

Curriculum Vitae

Personal details

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Languages	Fluent in English, French, Italian

Current position

Function	Organization/Department	Location
Associate professor	DPIA, University of Udine	Via delle Scienze, 206, 33100 Udine, Italy

Activities

• Teaching

- 2023-present: course of "Electronics" (bachelor's degree in "Management Engineering", U Udine, 60 h)
- 2023-present: course of "Physics" (bachelor's degree in "Building and territory technology", U Udine, 60 h)
- 2013, 2014: course of "Numerical methods" (60 h) at Phelma, Grenoble-INP.
- 2010, 2011, 2012, 2013, 2014 and 2015: course of "simulation of electronic devices" (15 h) at PHELMA, Grenoble-INP.
- 2006, 2007, 2008, 2009, 2010 and 2011 course of "Quantum transport simulation: NEGF methods" (8 h) at the summer school ESONN "European School On Nanosciences and Nanotechnologies".

• Supervision of students and post-docs (2005-Present)

- 16 PhD candidates
- 6 Post-docs

• Refereeing activities

- 24 PhD committees
- Reviewer for national agencies such as ANR (France), FNRS (Belgium), MIUR (Italy), FWF (Austria).
- Regular reviewer for several journals (IEEE TED, IEEE EDL, PRL, PRB, APL, JAP, ACS Nano, SciRep, ...)
- Member of technical conference committees (IEDM, ESSDERC, IWCN)

• Visiting positions

- 09/2021-09/2022: Visiting researcher at Dipartimento di Ingegneria Industriale e dell'Informazione, University of Udine, Italy

• Conference organization

- 2006: Scientific chair of the summer school MIGAS 2007, Autrans, France
- 2016: Member of the organizing committee of the IEEE-EDS Mini-colloquium in Grenoble, France
- 2018-2019: member of the technical committee of the IEDM conference
- 2018-2022: member of the technical committee of the ESSDERC conference
- 2020-2022: member of the technical committee of the IWCN conference

• National scientific qualifications

- October 2024: "Abilitazione scientifica Nazionale" (Italy), professore I fascia, settore: 09/E3, elettronica
- January 2022: "Abilitazione scientifica Nazionale" (Italy), professore II fascia, settore: 02/B2, fisica teorica della materia
- August 2018: "Abilitazione Scientifica Nazionale" (Italy), professore II fascia, settore: 09/E3, elettronica

• Management

- 2018-2023: Head of the "Computational Electronics" group of C2N (UMR 9001), Palaiseau, France. 4 permanent researchers and professors, 4-5 PhDs and post-doc

- 2012-2016: Head of the Modeling and Simulation group of IMEP-LAHC (UMR 5130), Grenoble, France. 3-4 permanent researchers and professors, 4-5 PhDs and post-docs
- **Member of doctoral teaching boards**
 - 2012- present: Doctoral teaching board of Dipartimento di Ingegneria Industriale e dell'Informazione, University of Udine, Italy
- **Memberships**
 - IEEE senior member

Previous academic positions

Start date	End date	Town	Organization	Function
10/2022	09/2023	Palaiseau (France)	CNRS-C2N	Research director (Directeur de Recherche)
06/2016	09/2022	Palaiseau (France)	CNRS-C2N	Research scientist (Chargé de Recherche)
11/2005	05/2016	Grenoble (France)	IMEP-LAHC	Research scientist (Chargé de recherche)
11/2004	10/2005	Grenoble (France)	CEA-LETI	Post-doc
01/2004	10/2004	Pisa (Italy)	University of Pisa	Post-doc

Education

- July 2012: “Habilitation à Diriger des Recherches” (French HDR) delivered by University of Grenoble, France.
- Nov. 2000 – Dec. 2003: PhD studies at Dipartimento di Ingegneria dell'Informazione, University of Pisa, Italy. Title: Modeling of electronic and spintronic nanostructures. PhD defense date: April 2004.
- Oct. 2002 – Jul. 2003: Research internship at Institut für Theoretische Festkörperphysik, Universität Karlsruhe, Germany
- Jun. 2000: Master in physics at Dipartimento di Fisica, University of Pisa, Italy

Scientific productions

- **Research Interests**

- Electronic and transport properties of nanowires and ultimate CMOS transistors
- Modeling and simulation of steep slope devices
- Ab-initio simulation of electronic and thermal properties of new materials for nanoelectronics
- Quantum transport in mesoscopic devices
- Scanning-gate microscopy
- Spin-dependent transport in 1D and 2D structures
- Charge fluctuations in single-electron transistors

