School of Electrical and Computer Engineering
Purdue University

January 2026

Name: Tillmann Christoph Kubis

Education:

Diploma	Nov. 2003	Physics Department, Technical Univ. Munich
PhD	Nov. 2009	Physics Department, Technical Univ. Munich

Professional and Honorary Society Memberships:

American Chemical Society	Member	2017 – present
American Physical Society	Regular member	2017 – present
Sigma Xi	Full member	2016 – present
Institute of Electrical and Electronics Engineering (IEEE)		
	Senior Member	2014 - present
German Physical Society (DPG)	Regular member	2004 – present

Honors and Awards:

[15] Named one of the Most Impactful Faculty Inventors of FY 2024
College of Engineering, Purdue University, 2024

[14] Named one of the Most Impactful Faculty Inventors of FY 2023,
College of Engineering, Purdue University, 2023

[13] Named one of the Most Impactful Faculty Inventors of FY 2022,
College of Engineering, Purdue University, 2022

[12] Named one of the Most Impactful Faculty Inventors of FY 2021,
College of Engineering, Purdue University, 2021

[11] Named Katherine Ngai Pesic & Silvaco Research Assistant Professor of Electrical and Computer Engineering, College of Engineering, Purdue University, 2021

[10] Named one of the Most Impactful Faculty Inventors of FY 2019,
College of Engineering, Purdue University, 2019

[9] Seed for Success Award of Purdue University, 2019

[8] Advisory board membership of the IWCN in acknowledgment of short-notice and successful coorganization of the international conference at Purdue University, 2015

[7] Intel award for contributions to the NEMO5 simulation software tool, 2013

[6] Co-author of two best student presentations (honorable mention) 15th International Workshop on Computational Electronics, 2012

[5] Co-author of the best student poster IEEE Nanotechnology Materials and Devices Conference (NMDC), 2011

[4] Doctoral degree in Physics "passed with distinction". 2009

[3] Students' award of teaching excellence (best exercise group, "Golden chalk"), Physics Department, Technische Universität München, Germany, 2008

[2] Students' award of teaching excellence (best exercise group, "Golden chalk"), Physics Department, Technische Universität München, Germany, 2005

[1] Diploma exams in Physics "passed with distinction", 2003

Professional Experience

2003 – 2009 Research Assistant: Physics Department, Technische Universität München, Germany

2010 - 2011 Post-Doctoral researcher: School of Electrical and Computer Engineering - Purdue University, IN, US

2011 – 2021 Research Assistant Professor: Network for Computational Nanotechnology - Purdue University, IN, US

2021 – 2022 Katherine Ngai Pesic & Silvaco Research Assistant Professor of Electrical and Computer Engineering, School of Electrical and Computer Engineering, Purdue University, IN, US

2016 – present School of Electrical and Computer Engineering – Purdue University, IN, US

2017 – present Center for Predictive Materials and Devices – Purdue University, IN, US

2019 – present Purdue Institute of Inflammation, Immunology and Infectious Disease, Purdue University, IN, US

2022 – present Katherine Ngai Pesic & Silvaco Associate Professor of Electrical and Computer Engineering, School of Electrical and Computer Engineering, Purdue University, IN, US

Consulting Activities

2017 – 2022	President of Quail Modeling LLC
2017 – 2019	President of LEDcentral LLC
2017 – 2018	Vicepresident of Nemoco LLC

Professional Society Activities

Organization:	International Workshop of Computational Electronics
Activity:	Workshop Co-Organizer, September 2015
Organization:	IEEE, Institute of Electrical and Electronics Engineers
Activity:	Member of TCAD committee, January 2026-2028

PhD Thesis Supervision Completed

Ganesh Hedge	December 2013, Modeling the atomic and electronic structure of Meta-Metal, Metal-Semiconductor and III-V/Oxide interfaces (co-mentoring with Prof. Klimeck)
Parijat Sengupta	January 2014, “THEORY OF TOPOLOGICAL INSULATORS AND ITS APPLICATIONS” (co-mentoring with Prof. Klimeck)
Yu He	December 2015, “ADVANCED BOUNDARY CONDITION METHOD IN QUANTUM TRANSPORT AND ITS APPLICATION IN NANODEVICES” (co-mentoring with Prof. Klimeck)
Yaohua Tan	May 2016, “TIGHT BINDING PARAMETERIZATION FROM AB-INITIO CALCULATIONS AND ITS APPLICATIONS” (co-mentoring with Prof. Klimeck)
Kai Miao	May 2017, “QUANTUM THERMAL TRANSPORT IN SEMICONDUCTOR NANOSTRUCTURE WITH DIFFUSION” (co-mentoring with Prof. Klimeck)
Junzhe Geng	August 2017, "MULTI-SCALE QUANTUM TRANSPORT MODELING OF LIGHT EMITTING DIODES"
Daniel Mejia	May 2018, “VISUAL ANALYTICS TO SUPPORT ATOMISTIC SIMULATIONS DESIGN”
Daniel Valencia	June 2018, “MODELING ELECTRONIC TRANSPORT IN METAL INTERCONNECTS”

Prasad Sarangapani	September 2018, “QUANTITATIVE PREDICTION OF NON-LOCAL MATERIAL AND TRANSPORT PROPERTIES THROUGH QUANTUM SCATTERING MODELS”
James Charles	September 2018, “MODELING NONLOCALITY IN QUANTUM SYSTEMS”
Xinchen Guo	October 2019, “GENERAL RESOURCE MANAGEMENT FOR COMPUTATIONALLY DEMANDING SCIENTIFIC SOFTWARE”
Kuang-Chung Wang	October 2019, “METHOD DEVELOPMENT IN THE NEGF FRAMEWORK: MAXIMALLY LOCALIZED WANNIER FUNCTION AND BÜTTIKER PROBE FOR MULTI-PARTICLE INTERACTION”
Yuanchen Chu	November 2019, “PREDICTIVE ELECTRO AND THERMAL QUANTUM TRANSPORT IN NANOSCALE DEVICES”
Daniel Lemus	April 2020, “LOW-RANK APPROXIMATION IN QUANTUM TRANSPORT SIMULATIONS”
Han-Wei Hsiao	May 2025, “ADVANCED QUANTUM MODELS FOR CORRUGATION AND DEFECTS IN TWO-DIMENSIONAL MATERIALS”

