Manasa Kaniselvan

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PhD candidate at ETH Zurich, originally from Canada. Working at the intersection of semiconductor physics, high performance computing, and geometric deep learning to advance large-scale semiconductor simulations at atomistic and *ab initio* levels of theory.

Skills - C++, Python (+PyTorch), high performance computing (CUDA/HIP, MPI, OpenMP), version control (git), scientific data visualization (Blender - intermediate), technical writing and presentation

Education

ETH Zurich — Zurich, Switzerland
Candidate for PhD, Information Technology and Electrical Engineering — November 2021–May 2026

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**
Advisor: Dr. Mathieu Luisier, Professor — September 1^{st} 2021 - 2026

- Developing multi-scale atomistic models for emerging memory devices, using methods such as Density Functional Theory (DFT), *ab initio* quantum transport, and Kinetic Monte Carlo. Incorporating equivariant graph neural networks to learn the electronic structure of individual material components, and adapting them for large-scale graphs which can describe structural disorder. Accelerating the developed codes on GPUs and multicore architectures.

PhD Intern - Samsung Semiconductor Inc — **San Jose, CA, USA**
Supervisor: Dr. Byounghak Lee, Principle Engineer — May 15^{th} 2023 - August 4^{th} 2023

- Accelerated a large-scale semiconductor process/device code by developing an algorithm to leverage internal symmetries. Presented implementation and results to the Samsung Electronics applications team in 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

- Investigated transistor devices made from strain-engineered 2D materials using DFT and quantum transport methods. Collaborated with experimental partners to fabricate and test devices.

Undergraduate Intern - Waterloo Institute for Nanotechnology — **Waterloo, ON, Canada**
Supervisor: Dr. Dayan Ban, Professor — January 1^{st} 2018 - September 1^{st} 2018

- Wrote a MATLAB code to simulate the operation of Resonant-Phonon Quantum Cascade Lasers (QCLs). Implemented global optimization methods to search for designs with higher-temperature lasing potential.

Undergraduate Intern - Adaptive Surface Technologies — **Cambridge, MA, USA**
Supervisor: Dr. Tehila Nahum, Principle Engineer — September 1^{st} 2016 - April 30^{th} 2017

- AST develops slippery coatings by infusing nano-porous surfaces with lubricants. Worked in a team of three engineers to formulate a food-safe slippery container coating for one of the largest companies in the consumer packaging industry.

Undergraduate Intern - National Institute of Materials Science — **Tsukuba, Ibaraki, Japan**
Supervisor: Dr. Genki Yoshikawa, Associate Professor — January 1^{st} 2016 - April 1^{st} 2016

- Optimized the morphology of drop-casted polymer films which served as active layers for a silicon nanosensor. Used COMSOL multiphysics to model sensor performance in the presence of film non-idealities.

Selected Awards

- NSERC PGSD-3 Doctoral Award ("Flexible Photovoltaics with 2D Material Heterostructures") - 63,000 CAD 2021
- Sanford Fleming Foundation (SFF) Teaching Assistant Excellence Award - 500 CAD 2021
- Waterloo Dean's Graduate Entrance Award - 5,000 CAD 2019
- NSERC Undergraduate Student Research Award ("Simulating semiconductor quantum structures") - 4,000 CAD 2018
- NSERC Undergraduate Student Research Award ("Modeling quantum cascade lasers") - 4,000 CAD 2017

Teaching & Supervision

Lectures

- **(Guest lecturer) Brain Inspired Computing: From Devices to Applications, ETH Zurich** April 2024
  Designed and delivered a lecture on device simulation approaches for non-volatile resistive memory.
- **(Co-Lecturer) 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. Served as a technical interviewer for applicants of the following cohort.

Student Project Supervisions

At ETH, masters' students can undertake semester- and thesis-projects proposed and led by PhD candidates. I have supervised 4 semester projects (for which students work 4 months part-time), and 2 theses (6 months full time).

- **Masters' thesis of Rayen Mahjoub, ETH Zurich** September 2024 - March 2025
  Adapting equivariant graph neural networks for electronic structure prediction of phase-change materials.
- **Masters' thesis of Alexander Maeder, ETH Zurich** September 2023 - March 2024
  Distributing iterative solvers for a GPU-accelerated Kinetic Monte Carlo code. Co-supervised with Dr. Alexandros Ziogas and Vincent Maillou. (***Thesis awarded the ETH Medal**)*
- **Masters' thesis of Jente Clarysse, ETH Zurich** April 2023 - October 2023
  Developing simulations of thermally-activated switching in resistive memory. (***Thesis awarded the ETH Medal***)
- **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). Co-supervised with Prof. Matheiu Luisier.
- **Bachelor thesis of Patrik Gjini, ETH Zurich** February 2022 - May 2022
  Implemented a Fast Multipole Method algorithm for Poisson's equation. Co-supervised with Dr. Marko Mladenovic.
- **Masters' semester project of Patrick Bütler, ETH Zurich** February 2022 - May 2022
  Investigating resistive switching in $MoTe_2$ with *ab-initio* Molecular Dynamics. Co-supervised with Jonathan Backmann.