- **European projects**

- 2005-2007: Network of Excellence FP6-EU SINANO – Project partner.
- 2008-2010: FP6-EU PULLNANO (PULLing the limits of NANOCmos electronics) – Project partner.
- 2007-2011: Network of Excellence FP7-EU NANOSIL (Silicon based NANOstructures and nanodevices) – Project partner.
- 2010-2013: FP7-EU NANOFUNCTION (Beyond CMOS Nanodevices for Adding Functionalities to CMOS) – Project partner.
- 2009-2012: ENIAC MODERN (MOdeling and DEsign of Reliable, process variation aware Nanoelectronic devices, circuits and systems) – Project partner.
- 2010-2013: FP7-EU SQWIRE (Silicon Quantum WIRE transistors) – Project partner.
- 2013-2017: FP7-EU COMPOSE3 (Compound Semiconductors for 3D integration) – Project partner.
- 2015-2017: H2020-ECSEL WAYTOGO FAST (Which Architecture Yields Two Other Generations of Fully depleted Advanced Substrate and Technologies) – Project partner.
- 2019-2022: IPCEI Nano 2022 (Modeling of SPAD devices) – Project partner.
- 2024-2027: HORIZON-CL4-2023 AttoSwitch – Project partner.

• National Projects

- 2006-2009: Project Cluster Région Rhône-Alpes (Impact des fluctuations atomistiques sur les composants de la nanoélectronique) – Partner principal investigator.
- 2008-2010: ANR PNANO2007 QUANTAMONDE (QUANTum and Atomistic MOdeling of NanoDEvices) – Partner principal investigator.
- 2008-2011: ANR PNANO2007 MICATEC (MICROscopie avancée du Transport Electronique Cohérente) – Partner principal investigator.
- 2011-2014: ANR P2N2010 QUASANOVA (QUAntum Simulations and Assessment of NanODEvice Architectures) – Partner principal investigator.
- 2014-2018: ANR P2N2013 MOSINAS (MOSFET à hétérostructure et film ultra mince d'InAs sur substrat silicium) – Partner principal investigator.
- 2014-2018: ANR P2N2013 NOODLES (NanODEvice mODEling for Low powER applicationS) – Principal investigator.
- 2020-2024: ANR 2020 2D-ON-DEMAND (Van der Waals heterostructures of 2D materials with on-demand band-structure) – Partner principal investigator.
- 2020-2024: ANR 2020 GeSPAD (Germanium-based single photon avalanche diodes) – Principal investigator.
- 2021-2025: ANR 2021 Tunne2D (Scalable tunneling diodes based on 2D materials) – Partner Principal investigator.
- 2021-2025: ANR 2021 Placho (Platform for multiscale simulation of hot carriers: electrons and phonons for energy harvesting) – WP leader.
- 2021-2025: ANR 2021 MixDFerro (Mixed Dimensional heterostructures under 2D Ferroelectric control) – WP leader