Master's and PhD Thesis Students Currently Being Supervised

Manas Pratap	PhD
Sidhaant Thakker	PhD

Teaching duties

- Co-instructor of ECE 60002 Concepts to Innovation I and II
- Mentor of Fall-2020-VIP-Startup (WL.202110.ENGR.47920.004) – “brainchild” student startup
- Mentor of Spring-2022-VIP-Startup (WL.202220.VIP.47920.004) “Glimpse” student startup
- Instructor and developer of hands-on course 595 Application oriented computational nanotechnology (in-person and asynchronous online)

Serial Journal Articles

[1] K.-H. Huang, N. Narendra, K. Yap, N. M. Morato, K. Chen, Y. Feng, R. G. Cooks, T. Kubis, and C. R. Ferreira, High-Throughput Small-Scale Platform for Synthesis, Characterization, and Modeling of Per- and Polyfluoroalkyl Substances Analogs, Environ. Sci. Technol. Lett. 12, 1437 (2025)

[2] H.-W. Hsiao, N. Narendra, and T. Kubis, Long range piezoelectricity effects in van der Waals heterobilayer systems beyond 1000 atoms, Journal of Physics: Condensed Matter 36, 265901 (2024)

[3] X. Guo, N. Narendra, G. Klimeck, and T. Kubis, General resource manager for computationally demanding scientific software (MARE), Engineering with Computers (2024)

[4] K. Wang, R. Grassi, Y. Chu, S. H. Sureshbabu, J. Geng, P. Sarangapani, X. Guo, M. Townsend, and T. Kubis, Introduction of multi-particle Büttiker probes -- Bridging the gap between drift diffusion and quantum transport, J. Appl. Phys. 128, 014302 (2020)

[5] D. Lemus, J. Charles, and T. Kubis, Mode-space-compatible inelastic scattering in atomistic nonequilibrium Green's function implementations, J. Comp. Elect. 19, 1389 (2020)

[6] D. Mejia, T. Kubis, and G. Klimeck, NemoViz: A visual interactive system for atomistic simulations design, Visualization in Engineering 6:6 (2018)

[7] Y. Chu, P. Sarangapani, J. Charles, G. Klimeck, and T. Kubis, Explicit screening full band quantum transport model for semiconductor nanodevices, J. Appl. Phys. 123, 244501 (2018)

[8] P. Sarangapani, C. Weber, J. Chang, S. Cea, M. Povolotskyi, G. Klimeck, T. Kubis, Atomistic tight-binding study of contact resistivity in Si/SiGe PMOS Schottky contact, IEEE Trans. on Nanotech. 17, 968 (2018)

[9] P. Long, J. Huang, M. Povolotskyi, P. Sarangapani, G. Valencia-Zapata, T. Kubis, M. Rodwell, G. Klimeck, Atomistic Modeling trap-assisted tunneling in hole tunnel Field Effect Transistors, Journal of Applied Physics 123, 174504 (2018)

[10] J. Geng, P. Sarangapani, K.-C. Wang, E. Nelson, B. Browne, C. Wordelman, J. Charles, Y. Chu, T. Kubis, G. Klimeck, Quantitative Multi-Scale, Multi-Physics Quantum Transport Modeling of GaN-Based Light Emitting Diodes, Phys. Status Solidi A, 1700662 (2018).

[11] K.-C. Wang, T. K. Stanev, D. Valencia, J. Charles, A. Henning, V. K. Sangwan, A. Lahiri, D. Mejia, P. Sarangapani, M. Povolotskyi, A. Afzalian, J. Maassen, G. Klimeck, M. C. Hersam, L. J. Lauhon, N. P. Stern, T. Kubis, Control of interlayer delocalization in 2H transition metal dichalcogenides, J. Appl. Phys. 122, 224302 (2017).

[12] Y. He, Y. Tan, Z. Jiang, M. Povolotskyi, G. Klimeck, and T. Kubis, Surface Passivation in Empirical Tight Binding, IEEE Trans. on Electron Devices 63, 954 (2016).

[13] J. Charles, P. Sarangapani, R. Golizadeh-Mojarad, R. Andrawis, D. Lemus, X. Guo, D. Mejia, J. E. Fonseca, M. Povolotskyi, T. Kubis, G. Klimeck, Incoherent transport in NEMO5: realistic and efficient scattering on phonons, J. Comput. Electron. 15, 1123 (2016).

[14] Z. Jiang, Y. Lu, Y. Tan, Y. He, M. Povolotskyi, T. Kubis, A. Seabaugh, P. Fay, G. Klimeck, Quantum Transport in AlGaSb/InAs TFETs With Gate Field In-Line With Tunneling Direction, IEEE Trans. on Elec. Dev., 62, 2445, (2015).

[15] R. Vedula, S. Mehrotra, T. Kubis, M. Povolotskyi, G. Klimeck, and A. Strachan, Optimal Ge/SiGe nanofin geometries for hole mobility enhancement: technology limit from atomic simulation, J. Appl. Phys. 117, 174312 (2015)

[16] P. Sengupta, T. Kubis, Y. Tan, and G. Klimeck, Proximity induced ferromagnetism, superconductivity, and finite-size effects on the surface states of topological insulator nanostructures, J. Appl. Phys. 117, 044304 (2015)

[17] G. Hedge, M. Povolotskyi, T. Kubis, J. Charles, G. Klimeck, An Environment-dependent Semi-Empirical Tight Binding Model Suitable for Electron Transport in Bulk Metals, Metal Alloys, Metallic Interfaces and Metallic Nanostructures II - Effect of Confinement and Homogeneous Strain on Cu Conductance, J. Appl. Phys. 115, 123703 (2014).

[18] G. Hedge, M. Povolotskyi, T. Kubis, J. Charles, and G. Klimeck, An Environment-dependent Semi-Empirical Tight Binding Model Suitable for Electron Transport in Bulk Metals, Metal Alloys, Metallic Interfaces and Metallic Nanostructures. I - Model and validation, J. Appl. Phys. 115, 123703 (2014).

[19] J. E. Fonseca, T. Kubis, M. Povolotskyi, B. Novakovic, A. Ajoy, G. Hedge, H. Ilatikhameneh, Z. Jiang, P. Sengupta, Y. Tan, and G. Klimeck, Efficient and realistic device modeling from atomic detail to the nanoscale, J. Comput. Electron. 12, 592 (2013).

