenovic, M. Luisier, A. Ziogas, "Accelerated Kinetic Monte Carlo Simulations of Atomistically-Resolved Resistive Memory Arrays". Submitted.
- C. Weilenmann, A. Ziogas, T. Zellweger, K. Portner, M. Mladenović, M. Kaniselvan, T. Moraitis, M. Luisier, A. Emboras, "Single Neuromorphic Memristor closely Emulates Multiple Synaptic Mechanisms for Energy Efficient Neural Networks". Under revision. Arxiv link: https://arxiv.org/abs/2402.16628

# OTHER CONFERENCE CONTRIBUTIONS

- 1. Manasa Kaniselvan, Marko Mladenovic, Patrik Gjini+, and Mathieu Luisier Modelling transport in valence change memory cells. Psi-k Conference, Lausanne, Switzerland, August 2022. Poster.
- 2. Manasa Kaniselvan, Marko Mladenovic, Patrik Gjini, and Mathieu Luisier Modelling transport in valence change memory cells. CECAM Workshop on "Quantum transport methods and algorithms: from particles to waves approaches", ETH Zürich, Switzerland, July 2022. Poster.
- 3. Manasa Kaniselvan. Engineering the Performance of 2D Transition Metal Dichalcogenide Nanotransistors through Quantum Transport Simulations. Nanotechnology Seminar delivered at the University of Waterloo, June 2021.
- 4. Boyu Wen, Chao Xu, Siyi Wang, Sm Shazzad Rassel, Manasa Kaniselvan, Chris Deimert, Zbigniew Wasilewski and Dayan Ban Novel 4-well THz QCL with hybrid injection/extraction channels. ITQW2019: Infrared Terahertz Quantum Workshop.
- 5. Mary Chen\*, Manasa Kaniselvan\*, Corin Seeleman\*, Danielle Smith\*. A Real-Time Non-Invasive Sensor for Monitoring Laser-Induced Temperature in Medical Applications. Waterloo Engineering Design Symposium 2019. Waterloo, ON, Canada. Oral presentation & poster.
- 6. UW Nano Robotics Group. Solenoid Actuated Microbot (SAM). 2018 IEEE IEEE International Conference on Robotics and Automation (ICRA). Brisbane, Australia. Competition & poster.
- 7. UW Nano Robotics Group. ElectroMagnetic Micro Actuation (EMMA): Version 2. 2016 IEEE International Conference on Robotics and Automation (ICRA). Stockholm, Sweden. Competition & poster
- 8. UW Nano Robotics Group. ElectroMagnetic Micro Actuation (EMMA) 2015 IEEE International Conference on Robotics and Automation (ICRA). Seattle, Washington, USA. Competition & poster

# PEER REVIEW ACTIVITY

Reviewer for: npj Computational Materials, IEEE Transactions on Electronic Devices, IEEE Electron Device Letters, Physical Review E, Physical Review Applied