Ali Rezaei (Dr. rer. nat.)

Quantum Simulation • HPC Performance Engineering • TCAD Modelling
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LinkedIn | Google Scholar | ResearchGate | Systems-Nuts | RoaRQ | Online CV

Professional Summary

Experienced in high-performance classical simulation of quantum computing and TCAD-based nano-electronic device modelling, with a strong track record in developing, maintaining and optimizing scalable simulation software across quantum, semiconductor, and superconducting domains – from quantum circuit emulators to NEGF-based solvers for nanoscale transistors.

Education

University of Urmia, Urmia, Iran *Sep 2007 – Aug 2011*
B.Sc. in Solid State Physics

IASBS, Zanjan, Iran *Sep 2012 – Apr 2015*
M.Sc. in Condensed Matter Physics
Thesis: *Thermoelectric properties of 3D topological insulators: effects of the gap and hexagonal warping*
Many-body Theory Group – supervised by Dr. Saeed H. Abedinpour and Dr. Jahan Abouie

University of Konstanz, Konstanz, Germany *Jan 2016 – Dec 2019*
Ph.D. (Dr. rer. nat.) in Condensed Matter Physics
Thesis: *Non-equilibrium and spin transport in hybrids of superconductors and magnets* – Grade: *Magna cum laude*
Quantum Transport Group – supervised by Prof. Dr. Wolfgang Belzig

Skills

Programming languages C, C++, Python, Fortran, Bash
HPC & Quantum Toolchains MPI, OpenMP, CUDA, SIMD intrinsics, Slurm, QuEST (co-dev.), QuESTlink, cuQuantum, Qiskit
Performance & Profiling Intel VTune, Intel MLC & PCM, Valgrind, Linux `perf`
DevOps & Build Git (+CI/CD), Jira, CMake, Catch2/CTest, Spack, Conda, Docker, Kubernetes
Scientific Tools MATLAB, GNU Octave, Wolfram Mathematica
EDA / TCAD Toolchains Synopsys Sentaurus, Silvaco Atlas, QuantumATK/QTX, OMEN/NEMO
Scientific Libraries Eigen, LAPACK/BLAS, OpenBLAS, ARPACK++, SuperLU, Quadpack, GMM(GetFEM), SciPy, NumPy, pandas, SymPy, matplotlib – among others
Personal Quick and continuous learner, strong communication and collaboration, team player, problem-solving and troubleshooting, detail-oriented, critical thinking, adaptability, positive attitude, and project management

Experience

Research Associate, University of Edinburgh (UK) *Feb 2024 – Present*
ICSA, EPCC & RoaRQ – Research Associate in **Quantum Computing HPC** (QuEST, C)
Co-developing QuEST v4 with a focus on optimisation prototyping and debunking performance bottlenecks through optimised algorithms.

- Low-level tuning: redesigned state-vector data layout, intrinsic SIMD (SSE2/AVX2/AVX-512) kernels, cache blocking, FMA, loop unrolling, and software prefetching.
- NUMA-aware execution: locality-sensitive task scheduler, thread pinning, and novel memory placement strategy to eliminate remote-access penalties and improve effective bandwidth.
- Micro-architectural profiling: located hotspots and memory-bandwidth limits with *Intel VTune*, Memory Latency Checker, Intel PCM, and Linux `perf`; insights fed back into the kernel design.
- Benchmarks show multifold speedups on single-node systems. Code available [here]; upstream merge pending completion of integration testing.

- Currently deploying: advanced memory tiering with fast NVMe SSD + CXL. MPI optimization and accelerator orchestration across multi-GPU (and FPGA) back-ends for scalable simulation on heterogeneous (CPU-GPU) clusters. Compression, and Circuit-knitting techniques to push classical simulations.

Research Associate, University of Glasgow (UK) *Aug 2020 – Dec 2023*
Device Modelling Group – **TCAD Software Developer** (NESS, C++)

- Co-developed, optimized, and extended a Non-Equilibrium Green's Function (NEGF) quantum-transport solver for both effective-mass and $k \cdot p$ Hamiltonians.
- Developed high-performance numerical algorithms for novel physics model: quantum tunnelling & interference, first-principles simulations with on-the-fly effective-mass extraction, finite-difference/-volume discretization schemes, statistical-variability workflows, Poisson–Schrödinger solver, and ML-accelerated NEGF, Josephson junction devices and silicon spin qubits.
- Designed next-generation Si and III–V devices including 3 nm GAA NSFETs, FinFET/planar MOSFETs, and resonant-tunnelling diodes for PUFs with Synopsys Sentaurus (SDEVICE), QuantumATK/QTX, Silvaco Atlas, and OMEN/NEMO – validating performance against industry roadmaps.
- Led CI/CD and HPC-scaling initiatives: migrated codebase to Git, containerized workflows, implemented unit testing, and tuned hybrid MPI + OpenMP parallelism
- Produced comprehensive documentation, tutorials and demos. Provided technical software support to academic and industrial partners, and onboarded/mentored junior developers.