[20] P. Sengupta, T. Kubis, Y. Tan, M. Povolotskyi, and G. Klimeck, Design principles for HgTe based Topological Insulator Devices, J. Appl. Phys. 114, 043702 (2013).

[21] S. R. Mehrotra, S.G. Kim, T. Kubis, M. Povolotskyi, M. S. Lundstrom, and G. Klimeck, Engineering Nanowire n-MOSFETs at Lg < 8 nm, IEEE Trans. Elect. Dev. 60, 2171 (2013).

[22] L. Zeng, Y. He, M. Povolotskyi, X.Y. Liu, G. Klimeck, T. Kubis, Low Rank Approximation Method for Efficient Green's Function Calculation of Dissipative Quantum Transport, J. Appl. Phys. 113, 213707 (2013)

[23] C. Deutsch, H. Detz, T. Zederbauer, A. M. Andrews, P. Klang, T. Kubis, G. Klimeck, M. E. Schuster, W. Schrenk, G. Strasser, K. Unterrainer, Probing scattering mechanisms with symmetric quantum cascade lasers, Optics Express 21, 7209 (2013).

[24] Y. Tan, M. Povolotskyi; T. Kubis, Y. He, Z. Jiang, G. Klimeck, T. Boykin, Empirical tight binding parameters for GaAs and MgO with explicit basis through DFT mapping, J. Comp. Electron. 12, 56 (2013).

[25] K. Fujita, M. Yamanishi, S. Furuta, K. Tanaka, T. Edamura, T. Kubis, and G. Klimeck, Indirectly pumped 3.7 THz InGaAs/InAlAs quantum-cascade lasers grown by metal-organic vapor-phase epitaxy, Optics Express 20, 20647 (2012).

[26] R. Kotlyar, T. Linton, R. Rios, M. Giles, S. Cea, K. Kuhn, M. Povolotskyi, T. Kubis, G. Klimeck, Does the low hole transport mass in <110> and <111> Si nanowires lead to mobility enhancements at high field and stress: a self-consistent tight-binding study, J. Appl. Phys. 111, 123718 (2012).

[27] H. Yasuda, T. Kubis, I. Hosako, and K. Hirakawa, Non-equilibrium Green's function calculation for GaN-based terahertz-quantum cascade laser structures, J. Appl. Phys. 111, 083105 (2012).

[28] S. Steiger, M. Povolotskyi, H.-H. Park, T. Kubis, and G. Klimeck, NEMO5: A Parallel Multiscale Nanoelectronics Modeling Tool, IEEE Transactions on Nanotechnology 10, 1464 (2011).

[29] S. Agarwal, M. Povolotskyi, T. Kubis, and G. Klimeck, Adaptive quadrature for sharply spiked integrands, J. Comput. Electron. 9, 252 (2010).

[30] P. Vogl and T. Kubis, The non-equilibrium Green's function method: an introduction, Journal of Computational Electronics, J. Comput. Electron. 9, 237 (2010).

[31] A. Matyas, T. Kubis, P. Lugli, and C. Jirauschek, Comparison between semiclassical and full quantum transport analysis of THz quantum cascade lasers, Physica E 42, 2628 (2010).

[32] T. Kubis, P. Vogl, Predictive Quantum Theory of Current and Optical Gain in Quantum Cascade Lasers, Laser Physics 19, 762 (2009).

[33] T. Kubis, P. Vogl, Microscopic theory of spin-filtering in non-magnetic semiconductor nanostructures, phys. stat. sol. (c) 5, 290 (2008).

[34] T. Kubis, C. Yeh, P. Vogl, Non-equilibrium quantum transport theory: Current and gain in quantum cascade lasers, J. Comput. Electron. 7, 432 (2008).

[35] T. Kubis, C. Yeh, P. Vogl, Quantum theory of transport and optical gain in quantum cascade lasers, phys. stat. sol. (c) 5, 232 (2008).

[36] S. Birner, T. Kubis, P. Vogl, Simulation of quantum cascade lasers - optimizing laser performance, Photonik international 2, 60 (2008).

[37] S. Birner, T. Zibold, T. Andlauer, T. Kubis, M. Sabathil, A. Trellakis, P. Vogl, nextnano: General Purpose 3-D Simulations, IEEE Transactions on Electron Devices 54, 2137 (2007).

[38] T. Kubis, P. Vogl, Self-consistent quantum transport theory: Applications and assessment of approximate models, J. Comput. Electron. 6, 183 (2007).

Serial Journal Correspondence or Letters

[1] K.-C. Wang, D. Valencia, J. Charles, A. Henning, M. E. Beck, V. K. Sangwan, L. J. Lauhon, M. C. Hersam, T. Kubis, Atomic-level charge transport mechanism in gate-tunable anti-ambipolar van der Waals Heterojunctions, Appl. Phys. Lett. 118, 083103 (2021)

[2] J. Charles, S. Kais, and T. Kubis, Introducing open boundary conditions in modeling nonperiodic materials and interfaces: the impact of the periodic assumption, ACS Matt. Lett. 2, 247 (2020)

[3] Y. Chu, J. Shi, K. Miao, Y. Zhong, P. Sarangapani, T. Fisher, G. Klimeck, X. Ruan and T. Kubis, Thermal boundary resistance predictions with non-equilibrium Green's function and molecular dynamics simulations, Appl. Phys. Lett. 115, 231601 (2019).

[4] K. Miao, S. Sadasivam, J. Charles, G. Klimeck, T. S. Fisher, and T. Kubis, Büttiker probes for dissipative phonon quantum transport in semiconductor nanostructures, Appl. Phys. Lett. 108, 113107 (2016).

[5] F. W. Chen, L. A. Jauregui, Y. Tan, M. Manfra, G. Klimeck, Y. P. Chen, and T. Kubis, In-surface confinement of topological insulator nanowire surface states, Appl. Phys. Lett. 107, 121605 (2015).

[6] P. Y. Long, M. Povolotskyi, B. Novakovic, T. Kubis, G. Klimeck, and M. J. W. Rodwell, Design and Simulation of Two-Dimensional Superlattice Steep Transistors, IEEE Electron. Dev. Lett. 35, 1212 (2014).

[7] Y. He, Y. Wang, G. Klimeck, and T. Kubis, Non-equilibrium Green's Functions Method: Non-trivial and Disordered Leads, Appl. Phys. Lett. 105, 213502 (2014).

