

Dr. Gabriele Penazzi



Personal information

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Experience

- 2010–Present **Research Scientist**, *Bremen Center for Computational Material Science, Physics Department, University of Bremen, Deutschland.*
- Research in the field of atomistic modelling of charge transport in nanostructured materials and devices
 - Students supervision and teaching
 - Co-author of awarded grant proposals
 - Co-organizer of international conferences
- 2009–2010 **Research Assistant**, *Department of Electronic Engineering, University of Rome Tor Vergata, Italy.*
- Research in the field of multiscale atomistic/finite element modelling of electronic devices
 - Students supervision and teaching
- 2006–Present **Founder member**, *Tiberlab S.r.l. - Spinoff of University of Rome "Tor Vergata", Italy.*
- TiberCAD TCAD development (www.tibercad.org) and training.

Education

- 2006–2010 **PhD in Learning and Sensing Systems Engineering**, *Department of Electronic Engineering, University of Rome Tor Vergata.*
Thesis Title: *Development of an atomistic/continuous simulation tool for nanoelectronic devices*
- 2003–2006 **MSc in Electronic Engineering**, *Department of Electronic Engineering, University of Rome Tor Vergata, 110/110 cum laude.*
Thesis title: *Development of a quantum transport simulator*
- 2000–2003 **Bachelor in Electronic Engineering**, *Department of Electronic Engineering, University of Rome Tor Vergata, 110/110 cum laude.*
Thesis title: *Experimental analysis of optical properties of Gallium Nitride*

Research interests

- Computational atomistic and multiscale charge transport modelling
- Charge transport in molecular systems and organic composites
- Non Equilibrium Green's Function base methods
- Nanostructured electronic materials and devices
- Density Functional Tight Binding theory and applications

Teaching

- 2014-2015 Lecturer in the class "Electronic Transport at Nanoscale", M.Sc. in Physics, University of Bremen
- 2013-Present Supervision of Bachelor students in Physics
- 2012-Present Lecturer in DFTB+ international tutorials and hands-on
- 2008-2010 Supervision of M.Sc. and Bachelor students in Electronic Engineering
- 2008-2010 Teaching assistant in the classes "Optoelectronic" and "Nanoelectronics", M.Sc. in Electronic Engineering, University of Rome "Tor Vergata"

Relevant professional activities

- 2015 Co-author awarded Eu Project SOPHIA proposal (Photovoltaic TNT Modeling) "MUSAS-ATOMISTIC".. Host agency ENEA, Italy
- 2015 Co-author of awarded DFG grant proposal "Time-dependent description of charge transport in molecular wires: bottom-up approach"
- 2014 Co-organizer of the International CECAM workshop "Charge Transport in Organic Materials", Bremen
- 2013 Co-organizer of the International CECAM workshop "Molecular Electronics: Quo Vadis", Bremen
- 2013 Co-author of awarded DFG grant proposal "Multi-scale approach for prediction of electrical properties of carbon nanotube reinforced polymers"
- 2010-present Developer for DFTB+ software (www.dftb-plus.org)
- 2007-present Developer for TiberCAD software (www.tibercad.org)

Computational skills

- Scientific programming in C/C++, Fortran, Python, Matlab
- Parallel programming OpenMP and MPI
- Experience with atomistic modelling: density functional and molecular dynamics
- Experience with Finite Element/Difference modelling (gmsh, libmesh)
- Version control systems (svn, git), automatic documentation (Sphinx, Doxygen)
- Data analysis and visualization