Ph.D. Researcher, University of Konstanz (DE) *Aug 2016 – Dec 2019*

- Analytical & numerical investigation of quantum transport properties (non-equilibrium and spin) in superconductor–ferromagnet (and –antiferromagnet) proximity-coupled heterostructures.
- Developed numerical packages utilizing the Eilenberger/Usadel quasiclassical Green's function methods and quantum circuit theory (Nazarov).
- Studied multiple phenomena in superconducting hybrids, including:
  - Generation, control, and detection of equal-spin triplet Cooper pairs in a spin-valve (S/FM) setup.
  - Spin-flip enhanced thermoelectricity in S/FM devices.
  - Induced spin-splitting in S/AFM devices.
- TA:
  - Quantum Field Theory of Nonequilibrium States (SS 2019)
  - Advanced Quantum Theory and Electrodynamics (WS 2017/2018)
  - Advanced Condensed Matter Physics (WS 2016/2017)

Research Interests

Quantum Computing & Algorithms, Quantum Simulation, Nano-/Quantum Device Modelling, TCAD Engineering, Quantum Transport, High-Performance Computing, ML for Physical Modelling, Condensed-Matter Theory

Publications

Quantum HPC

- **Ali Rezaei**, Luc Jaulmes, Maria Bahna, Oliver Thomson Brown, and Antonio Barbalace. "Low-Level and NUMA-Aware Optimization for High-Performance Quantum Simulation," arXiv:2506.09198 (2025).

Semiconductor Electronics

- Pranav Acharya, **Ali Rezaei**, Amretashis Sengupta, Tapas Dutta, Naveen Kumar, Patryk Maciazek, Asen Asenov, and Vihar Georgiev. "Analysis of Random Discrete Dopants Embedded Nanowire Resonant Tunnelling Diodes for Generation of Physically Unclonable Functions," *IEEE Trans. on Nanotechnology (TNANO)* (2024).
- Tapas Dutta, Fikru Adamu-Lema, Nikolas Xeni, **Ali Rezaei**, Ankit Dixit, Ismail Topaloglu, Vihar Georgiev, and Asen Asenov. "Predictive Simulation of Nanosheet Transistors Including the Impact of Access Resistance," in *Proc. IEEE SISPAD* (2024).
- Ankit Dixit, **Ali Rezaei**, Nikolas Xeni, Naveen Kumar, Tapas Dutta, Ismail Topaloglu, Preslav Alexandrov, Asen Asenov, and Vihar Georgiev. "Unravelling the Impact of Random Dopant Fluctuations on Si-based 3nm NSFET: A NEGF Analysis," in *Proc. IEEE NANO* (2024).
- Tongfei Liu, **Ali Rezaei**, Kaige Yang, Xuge Fan, Pranav Acharya, Vihar Georgiev, and Asen Asenov. "Study of Electron Mobility in Ultra-scaled Silicon Nanosheet FET," *Physica Scripta* **99**, 075410 (2024).
- Preslav Alexandrov, **Ali Rezaei**, Tapas Dutta, Nikolas Xeni, Asen Asenov, and Vihar Georgiev. "Convolutional Machine Learning Method for Accelerating Non-Equilibrium Green's Function Simulations in Nanosheet Transistors," *IEEE Trans. on Electron Devices (TED)* (2023).