[8] S. R. Mehrotra, M. Povolotskyi, D. C. Elias, T. Kubis, J. J. M. Law, M. J. W. Rodwell and G. Klimeck, Simulation study of thin-body ballistic n-MOSFETs involving transport in mixed Γ-L valleys, IEEE Elect. Dev. Lett. 34, 1196 (2013).

[9] Z. Jiang, M. A. Kuroda, Y. Tan, D. M. Newns, M. Povolotskyi, T. B. Boykin, T. Kubis, Gerhard Klimeck, and G. J. Martyna, Electron transport in nano-scaled piezoelectronic devices, Appl. Phys. Lett. 102, 193501 (2013).

[10] T. Liu, T. Kubis, G. Klimeck, and Q. J. Wang, Design of three-well indirect pumping terahertz quantum cascade lasers for high optical gain based on nonequilibrium Green's function analysis, Appl. Phys. Lett. 100, 122110 (2012).

[11] T. Kubis, S. R. Mehrotra, and G. Klimeck, Design concepts of terahertz quantum cascade lasers: Proposal for terahertz laser efficiency improvements, Appl. Phys. Lett. 97, 261106 (2010).

[12] C. Deutsch, A. Benz, H. Detz, P. Klang, M. Nobile, A. M. Andrews, W. Schrenk, T. Kubis, P. Vogl, G. Strasser, and K. Unterrainer, Terahertz Quantum Cascade Lasers based on Type II InGaAs/GaAsSb/InP, Appl. Phys. Lett. 97, 261110 (2010).

[13] H. Yasuda, T. Kubis, P. Vogl, N. Sekine, I. Hosako, K. Hirakawa, Nonequilibrium Green's function calculation for four-level scheme terahertz quantum cascade lasers, Appl. Phys. Lett. 94, 151109 (2009).

Regular Conference Proceedings and Presentations

[1] S. Moslemi-Tabrizi, P. Schvan, U. Kapoor, P. Blaise, and T. Kubis, Low-temperature Behavior in Nanowire Transistors by Quantum Transport Simulation, Silvaco luncheon during IEDM, San Francisco 2024

[2] H.-W. Hsiao, N. Narendra, and T. Kubis, DFTB Predictions of Twist Angle-Dependent Piezoelectricity in Heterobilayer Systems with 1000-2000 Atoms, APS March Meeting, Minneapolis 2024

[3] H.-W. Hsiao, N. Narendra, and T. Kubis, Solving Kohn-Sham Equations of Heterobilayer Systems Beyond 1000 Atoms: Twist Angle-dependent Piezoelectricity, IWCN 2023, Barcelona, Spain

[4] P. Blaise, T. Kubis, and E. Guichard, Nanowire transport and edge passivation, IWCN 2023, Barcelona, Spain

[5] P. Sarangapani, Y. Chu, J. Charles, and T. Kubis, Prediction of Urbach tails and band gap narrowing in bulk and confined III-V devices with atomistic non-equilibrium Green's functions, IWCN2019, Evanston, Illinois

[6] K.-C. Wang, S. H. Sureshbabu, Y. Chu, and T. Kubis: From semiclassical to quantum transport modeling including carrier recombination and generation, IWCN2019, Evanston, Illinois

[7] Y. Chu, J. Shi, K. Miao, Y. Zhong, P. Sarangapani, X. Ruan and T. Kubis: Thermal boundary resistance predictions with non-equilibrium Green's function and molecular dynamics simulations, IWCN2019, Evanston, Illinois

[8] J. Wang, K.-C. Wang, Y. Chu, and T. Kubis: Design of Ultraviolet Light Emitting Diodes Based on Hexagonal Boron Nitride, IWCN2019, Evanston, Illinois

[9] J. Charles, S. Kais, T. Kubis, Modeling Molecules in Interacting Environments, ACS National Meeting and Exposition 2018, New Orleans, Louisiana

[10] K.-C. Wang, P. Sarangapani, Y. Chu, and T. Kubis, Nonequilibrium Green's function method: Büttiker probes for carrier generation and recombination, SISPAD2018, Austin, Texas

[11] P. Sarangapani, Y. Chu, K.-C. Wang, D. Valencia, J. Charles, and T. Kubis, Nonequilibrium Green's function Method: Transport and Band Tail Prediction in Transition Metal Dichalcogenides, SISPAD2018, Austin, Texas

[12] Y. Chu, P. Sarangapani, J. Charles, G. Klimeck, and T. Kubis, Electron-only Explicit Screening Quantum Transport Model for Semiconductor Nanodevices, SISPAD2018, Austin, Texas

[13] J. Geng, P. Sarangapani, B. Browne, C. Wordelman, E. Nelson, T. Kubis, and G. Klimeck, Multi-Scale Nonequilibrium Green's Function Method for LEDs: Balance of Thermalization and Tunneling, IWCN2017, Windermere UK

