Ali Rezaei (Dr. rer. nat.)

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LinkedIn | Google Scholar | ResearchGate | Systems-Nuts | RoaRQ | Online CV

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

- Analytical & numerical investigation of quantum transport properties (non-equilibrium and spin) in superconductor–ferromagnet (and –antiferromagnet) proximity-coupled heterostructures.
- Developed numerical packages (Fortran, MATLAB, Python) 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 Roles:
 - Quantum Field Theory of Nonequilibrium States (SS 2019)
 - Advanced Quantum Theory and Electrodynamics (WS 2017/2018)
 - Advanced Condensed Matter Physics (WS 2016/2017)

Academic Employment

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 bottle-necks through optimised algorithms that achieve several-fold speed-ups - code available [here]; upstream merge pending completion of integration testing.

- 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 that nearly eliminates remote-access penalties and improves 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.
- Under implementation: 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. 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.

Skills

Programming languages

C, C++, Python, Fortran 90/95, 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

Scientific Libraries Eigen, LAPACK/BLAS, OpenBLAS, ARPACK++, SuperLU, Quadpack, GMM(GetFEM), SciPy, NumPy, pandas, SymPy, matplotlib – among others

EDA / TCAD Toolchains

Synopsys Sentaurus, Silvaco Atlas, QuantumATK/QTX, OMEN/NEMO

Soft Quick and continuous learner, strong communication and collaboration, team player, problem-solving and troubleshooting, detail-oriented, critical thinking, adaptability, positive attitude

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

• Preprints in preparation

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

- Advanced Data Science with IBM Specialization
 - IBM badge: Fundamentals of 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.