Languages

Italian **Mother tongue**

English **Fluent**
German **Intermediate - B2**

Journal articles

- 2016 Auf der Maur, M., A. Pecchia, G. Penazzi, W. Rodrigues, and A. Di Carlo. "Efficiency Drop in Green InGaN / GaN Light Emitting Diodes: The Role of Random Alloy Fluctuations". In: *Physical Review Letters* 116.2, p. 027401.
Penazzi, G., A. Pecchia, V. Gupta, and T. Frauenheim. "A Self Energy Model of Dephasing in Molecular Junctions". In: *The Journal of Physical Chemistry C*.
- 2015 Bhandary, S., G. Penazzi, J. Fransson, T. Frauenheim, O. Eriksson, and B. Sanyal. "Controlling Electronic Structure and Transport Properties of Zigzag Graphene Nanoribbons by Edge Functionalization with Fluorine". In: *The Journal of Physical Chemistry C* 36, p. 119.
Markov, S., G. Penazzi, Y. Kwok, A. Pecchia, B. Aradi, T. Frauenheim, and G. Chen. "Permittivity of oxidized ultra-thin silicon films from atomistic simulations". In: *IEEE Electron Device Letters* 36, pp. 1076–1078.
- 2014 López, M., A. Pecchia, M. Auf der Maur, F. Sacconi, G. Penazzi, and A. Di Carlo. "Atomistic simulations of InGaN/GaN random alloy quantum well LEDs". In: *physica status solidi (c)* 11.3, pp. 632–634.
- 2013 Auf der Maur, M., A. Pecchia, G. Penazzi, F. Sacconi, and A. Carlo. "Coupling atomistic and continuous media models for electronic device simulation". In: *Journal of Computational Electronics* 12, pp. 553–562.
Deák, P., B. Aradi, A. Gagliardi, H. A. Huy, G. Penazzi, B. Yan, T. Wehling, and T. Frauenheim. "Possibility of a Field Effect Transistor Based on Dirac Particles in Semiconducting Anatase-TiO₂ Nanowires". In: *Nano Letters* 13.3, pp. 1073–1079.
Penazzi, G., J. M. Carlsson, C. Diedrich, G. Olf, A. Pecchia, and T. Frauenheim. "Atomistic modeling of charge transport across a carbon nanotube-polyethylene junction." In: *Journal of Physical Chemistry C* 117, pp. 8020–8027.
- 2011 Auf der Maur, M., G. Penazzi, G. Romano, F. Sacconi, A. Pecchia, and A. Di Carlo. "The multiscale paradigm in electronic device simulation". In: *Electron Devices, IEEE Transactions on* 99, pp. 1–8.
- 2010 Auf der Maur, M., F. Sacconi, G. Penazzi, G. Romano, M. Povolotskyi, A. Pecchia, and A. Di Carlo. "Concurrent multiscale simulation of electronic devices". In: *Journal of computational electronics* 9.3, pp. 262–268.
Penazzi, G., A. Pecchia, F. Sacconi, and A. Di Carlo. "Calculation of optical properties of a quantum dot embedded in a GaN/AlGaIn nanocolumn". In: *Superlattices and Microstructures* 47.1, pp. 123–128.
- 2009 Auf der Maur, M., F. Sacconi, G. Penazzi, M. Povolotskyi, G. Romano, A. Pecchia, and A. Di Carlo. "Coupling atomistic and finite element approaches for the simulation of optoelectronic devices". In: *Optical and quantum electronics* 41.9, pp. 671–679.
- 2008 Auf der Maur, M., M. Povolotskyi, F. Sacconi, A. Pecchia, G. Romano, G. Penazzi, and A. Di Carlo. "TiberCAD: towards multiscale simulation of optoelectronic devices". In: *Optical and quantum electronics* 40.14, pp. 1077–1083.

Pecchia, A., G. Penazzi, L. Salvucci, and A. Di Carlo. "Non-equilibrium Green's functions in density functional tight-binding: method and applications". In: *New Journal of Physics* 10, p. 065022.