[14] Y. Chu, P. Sarangapani, J. Charles, M. Povolotskyi, G. Klimeck and T. Kubis, Nonequilibrium Green's function method: Performance prediction of band-to-band tunneling devices in electron-only representation, IWCN2017, Windermere UK
[15] K.-C. Wang, T. Kosev Stanev, D. Valencia, J. Charles, P. Sarangapani, A. Henning, V. K. Sangwan, A. Lahiri, M. Povolotskyi, A. Afzalian, G. Klimeck, M. Lundstrom, M. C. Hersam, L. J. Lauhon, N. P. Stern, and T. Kubis, Stark effect in the photoluminescence of transition metal dichalcogenide structures, IWCN2017, Windermere UK
[16] J. Charles, P. Sarangapani, Y. Chu, G. Klimeck, and T. Kubis, Non-Local Scattering with a New Recursive Nonequilibrium Green's Function Method, IWCN2017, Windermere UK
[17] P. Sarangapani, Y. Chu, J. Charles, G. Klimeck, and T. Kubis, Non-equilibrium Green's function method: Band tail formation in non-local polar optical phonon scattering, IWCN2017, Windermere UK
[18] X. Guo, K.-C. Wang, J. Charles, J. Geng, D. Mejia, D. Valencia, D. Lemus, J. E. Fonseca, G. Klimeck, and T. Kubis, NEMO5, Xeon Phi and hStreams: Physics of Ultrascaled 2D Nanotransistors, Supercomputing 2016, Salt Lake City, UT
[19] K.-C. Wang, D. Valencia, J. Charles, Y. He, M. Povolotskyi, G. Klimeck, J. Maassen, M. Lundstrom, T. Kubis, NEMO5: Predicting MoS2 Heterojunctions, International Conference on Simulation of Semiconductor Processes and Devices 2016,
[20] X. Guo, K.-C. Wang, J. Charles, J. Geng, D. Mejia, D. Valencia, D. Lemus, J. E. Fonseca, G. Klimeck, and T. Kubis, MPI + hStreams in NEMO5: Partitioning Xeon Phi, Intel Xeon Phi User Group (IXPUG) 2016, Chicago, IL
[21] J. Geng, P. Sarangapani, E. Nelson, C. Wordelman, B. Browne, T. Kubis, and G. Klimeck, Multi-Scale, Multi-Physics NEGF Quantum Transport for Nitride LEDs, 16th International Conference NUSOD
[22] P. Long, J. Z. Huang, M. Povolotskyi, D. Verreck, J. Charles, T. Kubis, G. Klimeck, M. J. W. Rodwell, B. H. Calhoun, A tunnel FET design for high-current, 120mV operation, Electron Devices Meeting (IEDM) (2016).
[23] F. W. Chen, M. Manfra, G. Klimeck, and T. Kubis, NEMO5: Why Must We Treat Topological Insulator Nanowires Atomically?, IWCE2015, West Lafayette, IN, USA
[24] Y. P. Tan, M. Povolotskyi, T. Kubis, T. B. Boykin, and G. Klimeck, Transferable Tight Binding Model for Strained Group IV and III-V Heterostructures, IWCE2015, West Lafayette, IN, USA
[25] A. Afzalian, J. Huang, H. Ilatikhameneh, J. Charles, D. Lemus, J. Bermeo Lopez, S. Perez Rubiano, T. Kubis, M. Povolotskyi, G. Klimeck, M. Passlack, and Y.-C. Yeo, Mode Space Tight Binding Model for Ultra-Fast Simulations of III-V Nanowire MOSFETs and Heterojunction TFETs, IWCE2015, West Lafayette, IN, USA

[26] Y. Tan, M. Povolotskyi, T. Kubis, T. B. Boykin and G. Klimeck, Tight Binding analysis of Si/GaAs UTBs with subatomic resolution, IWCE2014, Paris, France
[27] H. Ilatikhameneh, B. Novakovic, Y. Tan, T. Kubis, M. Povolotskyi, R. Rahman and G. Klimeck, Transport properties of 2D material transistors, IWCE2014, Paris, France
[28] K. Miao, H. Ilatikhameneh, Y. He, M. Povolotskyi, G. Klimeck, T. Kubis and T. S. Fisher, Thermal transport across strain relaxed Si/Ge interfaces, IWCE2014, Paris, France
[29] P. Sarangapani, Y. Tan, J. Charles, T. A. Ameen, M. Povolotskyi, T. Kubis and G. Klimeck, Atomistic Tight Binding Simulations with Real Space Basis Functions: Optical Properties of Multi Million Atom Systems, IWCE2014, Paris, France.
[30] Y. He, T. Kubis, M. Povolotskyi, J. Fonseca, G. Klimeck, Quantum Transport in NEMO5: Algorithm Improvements and High Performance Implementation, SISPAD 2014, Yokohama, Japan
[31] J. Charles, M. Povolotskyi, Y. He, Y. Maeda, D. Lemus, T. Kubis, G. Klimeck, T. Sakurai, Applications of Eigenvalue Solvers in Nanoelectronic Device Modeling, EPASA2014, Tsukuba-city, Japan
[32] Y. Wang, Y. He, G. Klimeck, and T. Kubis, Nonequilibrium Green's Function Method: Algorithm for Regular and Irregular Leads, IWCE2013, Nara, Japan
[33] Z. Jiang, M.A. Kuroda, Y. Tan, D.M. Newns, G.J. Martyna, M. Povolotskyi, T.B. Boykin, T. Kubis, and G. Klimeck, Tight-Binding Modeling of Intermediate Valence Compound SmSe for Piezoelectronic Devices, IWCE2013, Nara, Japan
[34] Y. He, L. Zeng, T. Kubis, M. Povolotskyi, and G. Klimeck, Efficient solution algorithm of non-equilibrium Green's functions in atomistic tight binding representation, IWCE2012, Madison, Wisconsin
[35] L. Zeng, Y. He, T. Kubis, M. Povolotskyi, X. Y. Liu, and G. Klimeck, Efficient solution algorithm of non-equilibrium Green's functions in effective mass approximation, IWCE2012, Madison, Wisconsin
[36] Z. Jiang, Y. He, Y. Tan, M. Povolotksyi, T. Kubis, and G. Klimeck, Quantum Transport in GaSb/InAs Nanowire TFET with Semiclassical Charge Density, IWCE2012, Madison, Wisconsin
[37] P. Sengupta, T. Kubis, M. Povolotskyi, and G. Klimeck, Tight binding based electronic structure calculation for topological insulators and broken-gap devices, IWCE2012, Madison, Wisconsin
[38] J. Fonseca, T. Kubis, M. Povolotksyi, Y. He, H. Ilatikhameneh, Z. Jiang, S. Kim, D. Meija, J. M. Sellier, P. Sengupta, Y. Tan, and G. Klimeck, NEMO5, a Parallel, Multiscale, Multiphysics Nanoelectronics Modeling Tool, SISPAD 2012, Denver, Colorado
[39] T. Kubis and G. Klimeck, Conceptual design improvements for terahertz quantum cascade lasers need for molecule detection, NanoDDS 2011, Brooklyn, NewYork

[40] C. Deutsch, A. Benz, H. Detz, P. Klang, M. Nobile, A. M. Andrews, W. Schrenk, T. Kubis, P. Vogl, G. Strasser and K. Unterrainer, InGaAs/GaAsSb Terahertz Quantum Cascade Lasers, EDISON 2011, Santa Barbara, California

[41] T. Kubis, P. Vogl, How periodic are terahertz quantum cascade lasers?, EDISON 2009, Montpellier, France

[42] A. Matyas, T. Kubis, P. Lugli, and C. Jirauschek, Carrier transport in THz quantum cascade lasers: Are Green's functions necessary? , EDISON 2009, Montpellier, France