Publications

Papers in peer-reviewed journals

1. P. Grigolini, M.G. Pala, L. Palatella, and R. Roncaglia, "Towards the thermo-dynamics of localization processes", *Physical Review E* vol. 62, p. 3429 (2000).
2. P. Grigolini, M.G. Pala, and L. Palatella, "Quantum measurement and entropy production", *Physics Letters A* vol. 285, p. 49 (2001).
3. M.G. Pala and G. Iannaccone, "A three-dimensional solver of the Schrödinger equation in momentum space for the detailed simulation of nanostructures", *Nanotechnology* vol. 13, p. 369 (2002).
4. M.G. Pala, G. Iannaccone et al., "Extraction of parameters of surface states from experimental test structures", *Nanotechnology* vol. 13, 373 (2002).
5. M. Bologna, P. Grigolini, M.G. Pala, and L. Palatella, "Decoherence, wave function collapses and non-ordinary statistical mechanics", *Chaos, Solitons & Fractals* vol. 17, p. 601 (2002).
6. M.G. Pala and G. Iannaccone, "Modeling decoherence effects on the transport properties of mesoscopic devices", *J. Comp. Electronics* vol. 2, p. 399 (2003).
7. M.G. Pala, M. Governale, J. König, and U. Zülicke, "Universal Rashba spin precession of two-dimensional electrons and holes", *Europhysics Letters* vol. 65, p. 850 (2004).
8. M.G. Pala, M. Governale, J. König, U. Zülicke, and G. Iannaccone, "Two-dimensional hole precession in an all-semiconductor spin field-effect-transistor", *Physical Review B* vol. 69, p. 045304 (2004).
9. M.G. Pala and G. Iannaccone, "Statistical model of dephasing in mesoscopic devices introduced in the scattering matrix formalism", *Physical Review B* vol. 69, p. 235304 (2004).
10. M.G. Pala and G. Iannaccone, "Effect of dephasing on the current statistics of mesoscopic devices", *Physical Review Letters* vol. 93, p. 25683 (2004).
11. G. Fiori, M.G. Pala, and G. Iannaccone, "Three-dimensional simulation of realistic Single Electron Transistors", *IEEE Transactions on Nanotechnology* vol. 4, p. 415 (2005).
12. M.G. Pala, M. Governale, U. Zülicke, and G. Iannaccone, "Rashba spin precession in quantum Hall edge channels", *Physical Review B* vol. 71, p. 115306 (2005).
13. M.G. Pala, G. Iannaccone, and G. Curatola, "Numerical simulation of ballistic magnetoconductance and magnetic focusing in strained Si-SiGe cavities", *Nanotechnology* vol. 16, p. S206 (2005).
14. M.G. Pala, C. LeRoyer, G. LeCarval, and L. Clavelier, "Modeling of non-equilibrium transport effects in Fully-Depleted GeOI-MOSFETs", *J. Comp. Electronics* vol. 5, p. 241 (2006).
15. Th. Schäpers, V. A. Guzenko, M.G. Pala, U. Zülicke, M. Governale, J. Knobbe, and H. Hardtdegen, "Suppression of weak antilocalization in GaInAs/InP narrow quantum wires", *Physical Review B* vol. 74, p. 081301(R) (2006).
16. M.G. Pala, M. Governale, and J. König, "Non-Equilibrium Josephson and Andreev Current through Interacting Quantum Dots", *New Journal of Physics* vol. 9, p. 278 (2007).
17. F. Martins, B. Hackens, M.G. Pala, et al., "Imaging electron wave functions inside open quantum rings", *Physical Review Letters* vol. 99, p. 136807 (2007).

