

# 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 develop atomistic semiconductor device simulations at experimentally-relevant scales.

**Skills** - C++, Python (+PyTorch), High Performance- / GPU-Computing (CUDA/HIP, MPI, OpenMP), Numerical methods

## EDUCATION

<b>ETH Zurich</b> Candidate for PhD, Information Technology and Electrical Engineering	Zurich, Switzerland November 2021–May 2026
<b>University of Waterloo</b> Master of Applied Science (MAsc), Electrical and Computer Engineering	Waterloo, ON, Canada September 2019–May 2021
<b>University of Waterloo</b> Bachelor of Applied Science (BAsc), Nanotechnology Engineering.	Waterloo, ON, Canada September 2014–May 2019

## EXPERIENCE

<b>Scientific Assistant &amp; PhD Candidate - ETH Zürich</b> Advisor: Dr. Mathieu Luisier, Professor	<b>Zürich, Switzerland</b> September 1 <sup>st</sup> 2021 - 2026
<ul style="list-style-type: none"><li>– Developing multi-scale atomistic simulations for emerging memory devices, using Density Functional Theory (DFT), Molecular Dynamics (MD), <i>ab initio</i> quantum transport, Kinetic Monte Carlo, and Graph Neural Networks.</li><li>– Accelerating the developed custom scientific and ML applications on GPUs and distributing them on supercomputers.</li><li>– Working with experimental collaborators at IBM to fabricate conceptualized devices and investigate their operation.</li></ul>	
<b>PhD Intern - Samsung Semiconductor Inc</b> Supervisor: Dr. Byoungnak Lee, Principle Engineer	<b>San Jose, CA, USA</b> May 15 <sup>th</sup> 2023 - August 4 <sup>th</sup> 2023
<ul style="list-style-type: none"><li>– Accelerated a large-scale semiconductor process/device code by developing an algorithm to leverage symmetries in atomic structures. Presented implementation and results to the Samsung Electronics applications team in Korea.</li></ul>	
<b>Research Assistant &amp; MAsc Student - University of Waterloo</b> Advisor: Dr. Youngki Yoon, Associate Professor	<b>Waterloo, ON, Canada</b> September 1 <sup>st</sup> 2019 - September 1 <sup>st</sup> 2021
<ul style="list-style-type: none"><li>– Investigated transistor devices made from strain-engineered 2D materials using DFT and quantum transport methods. Collaborated with experimental partners to fabricate and test devices.</li></ul>	
<b>Undergraduate Intern - Waterloo Institute for Nanotechnology</b> Supervisor: Dr. Dayan Ban, Professor	<b>Waterloo, ON, Canada</b> January 1 <sup>st</sup> 2018 - September 1 <sup>st</sup> 2018
<ul style="list-style-type: none"><li>– Wrote a MATLAB code to simulate Resonant-Phonon Quantum Cascade Lasers (QCLs) by solving the Schroedinger Equation. Implemented global optimization methods to search for designs with higher-temperature lasing potential.</li></ul>	
<b>Undergraduate Intern - Adaptive Surface Technologies</b> Supervisor: Dr. Tehila Nahum, Principle Engineer	<b>Cambridge, MA, USA</b> September 1 <sup>st</sup> 2016 - April 30 <sup>th</sup> 2017
<ul style="list-style-type: none"><li>– 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.</li></ul>	
<b>Undergraduate Intern - National Institute of Materials Science</b> Supervisor: Dr. Genki Yoshikawa, Associate Professor	<b>Tsukuba, Ibaraki, Japan</b> January 1 <sup>st</sup> 2016 - April 1 <sup>st</sup> 2016
<ul style="list-style-type: none"><li>– 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.</li></ul>	

## SELECTED AWARDS (CAD)

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- National Science and Eng. Research Council of Canada (NSERC) PGSD-3 Doctoral Award - \$63,000 2021
- Sanford Fleming Foundation (SFF) Teaching Assistant Excellence Award - \$500 2021
- Waterloo Graduate Research Studentship (with MASc offer) - \$35,000 2019–2021
- Waterloo Dean's Graduate Entrance Award - \$5,000 2019
- NSERC Undergraduate Student Research Awards - \$4,000 2018
- NSERC Undergraduate Student Research Award - \$4,000 2017
- NIMS (Japan) Internship Program Fellowship - \$5,700 2016
- Waterloo President's (Entrance) Scholarship - \$2,000 2014

## TEACHING & SUPERVISION

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### Lectures

- **(Guest lecturer) Brain Inspired Computing: From Devices to Applications, ETH Zurich** April 2024  
Designed and delivered a lecture on atomistic device simulation approaches for non-volatile resistive memory.
- **(Lecturer) Digital Electronics, Ashesi University (collaboration with ETH Zurich)** February 2024, & March 2025  
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.