[43] H. Yasuda, T. Kubis, P. Vogl, N. Sekine, I. Hosako, and K. Hirakawa, Non-equilibrium Green's function calculation for four-level scheme terahertz quantum cascade lasers, EDISON 2009, Montpellier, France

[44] T. Kubis, P. Vogl, Non-equilibrium quantum transport theory: Current and gain in quantum cascade lasers, IWCE2010, Amherst, Massachusetts

[45] T. Kubis, P. Vogl, Microscopic theory of spin-filtering in non-magnetic semiconductor nanostructures, HCIS15, Tokyo, Japan

[46] T. Kubis, P. Vogl, Quantum theory of transport and optical gain in quantum cascade lasers, HCIS15, Tokyo, Japan

[47] T. Kubis, P. Vogl, Self-consistent Quantum Transport Theory: Applications and Assessment of Approximate Models, IWCE2006, Vienna, Austria

[48] T. Kubis, S. Birner, P. Vogl, C. Jirauschek, Non-equilibrium quantum transport theory for quantum cascade lasers, ICPS28, Vienna, Austria

[49] T. Kubis, A. Trellakis, P. Vogl, Self-consistent quantum transport theory of carrier capture in heterostructures, HCIS14, Chicago, Illinois

Invited Conference Presentations

[1] L. Melican, D. Lemus, and T. Kubis, Mode space in DFTB quantum transport in the nanodevice simulation tool NEMO5, 2024 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), San Jose, 2024

[2] T. Kubis, Victory Atomistic – Updates on 2D Materials, CNTs, and How We Bridge Atomistic Simulations and TCAD, SURGE Virtual Event North America 2022

[3] T. Kubis, Latest quantum transport models for atomistic material and device performance predictions, VLSI-TSA, Hsinchu, Taiwan, 2022

[4] T. Kubis, Self-energies in Atomistic Quantum Transport for Energy Transfer at Irregular Interfaces, IEDM, San Francisco, 2021

[5] T. Kubis, Victory Atomistic: Fully Customizable Atomistic Simulation Toolbox, SURGE Virtual Event North America 2021

[6] T. Kubis, State-of-the-art Quantum Transport Simulation with NEMO5 & Victory Atomistic, SURGE Virtual Event North America 2020

[7] J. Charles, P. Sarangapani, and T. Kubis, Atomistic Green's functions: the beauty of self-energies, ESSDERC 2020, Grenoble, France

[8] X. Guo, D. Lemus, J. Charles, and T. Kubis, Resource control in NEMO5's quantum transport calculations, IWCN2019, Evanston, Illinois

[9] K.-C. Wang, P. Sarangapani, Y. Chu, and T. Kubis, Self-energies: enabling multiphysics and multiscaling in optoelectronic quantum transport modeling, NUSOD 2018, Hongkong, PR China

[10] X. Guo, D. Lemus, D. Mejia, J. Fonseca, G. Klimeck, and T. Kubis, NEMO5: A Parallelized Multi-Scale and Multi-Physics Nanodevices Simulation Software, SIAM Conference on Computational Science and Engineering (CSE) 2017, Atlanta, GA

[11] T. Kubis, J. Geng, G. Klimeck, NEMO5: Efficient modeling of quantum transport in light emitting diodes, OPTO SPIE Photonics West 2017, San Francisco, California

[12] T. Kubis, Y. He, R. Andrawis, and G. Klimeck, General Retarded Contact Self-energies in and beyond the Non-equilibrium Green's Function Method, Journal of Physics: Conference Series, 696, 012019 (2016).

[13] T. Kubis, Transport in realistic nanoscale devices with NEMO5, SRC Annual Executive Review 2015 – Intel Hillsboro, Oregon

[14] T. Kubis, Contact self-energies: More than simple boundary conditions, Progress in Nonequilibrium Green's functions VI – Lund, Sweden, 2015

[15] P. Vogl, T. Kubis, P. Greck, The nonequilibrium Green's functions method and descendants: ways to avoid and to go, IWCE2010, Pisa, Italy

[16] T. Kubis, G. Klimeck, Rough interfaces in THz quantum cascade lasers, IWCE2010, Pisa, Italy

[17] T. Kubis, G. Klimeck, and P. Vogl, Prediction of novel and efficient THz quantum cascade lasers, IQCLSW 2010, Florence, Italy

[18] T. Kubis, P. Vogl, Predictive quantum theory of current and optical emission in quantum cascade lasers, OPTO SPIE Photonics West 2009, San Jose, California

[19] T. Kubis, P. Vogl, Predictive quantum theory of current and optical gain in quantum cascade lasers, Lphys'08, Trondheim, Norway

Invited Lectures

[1] "Non-equilibrium quantum transport theory of quantum cascade lasers," ECE Seminar, Technical University of Munich, Munich, Germany, November 30, 2006.

[2] "Self-consistent quantum transport theory in semiconductor heterostructures: challenges, pitfalls and solutions", Physics Seminar, University of Regensburg, Regensburg, Germany, May 6, 2007.

[3] "Nonequilibrium Green's functions theory: Transport and optical gain in THz quantum cascade lasers", Birck seminar, Purdue University, West Lafayette, IN, March 26, 2010.

[4] "Introduction to nonequilibrium Green's function method: challenges, solutions and applications", ECE Seminar, University of Chicago, Chicago, IL, November 30, 2011.

[5] "NEMO5 Overview Presentation", NCN Summerschool 2012, Purdue University, West Lafayette, IN, July 17, 2012.

[6] "Self-energies: Opening Doors for Nanotechnology", Predictive Science Faculty Seminar, Purdue University, West Lafayette, IN, April 4, 2016.

[7] "NEMO5 and 2D Materials: Tuning Bandstructures, Wave Functions and Electrostatic Screening", ECE Seminar, Purdue University, West Lafayette, IN, October 19, 2016.

[8] "Nonequilibrium Green's Functions: Reliably Predicting Chemical Reactions", Physical Chemistry Seminar, Purdue University, West Lafayette, IN, February 15, 2017.

[9] "Nonequilibrium Green's Functions: A Powerful Many-Body Method", Physics Seminar, The University of Toledo, OH, October 5, 2017.

[10] "Atomistic Device Simulations", Silvaco User Global Event, Santa Clara, CA, October 9, 2018.