Student Design Team Positions

Technical Lead - UW Nano Robotics Group (UWNRG) Waterloo, ON, Canada
January 2015 - July 2019

- UWNRG is an undergraduate student design team which designs micro-robotic actuation systems to compete at the annual IEEE International Conference for Robotics and Automation (ICRA) Microbotics Challenges.
- Led the development of the microbot SAM (Solenoid Actuated Microbot). Completing the competition challenges required cleanroom fabrication work, electrical setup, and basic image recognition/pathfinding.
- Acquired funding for lab expenses, equipment, cleanroom usage, and conference travel costs. Competition Record: 3rd place (ICRA 2015, Seattle USA), 1st place (ICRA 2016, Stockholm Sweden), 2nd place (ICRA 2018, Brisbane Australia).

Publications (Journal/Reviewed Conferences)

'*' = equal contribution

Under Review:

1. C. Xia*, **M. Kaniselvan***, A. Ziogas, M. Mladenović, A. Maeder+, and M.Luisier, "Learning the Hamiltonians of Disordered Materials with Equivariant Graph Networks". Submitted to the *[anonymized for double blind review]*.

2. **M. Kaniselvan**, Y. Jeon, M. Mladenović, M.Luisier, and D. Akinwande, "Mechanisms of Resistive Switching in 2D Layered Materials". Under review at *Nature Materials*.

Published:

3. **M. Kaniselvan***, A. Maeder*, M. Mladenovic, M. Luisier, A. Ziogas, "Accelerated Kinetic Monte Carlo Simulations of Atomistically-Resolved Resistive Memory Arrays". (accepted) *International Conference for High Performance Computing, Networking, Storage, and Analysis (SC24)*, November 2024

4. M. Luisier, J. Backman, J. Cao, L. Deuschle, **M. Kaniselvan**, Y. Lee, A. Maeder, V. Maillou, M. Mladenovic, N. Vetsch, A. Winka, C. H. Xia, and A. N. Ziogas, "Nanoscale Device Modeling beyond the Ballistic Limit of Transport and Fixed Geometries". *IEEE International Electron Device Meeting (IEDM), December 2024*.

5. 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". *Nature Communications*, August 2024. doi: 10.1038/s41467-024-51093-3 ***(*Editor's Pick)***

6. **M. Kaniselvan**, M. Mladenović, J. Clarysse, and M. Luisier, "Insights behind multi-level conductance transitions in HfO_x memristors". *Device Research Conference (DRC)*, June 2024.

7. Alexander Maeder, **Manasa Kaniselvan**, Marko Mladenovic, Mathieu Luisier and Alexandros Nikolaos Ziogas, "A Distributed Conjugate Gradient Solver for Kinetic Monte Carlo simulations under applied fields." *Platform for Advanced Scientific Computing (PASC24)*, June 2024. Poster.

8. 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

9. Marko Mladenovic, **Manasa Kaniselvan**, Christoph Weilenmann, Alexandros Emboras, and Mathieu Luisier "Termination-Dependence of Resistive Switching in $SrTiO_3$-based Valence Change Memory." *International Workshop on Computational Nanotechnology (IWCN)*, June 2023.

10. **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]

11. 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

12. **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 (SISPAD)*, October 2022 doi: 10.10632F5.0053789.

13. **M. Kaniselvan**, M. Sritharan, and Y. Yoon, "Mitigating Tunneling Leakage in Ultrascaled HfS_2 pMOS Devices with Uniaxial Strain," *IEEE Electron Device Letters*, June 2022 doi:10.1109/LED.2022.3179228 ***(*Editor's Pick)***

14. **M. Kaniselvan** and Y. Yoon, "Strain-tuning $PtSe_2$ 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

15. G. Han, **M. Kaniselvan**, and Y. Yoon, "Photoresponse of $MoSe_2$ 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

16. M. Naqi*, **M. Kaniselvan***, S. Choo*, G. Han, S. Kang, J. Kim, Y. Yoon, and S. Kim, "Ultrasensitive Multilayer MoS_2-Based Photodetector with Permanently Grounded Gate Effect," *Advanced Electronic Materials*, vol. 6, no. 4, p. 1901256, Feb. 2020. doi: 10.1002/aelm.201901256.