### 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 3 theses (6 months full time).

- **Masters' thesis of Rayen Mahjoub, ETH Zurich** September 2024 - March 2025  
Investigating the crystalline-amorphous phase changes of Germanium-Antimony-Tellurium (GST) compounds.
- **Masters' thesis of Alexander Maeder, ETH Zurich** September 2023 - March 2024  
Distributing iterative solvers for a GPU-accelerated Kinetic Monte Carlo code. (*\*Thesis awarded the ETH Medal*)  
Currently: PhD student in the same group
- **Masters' thesis of Jente Clarysse, ETH Zurich** April 2023 - October 2023  
Developing atomistic simulations of thermally-activated switching in resistive memory. (*\*Thesis awarded the ETH Medal*)  
Currently: Associate at Boston Consulting Group
- **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  
Performing quantum transport simulations on Interband Cascade Lasers (ICLs). Currently: PhD student at National University of Singapore
- **Bachelor thesis of Patrik Gjini, ETH Zurich** February 2022 - May 2022  
Implemented a Fast Multipole Method algorithm for Poisson's equation. Currently: Master thesis student in the same group
- **Masters' semester project of Patrick Bütler, ETH Zurich** February 2022 - May 2022  
Investigating resistive switching in MoTe<sub>2</sub> with *ab-initio* Molecular Dynamics. Currently: PhD student at IBM Zurich

### 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/PEER-REVIEWED FULL CONFERENCE PAPERS)

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‘\*’ = equal contribution

‘+’ = supervised masters’ students (work done for their thesis)

### In preparation:

1. **M. Kaniselvan**, A. Maeder, R. Mahjoub+, C. Xia, A. Ziogas and M. Luisier, “Enabling Large-scale Electronic Structure Calculations with Topology-aware Distribution of Graph Neural Networks”. In preparation.
2. P. Solomon, **M. Kaniselvan**, H. Miyazoe, B. Khan, T. Ando, and M. Luisier, “Atomistic Origin of RTN-like centers created and Annihilated by RRAM write Processes”. In preparation.
3. **M. Kaniselvan**, K. Portner, D. Falcone, V. Bragaglia, B. Offrein, and M. Luisier, “Factors Influencing the Electroforming Kinetics of  $\text{HfO}_x/\text{Ti}$  RRAM devices”. In preparation.

### Submitted/Under Review:

4. M. Mladenović, **M. Kaniselvan**, C. Weilenmann, A. Emboras, and M. Luisier, “Termination-Dependent Resistive Switching in  $\text{SrTiO}_3$  Valence Change Memory Cells”. Under review at *ACS Applied Electronic Materials*.
5. C. Xia\*, **M. Kaniselvan\***, A. Ziogas, M. Mladenović, A. Maeder, and M. Luisier, “Learning the Hamiltonians of Disordered Materials with Equivariant Graph Networks”. Under review at *[Anonymized for double-blind review]*. Preprint available: <https://arxiv.org/abs/2501.19110>
6. **M. Kaniselvan**, J. Clarysse+, M. Mladenović, and M. Luisier, “Atomistic simulations of failure mechanisms in ultrascaled  $\text{HfO}_x$  RRAM arrays”. Submitted to the *Device Research Conference (DRC)*.

### Accepted/Published:

7. **M. Kaniselvan**, Y. Jeon, M. Mladenović, M. Luisier, and D. Akinwande, “Mechanisms of Resistive Switching in 2D Layered Materials”. Accepted at *Nature Materials*, January 2025.
  8. **M. Kaniselvan\***, A. Maeder\*+, M. Mladenovic, M. Luisier, A. Ziogas, “Accelerated Kinetic Monte Carlo Simulations of Atomistically-Resolved Resistive Memory Arrays”. Proceedings of the *International Conference for High Performance Computing, Networking, Storage, and Analysis (SC24)*, November 2024. doi: 10.1109/SC41406.2024.00097. (*\*Reproducibility Award Finalist*)
  9. 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*)
  10. 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
  11. **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 Front Cover - designed by me*)
- In the media:** [Covered by ETH] [Covered by the Werner Siemens Foundation]
12. 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 Back Cover*)
  13. **M. Kaniselvan**, M. Sritharan, and Y. Yoon, “Mitigating Tunneling Leakage in Ultrascaled  $\text{HfS}_2$  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  $\text{PtSe}_2$  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  $\text{MoSe}_2$  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  $\text{MoS}_2$ -Based Photodetector with Permanently Grounded Gate Effect,” *Advanced Electronic Materials*, vol. 6, no. 4, p. 1901256, Feb. 2020. doi: 10.1002/aelm.201901256.

## OTHER PEER-REVIEWED CONFERENCE CONTRIBUTIONS

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17. 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.
18. **M. Kaniselvan**, M. Mladenović, J. Clarysse+, and M. Luisier, “Insights behind multi-level conductance transitions in  $\text{HfO}_x$  memristors”. Proceedings of the *Device Research Conference (DRC)*, June 2024. doi: 10.1109/DRC61706.2024.10605556
19. 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.
20. Marko Mladenovic, **Manasa Kaniselvan**, Christoph Weilenmann, Alexandros Emboras, and Mathieu Luisier “Termination-Dependence of Resistive Switching in  $\text{SrTiO}_3$ -based Valence Change Memory.” *International Workshop on Computational Nanotechnology (IWCN)*, June 2023.
21. **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.
22. **UW Nano Robotics Group**. *Solenoid Actuated Microbot (SAM)*. 2018 IEEE IEEE International Conference on Robotics and Automation (ICRA). Brisbane, Australia. Competition & poster.
23. **UW Nano Robotics Group**. *ElectroMagnetic Micro Actuation (EMMA): Version 2*. 2016 IEEE International Conference on Robotics and Automation (ICRA). Stockholm, Sweden. Mobile microbotics competition & poster
24. **UW Nano Robotics Group**. *ElectroMagnetic Micro Actuation (EMMA)* 2015 IEEE International Conference on Robotics and Automation (ICRA). Seattle, Washington, USA. Mobile microbotics competition & poster