[11] "Quantum Transport Simulations for 21st Century Electronics, Coloquio del ICF, Universidad Nacional Autonoma de Mexico, Mexico City, June 15, 2022

[12] Atomistic Quantum Code Library – Heat, Spin and Charge Transport in Nanodevices and Molecular Chemistry, TU-Munich, Germany, June 16, 2023

[13] Ideas to Innovation Pathway, Universidade de São Paulo, Brazil, November 21-24, 2023

Published Reviews

[1] P. Sarangapani, J. Charles, and T. Kubis, "Tuning band tails in mono and multilayered transition metal dichalcogenides: A detailed assessment and a quick-reference guide", Phys. Rev. Applied 17, 024005 (2022)

[2] N. Narendra, X. Chen, J. Wang, J. Charles, R. G. Cooks, T. Kubis, Quantum mechanical modeling of reaction rate acceleration in microdroplets, J. Phys. Chem. A 124, 4984 (2020)

[3] Prasad Sarangapani, Yuanchen Chu, James Charles, Gerhard Klimeck, and Tillmann Kubis, Band-tail formation and band-gap narrowing driven by polar optical phonons and charged impurities in atomically resolved III–V semiconductors and nanodevices, Phys. Rev. Applied 12, 044045 (2019)

[4] S. Sadasivam, N. Ye, J. P. Feser, J. Charles, K. Miao, T. Kubis, and T. S. Fisher, Thermal transport across metal silicide-silicon interfaces: First-principles calculations and Green's function transport simulation, Phys. Rev. B 95, 085310 (2017)

[5] Y. P. Tan, M. Povolotskyi, T. Kubis, T. Boykin, and G. Klimeck, Tight-binding analysis of Si and GaAs ultrathin bodies with subatomic resolution, Phys. Rev. B 92, 085301 (2015)

[6] C. Jirauschek and T. Kubis, Modeling techniques for quantum cascade lasers, Appl. Phys. Rev. 1, 011307 (2014).

[7] S. Steiger, M. Salmani-Jelodar, D. Areshkin, A. Paul, T. Kubis, M. Povolotskyi, H.-H. Park, and G. Klimeck, Enhanced valence force field model for the lattice properties of gallium arsenide, Phys. Rev. B 84, 155204 (2011).

[8] T. Kubis, P. Vogl, Assessment of approximations in nonequilibrium Green's function theory, Phys. Rev. B 83, 195304 (2011).

[9] T. Kubis, C. Yeh, P. Vogl, A. Benz, G. Fasching, C. Deutsch, Theory of nonequilibrium quantum transport and energy dissipation in terahertz quantum cascade lasers, Phys. Rev. B 79, 195323 (2009).

Pending Publications

[1] N. Narendra and T. Kubis, Ultrasensitive, universal single-ion nanodetector, ACS Nano Lett. under review

[2] M. Pratap, L. Melican, and T. Kubis, Selective State Filtering in NEGF: A method for Quantum State Sensitivity Analysis, J. Comp. Electronics under review

[3] Nanometer-scale carbon nanotube field-effect transistor mass analyzer, in preparation for Journal of the American Society for Mass Spectrometry

[4] N. Narendra, R. G. Cooks, and T. Kubis, Quantum Mechanics of Molecules in their Explicit Environment: Shifting Reaction Pathways at Droplet Surfaces, resubmission in preparation for Physical Chemistry Chemical Physics

Patents Approved and Patent Applications

1. T. Kubis, Light emitting device and method of making the same, Patent granted, US Patent 12,477,863, November 2025
2. T. Kubis, System and methods for fabrication of quantum computing networks, NATL patent filed, US 19/481,852, November 2025
3. T. Kubis, C. Ferreira, J. Appenzeller, N. Narendra, Semiconductor/insulator heterostructure-based analyzer, Provisional patent filed, US 63/921,760, November 2025
4. T. Kubis, System and methods for thermal management of 2D materials, Provisional patent filed, US 63/872,266, August 2025
5. T. Kubis, H.-W. Hsiao, D. Lemus, L. Melican, Methods and systems for enabling density functional quantum transport simulations, Provisional patent filed, US 63/863,785, August 2025
6. C. Steele, R. Baretto, F. Berry, T. Kubis, J. Condron, New photocatalyst for photodegradation of unwanted, Provisional patent files, US 63/855,667, August 2025
7. C. Ferreira, T. Kubis, N. Gutierrez, Excretable therapeutic system and method for PFAS clearance, Provisional patent filed, US 63/854,985, July 2025
8. T. Kubis, F. Berry, Light energy harvesting systems and methods, US patent application filed, US 19/283,544, July 2025
9. T. Kubis, Y. Chu, K.-C. Wang, Method of modeling interactions between many particles, Patent granted, US Patent 12,190,028, July 2025

10. C. Ferreira, T. Kubis, K-H Huang, Remediation of per- and polyfluoroalkyl substances (PFAS) by chemical derivation, US Patent application filed, US 63/845,182, July 2025
11. R. Barreto, F. Berry, J. Condron, T. Kubis, C. Steele, A device for pigmenting lumber, US-patent application filed, US 63/829,366, June 2025
12. T. Kubis, C. Ferreira, N. Narendra, Carbon nanotube-based ion analyzer, PCT-patent application filed, PCT/US25/17531, February 2025
13. T. Kubis, H.-W. Hsiao, "Piezoelectricity of 2D Heterobilayer Systems", US Patent application filed, US 18/943,654, November 2024
14. T. Kubis, F. Berry, "Waveguide Based Light Collection and Distribution Devices", Provisional Patent filed, US 63/712,761, October 2024
15. T. Kubis, J. Charles, "Enhanced cascade field effect transistor", US Patent 12,132,102B2, October 2024
16. T. Kubis, F. Berry, "Telasol – LEDs and optical devices to harvest light energy", Provisional Patent filed, US63/677,829, July 2024
17. G. Klimeck, T. Kubis, J. Geng, "Method and system for realistic and efficient simulation of light emitting diodes having multi-quantum-wells", US Patent 12,050,844B2, July 2024
18. T. Kubis, D. Lemus, H.-W. Hsiao, L. Melican, "Low rank approximation for density functional theory representations", Provisional Patent filed, US63/665,532, June 2024
19. T. Kubis, "Low-cost Fabrication Method for Charge and Current Based Quantum Computing Networks", PCT Patent filed, PCT/US24/28721, May 2024
20. T. Kubis, N. Narendra, C. Ferreira, "CNT Based Mass Spectrometer", Provisional Patent filed, US 63/562,888, March 2024
21. T. Kubis, H.-W. Hsiao, "Piezoelectric heterosystems and methods of manipulating the properties thereof", Provisional Patent filed, US 63/548,171, November 2023
22. T. Kubis, "Flexible nanoparticle based light collection and distribution devices", Provisional Patent filed, US 63/544,534, October 2023
23. C. Steele, T. Kubis, "In-flow photoreactor system and method", Provisional Patent filed, US 63/544,530, October 2023
24. T. Kubis, J. Charles, and D. Lemus, "System architecture and methods of determining device behavior", Patent granted, US Patent 11,768,981, September 2023.
25. T. Kubis, "Systems and Methods for Generating Computational models of materials, interfaces, and devices", U.S. Patent application filed, July 2023
26. T. Kubis, "Semiconductor device and method of making the same", Patent granted, US Patent 11,682,749, June 2023