Conference proceedings

- 2015 Markov, S., Y. Kwok, G. Chen, G. Penazzi, B. Aradi, T. Frauenheim, and A. Pecchia. "Atomic level simulation of permittivity of oxidized ultra-thin Si channels". In: SISPAD. IEEE, pp. 40–43. DOI: 10.1109/SISPAD.2015.7292253.
- 2014 Markov, S., C. Yam, G. Chen, B. Aradi, G. Penazzi, and T. Frauenheim. "Towards atomic level simulation of electron devices including the semiconductor-oxide interface". In: SISPAD. IEEE, pp. 65–68. DOI: 10.1109/SISPAD.2014.6931564.
- Penazzi, G., P. Deák, B. Aradi, T. Wehling, A. Gagliardi, H. A. Huy, B. Yan, and T. Frauenheim. "TiO₂ Nanowires as a Wide Bandgap Dirac Material: a numerical study of impurity scattering and Anderson disorder". In: *MRS Proceedings*. MRS. Cambridge University Press.
- 2013 Lopez, M., M. Auf der Maur, A. Pecchia, F. Sacconi, G. Penazzi, and A. Di Carlo. "Simulation of Random Alloy Effects in InGaN/GaN LEDs". In: NUSOD. Vancouver, Canada: IEEE.
- 2011 Baretin, D., A. Pecchia, G. Penazzi, M. Auf der Maur, B. Lassen, M. Willatzen, and A. Di Carlo. "Comparison of continuum and atomistic methods for the analysis of InAs/GaAs quantum dots". In: *Numerical Simulation of Optoelectronic Devices (NUSOD), 2011 11th International Conference on*, pp. 177–178. DOI: 10.1109/NUSOD.2011.6041203.
- 2010 Pecchia, A., G. Penazzi, and A. Di Carlo. "Point defect scattering in silicon nanowires". In: *Proc. 14th International Workshop on Computational Electronics (IWCE)*.
- Romano, G., G. Penazzi, and A. Di Carlo. "Multiscale thermal modeling of GaN/AlGaIn quantum dot LEDs". In: SPIE, pages. DOI: 10.1117/12.842645.
- Sacconi, F., G. Penazzi, A. Pecchia, M. Auf der Maur, and A. Di Carlo. "Optoelectronic and transport properties of nanocolumnar InGaIn/GaN quantum disk LEDs". In: SPIE, pages. DOI: 10.1117/12.840533.
- 2009 Auf der Maur, M., M. Povolotskyi, F. Sacconi, G. Romano, G. Penazzi, A. Pecchia, and A. Di Carlo. "Multiscale-Multiphysics Simulation of Nanostructured Devices: the TiberCAD Project". In: *Computational Electronics, 2009. IWCE '09. 13th International Workshop on*, pp. 1–4. DOI: 10.1109/IWCE.2009.5091126.
- Penazzi, G., A. Pecchia, F. Sacconi, M. Auf der Maur, M. Povolotskyi, G. Romano, and A. Di Carlo. "Simulations of Optical Properties of a GaIn Quantum Dot Embedded in a AlGaIn Nanocolumn within a Mixed FEM/atomistic Method". In: *Computational Electronics, 2009. IWCE '09. 13th International Workshop on*, pp. 1–4. DOI: 10.1109/IWCE.2009.5091153.

- 2008 Di Carlo, A., M. Auf der Maur, F. Sacconi, A. Pecchia, M. Povolotskyi, G. Penazzi, and G. Romano. "Multiscale Atomistic Simulations of High-k MOSFETs". In: *Nanotechnology, 2008. NANO '08. 8th IEEE Conference on*, pp. 377–378. DOI: 10.1109/NANO.2008.116.
- Sacconi, F., G. Romano, G. Penazzi, M. Povolotskyi, M. Auf der Maur, A. Pecchia, and A. Di Carlo. "Electronic and transport properties of GaN/AlGaIn quantum dot-based p-i-n diodes". In: *Simulation of Semiconductor Processes and Devices, 2008. SISPAD 2008. International Conference on*, pp. 177–180. DOI: 10.1109/SISPAD.2008.4648266.
- 2007 Pecchia, A., G. Penazzi, and A. Di Carlo. "Efficient Green's Function Algorithms for Atomistic Modeling of Si Nanowire FETs". In: *Proc. Simulation of Semiconductor Processes and Devices (SISPAD)*. Springer Vienna.

Invited talks

- 2015 CECAM workshop "Open quantum systems computational methods", 2015 Hong Kong. Title: "DFTB modeling of electronic materials and devices: current status and perspectives"
- 2015 CECAM workshop "Development of next generation accurate approximate DFT/B methods", 2015 Bremen, Germany. Title: "DFTB modeling of electronic materials and devices: current status and perspectives"
- 2014 CECAM workshop "High performance models of charge transport in large scale systems", 2014 Bremen, Germany. Title: "Tight binding modeling of charge transport in disordered materials"
- 2013 543 WE-Heraus Seminar "Electron Transport through Atoms, Molecules and Nanowires: Advances in Experiment and Theory", 27-31 October 2013 Bad Honnef, Germany. Title: "DFTB for charge transport: method and applications"