- Naveen Kumar, César Pascual García, Ankit Dixit, **Ali Rezaei**, and Vihar Georgiev. "Charge Dynamics of Amino Acids Detection and the Effect of Steric Hindrance on FinFET-based Electrolyte-Gated Sensor," *Solid-State Electronics* **210**, 108789 (2023).
- Naveen Kumar, Ankit Dixit, **Ali Rezaei**, Tapas Dutta, César Pascual García, Vihar Georgiev. "Insights into the Ultra-Steep Subthreshold Slope Gate-all-around Feedback-FET for memory and sensing applications," *IEEE NMDC* (2023).
- Naveen Kumar, César Pascual García, Ankit Dixit, **Ali Rezaei**, Asen Asenov, Vihar Georgiev. "Electrolyte Gated FET-based Sensing of Immobilized Amphoteric Molecules Including the Variability in Affinity of the Reactive Sites," *IEEE SISPAD* (2023).
- Preslav Alexandrov, **Ali Rezaei**, Nikolas Xeni, Tapas Dutta, Asen Asenov and Vihar Georgiev. "Fully Convolutional Generative Machine Learning method for accelerating Non-Equilibrium Green's Function simulations," *IEEE SISPAD* (2023).
- Daniel Nagy, **Ali Rezaei**, Nikolas Xeni, Tapas Dutta, Fikru Adamu-Lema, Ismail Topaloglu, Vihar P Georgiev, Asen Asenov, "Hierarchical simulation of nanosheet field effect transistor: NESS flow," *Solid-State Electronics* **199**, 108489 (2023).
- **Ali Rezaei**, Patryk Maciazek, Amretashis Sengupta, Tapas Dutta, Cristina Medina-Bailon, Asen Asenov, Vihar P Georgiev, "Statistical device simulations of III-V nanowire resonant tunneling diodes as physical unclonable functions source," *Solid-State Electronics* **194**, 108339 (2022).
- Tapas Dutta, Cristina Medina-Bailon, **Ali Rezaei**, Daniel Nagy, Fikru Adamu-Lema, Nikolas Xeni, Yassine Abourrig, Naveen Kumar, Vihar P Georgiev, Asen Asenov, "Tcad simulation of novel semiconductor devices," *IEEE 14th International Conference on ASIC (ASICON)* (2021).
- Cristina Medina-Bailon, Tapas Dutta, **Ali Rezaei**, Daniel Nagy, Fikru Adamu-Lema, Vihar Georgiev, Asen Asenov, "Simulation and modeling of novel electronic device architectures with NESS (nano-electronic simulation software): A modular nano TCAD simulation framework," *Micromachines* **12**, 680 (2021).
- Cristina Medina-Bailon, Tapas Dutta, Fikru Adamu-Lema, **Ali Rezaei**, Daniel Nagy, Vihar P. Georgiev, Asen Asenov, "Nano-Electronic Simulation Software (NESS): A Novel Open-Source TCAD Simulation Environment," *JoMM* **3**, 20030407 (2020).

Superconducting Electronics

- **Ali Rezaei**, Robert Hussein, Akashdeep Kamra, and Wolfgang Belzig, "Phase-controlled spin and charge currents in superconductor-ferromagnet hybrids," *Phys. Rev. Research* **2**, 033336 (2020).
- **Ali Rezaei**, Akashdeep Kamra, Peter Machon, and Wolfgang Belzig, "Spin-flip enhanced thermoelectricity in superconductor-ferromagnet bilayers," *New J. Phys.* **20**, 073034 (2018).
- Akashdeep Kamra, **Ali Rezaei**, and Wolfgang Belzig, "Spin-splitting induced in a superconductor by an anti-ferromagnetic insulator," *Phys. Rev. Lett.* **121**, 247702 (2018).

Topological Insulators

- **Ali Rezaei**, A. Sabzalipour, S. H. Abedinpour, J. Abouie. "Effect of hexagonal warping on the surface electrical conductivity of a topological insulator," in *Proc. of the 12th Condensed Matter Physics Conference of the Physical Society of Iran*, Isfahan Univ. of Technology (2015).
- **Ali Rezaei**, S. H. Abedinpour, J. Abouie. "Thermoelectric properties of topological insulators doped with impurities," in *Proc. of the 21st IPM Spring School*, Tehran, Iran (2014).

Awards and Honors

- Certificate of training in the IRTG Nano (SFB 767) – University of Konstanz, Germany (Dec 2019).
- Best Scientific Poster Prize at the 697th WE-Heraeus-Seminar *"Superconductivity in Low Dimensional and Interacting Systems"* – Physikzentrum Bad Honnef, Germany (Jun 2019).
- Ranked 120/30,000+ (top 0.4 %) in the M.Sc. National University Entrance Exam (Condensed Matter Physics), Iran (Sep 2012).

Additional Certifications

- **IBM Quantum**
  - IBM badge: Variational Algorithm Design
  - IBM badge: Quantum Algorithms
  - IBM badge: Quantum Information
- **Advanced Data Science with IBM Specialization**

  - IBM badge: Scalable Data Science
  - IBM badge: Advanced Machine Learning and Signal Processing
  - IBM badge: Applied AI with Deep Learning
- **IBM Data Science Professional Certificate**
  - IBM badge: Data Science Orientation
- **Machine Learning** (Stanford University)
  - Covered supervised learning (regression, neural networks, SVMs); unsupervised learning (K-means, PCA, anomaly detection); recommender systems; and large-scale machine learning.
- **SQL for Data Science** (UCDavis)
- **Object-Oriented Data Structures in C++** (University of Illinois)
- **Workshop on Scientific Presenting for Physicists** (University of Konstanz)

References

Available upon request.