27. T. Kubis, “System and Methods for Fabrication of Quantum Computing Networks”, Provisional Patent filed, US 63/465,905, May 2023

28. T. Kubis, “Light emitting device and method of making the same”, Patent granted US Patent 11,605,756, March 2023

29. T. Kubis and J. Charles, “Method of identifying properties of molecules under open boundary conditions”,
Patent granted US Patent 11,508,463, November 2022;
Continuation filed US 18/160,578, January 2023

30. T. Kubis and P. Sarangapani, “Method of modeling many particle system”, Patent granted US Patent 11,372,948, August 2022

31. T. Kubis and J. Charles, “Enhanced cascade field effect transistor”, U. S. Patent granted US Patent 11,362,200, August 2022

32. T. Kubis and R. Martinez, “Flexible nanostructure based light collection and distribution devices”, Provisional Patent filed US 63/391,204, July 2022

33. T. Kubis and H.-W. Hsiao, “DFTB Parameterization Method to Faithfully Reproduce Various Observables”, Provisional Patent filed US 63/388,997, July 2022

34. T. Kubis, “System and Methods for Fabrication of Quantum Computing Networks”, Provisional Patent filed US 63/339,235, May 2022

35. T. Kubis and R. Martinez, “Water Desalination via Electrostatic Rapid Water Transport through Polymeric Carbon Nanotube Membranes”, Provisional Patent filed US 63/336,712, April 2022

36. T. Kubis, “Semiconductor device and method of making the same”, U.S. Patent granted US Patent 11,152,542, October 2021

37. T. Kubis, J. Charles, and D. Lemus, “Hybrid Simulation Approach of Atomistic Quantum Transport and Semiclassical Drift Diffusion”, U.S. Patent application filed September 2021

38. G. Klimeck, T. Kubis, and J. Geng, “Method and system for realistic and efficient simulation of light emitting diodes having multi-quantum-wells”, US Patent granted US Patent 11,093,667, August 2021

39. T. Kubis and P. Sarangapani, “Cascade tunneling field effect transistor”, U. S. Patent granted US Patent 10,763,367, November 2020.

40. T. Kubis, J. Charles, and D. Lemus, “Open-closed hybrid boundary quantum property method”, U.S. Patent application filed September 2020.

41. T. Kubis and P. Sarangapani, “Predictive and automatic determination of nonlocal scattering scaling factor”, U. S. Patent application filed November 2019.

42. T. Kubis and J. Charles, “General Cascade Field Effect Transistor Concept”, U. S. Patent application filed June 3, 2019.

43. T. Kubis, “Staggered 2D LEDs for Multi-Purpose Lighting”, U. S. Patent application filed August 2019.

44. T. Kubis and X. Guo, “Machine Learning and Dynamic Resource Management Platform”, U. S. Patent application filed April 2019.

45. T. Kubis, Y. Chu, and K.-C. Wang, “Method of modeling interactions between many particles”, U. S. Patent application filed August 2019.

46. G. Klimeck, M. Povolotskyi, T. C. Kubis, and G. Hedge, “Physical modeling of electronic devices/systems," U. S. Patent granted US9858365B2 January 02, 2018

47. T. Kubis, “System and methods of processing liquid therein”, U. S. Patent application filed April 3, 2017.

48. G. Klimeck, T. C. Kubis, and J. Geng, “Realistic and Efficient Model for LED Devices”, U. S. Patent application filed May 22, 2017.

49. T. C. Kubis and J. A. Charles, “Open Boundary Conditions for Quantum Models in Fluids”, U. S. Patent application filed June 29, 2017.

50. T. Kubis, Y. Chu, and K.-C. Wang, “Generalized Büttiker probes”, U. S. Patent application filed August 2018.

51. T. Kubis, J. Charles, and D. Lemus, “Method of modelling many-particle systems”, U. S. Patent application filed September 2018.

52. T. Kubis and P. Sarangapani, “Predictive and Automatic Determination of Nonlocal Scattering Scaling Factor”, U. S. Patent application filed November 2018.

Activities as a Referee

Nature Partner Journals Computational Materials
AVS Quantum Science
Nature Communications Physics
Physical Review Applied
Journal of Physics: Condensed Matter
AIP Advances
Physical Review Letters
Journal of Physical Review B
Applied Physics Letters
Journal of Applied Physics
Optics Express
IEEE Transactions on Electron Devices
Journal of Quantum Electronics
Journal of Selected Topics in Quantum Electronics

Journal of Computational Electronics
European Journal of Physics
Nanomaterials and Nanotechnology Journal
New Journal of Physics
Physica Status Solidi
Journal of Physics D: Applied Physics
Scientific Reports
Reviews of Modern Physics
Philosophical Magazine
Opto-Electronics Review
IEEE Electron Device Letters

Special Projects, Short Courses, etc. -- Contribution

Lecturer, "NEMO5 lectures and hands-on tutorial series", Training for Intel engineers, Hillsboro, OR, June 24 – 26, 2014.

Other Activities:

Member of advisory board committee of international workshop of computational nanotechnology, 2015 - present.

Head-organizer, Summit on Big Data and Cyberinfrastructure in Material Science, Chicago, November 21-22, 2019.

Member of the standing committee for ECE Junior Faculty Recruitment (2023-2024 until committee was dissolved)

Head of search committee for Silicon Valley professor of engineering practice (2025 – present)