18. C. Buran, M.G. Pala, M. Bescond, and M. Mouis, "Full-three-dimensional quantum approach to evaluate the surface-roughness-limited magnetoresistance mobility in SNWT", *J. Comp. Electronics* vol. 7, p. 328-331 (2008).
19. M.G. Pala, B. Hackens, F. Martins, H. Sellier, V. Bayot, S. Huant, and T. Ouisse, "Local density of states in mesoscopic samples from scanning gate microscopy", *Physical Review B* vol. 77, p. 125310 (2008).
20. M. Governale, M.G. Pala, and J. König, "Real-time diagrammatic approach to transport through interacting quantum dots with normal and superconducting leads", *Physical Review B* vol. 77, p. 134513 (2008).
21. S. Poli, M.G. Pala, T. Poiroux, S. Deleonibus, and G. Baccarani, "Size Dependence of Surface-Roughness-Limited Mobility in Silicon-Nanowire FETs", *IEEE-Transactions on Electron Devices* vol. 55, p. 2968 (2008).
22. D. Futterer, M. Governale, M.G. Pala, and J. König, "Nonlocal Andreev transport through an interacting quantum dot", *Physical Review B* vol. 79, p. 054505 (2009).
23. S. Poli S, M.G. Pala and T. Poiroux, "Full Quantum Treatment of Remote Coulomb Scattering in Silicon Nanowire FETs", *IEEE-Transactions on Electron Devices* vol. 56, p. 1191 (2009).
24. M. Bescond, M. Lannoo, F. Michelini, L. Raymond, M.G. Pala, "3D real-space quantum transport simulation of nanowire MOS transistors: Influence of the ionized doping impurity", *Microelectronics Journal*, vol. 40, p. 756 (2009).
25. M.G. Pala, S. Baltazar, F. Martins et al., "Scanning gate microscopy of quantum rings: effects of an external magnetic field and of charged defects", *Nanotechnology* vol. 20, p. 264021 (2009).
26. K. Rogdakis, S. Poli, E. Bano, K. Zekentes, and M.G. Pala, "Phonon- and surface-roughness-limited mobility of gate-all-around 3C-SiC and Si nanowire FETs", *Nanotechnology* vol. 20, 295202 (2009).
27. C. Buran, M.G. Pala, M. Bescond, et al., "Three-Dimensional Real-Space Simulation of Surface Roughness in Silicon Nanowire FETs", *IEEE-Transactions on Electron Devices* vol. 56, p. 2186-2192 (2009).
28. E. Buccafurri, R. Clerc, F. Calmon, M. Pala, A. Poncet, G. Ghibaudo, "Performances comparison of Si and GaAs based resonant tunneling diodes", *Physica status solidi (c)*, vol. 6, p. 1408-1411 (2009).
29. M.G. Pala, C. Buran, S. Poli, and M. Mouis, "Full quantum treatment of surface roughness effects in Silicon nanowire and double gate FETs", *J. Comp. Electronics* vol. 8, p. 374 (2009).
30. S. Poli and M.G. Pala, "Channel-Length Dependence of Low-Field Mobility in Silicon-Nanowire FETs", *IEEE Electron Device Letters* vol. 30, p. 1212 (2009).
31. B. Hackens, F. Martins, S. Faniel, C. A. Dutu, H. Sellier, S. Huant, M. Pala, L. Desplanque, X. Wallart, V. Bayot, "Imaging Coulomb Islands in a Quantum Hall Interferometer", *Nature Communications* vol. 1, p. 39 (2010).
32. D. J. Eldridge, M.G. Pala, M. Governale, J. König, "Superconducting proximity effect in interacting double-dot systems", *Physical Review B* vol. 82, p. 184507 (2010).
33. S. Estevez Hernandez, M. Akabori, K. Sladek, Ch. Volk, S. Alagha, H. Hardtdegen M.G. Pala, N. Demarina, D. Grützmacher, Th. Schäpers, "Spin-orbit coupling and phase-coherence in InAs nanowires", *Physical Review B* vol. 82, p. 235303 (2010).
34. A. Braggio, M.G. Pala, M. Governale, J. König, "Superconducting proximity effect in interacting quantum dots revealed by shot noise", *Solid-State Communications* vol. 151, p. 155 (2011).
35. F. Martins, B. Hackens, H. Sellier, P. Liu, M.G. Pala, S. Baltazar, L. Desplanque, X. Wallart, V. Bayot, S. Huant, "Scanning-gate microscopy of semiconductor nanostructures: an overview", *Acta Physica Polonica A* vol. 119, p. 569-575 (2011).
36. A. Cresti, M.G. Pala, S. Poli, M. Mouis and G. Ghibaudo, "A comparative study of surface-roughness induced variability in Si nanowire and double-gate FETs", *IEEE-Transactions on Electron Devices* vol. 58, p. 2274-2281 (2011).
37. H. Sellier, B. Hackens, M.G. Pala et al., "On the imaging of electron transport in semiconductor quantum structures by scanning-gate microscopy: successes and limitations", *Semicond. Science and technology* vol. 26, p. 064008 (2011).
38. M.G. Pala, S. Baltazar, P. Liu, H. Sellier, B. Hackens, F. Martins, V. Bayot, X. Wallart, L. Desplanque, S. Huant, "Transport inefficiency in branched-out mesoscopic networks: An analog of the Braess paradox", *Physical Review Letters* vol. 108, p. 076802 (2012).
39. A. Bekaddour, M.G. Pala, N. Chabane-Sari and G. Ghibaudo, "Deterministic method to evaluate the threshold voltage variability induced by discrete trap charges in Si nanowire FETs", *IEEE-Transactions on Electron Devices* vol. 59, p. 1462-1467 (2012).
40. F. Conzatti, M.G. Pala, D. Esseni, "Surface Roughness Induced Variability in Nanowire InAs Tunnel-FETs", *IEEE-Electron Device Letters* vol. 33, p. 806-808 (2012).
41. F. Conzatti, M.G. Pala, D. Esseni, E. Bano, L. Selmi, "Strain Induced Performance Improvements in InAs Nanowire Tunnel-FETs", *IEEE-Transactions on Electron Devices* vol. 59, p. 2085-2092 (2012).
42. M. Pala, H. Sellier, B. Hackens, F. Martins, V. Bayot, S. Huant, "A new transport phenomenon in nanostructures: A mesoscopic analog of the Braess paradox encountered in road networks", *Nanoscale Res. Lett.* vol. 7, p. 472 (2012).
43. F. Martins, S. Faniel, B. Rosenow, H. Sellier, S. Huant, M.G. Pala, L. Desplanque, X. Wallart, V. Bayot, and B. Hackens, "Coherence and Coulomb blockade in ultrasmall quantum Hall islands", *New Journal of Physics* vol. 15, p. 013049 (2013).
44. F. Martins, S. Faniel, B. Rosenow, H. Sellier, S. Huant, M.G. Pala, et al., "Coherent tunnelling across a quantum point contact in the quantum Hall regime", *Scientific Reports* vol. 3, pp. 1-5 (2013).
45. F. Conzatti, M.G. Pala, D. Esseni and E. Bano, "Investigation of localized versus uniform strain as a performance booster in InAs Tunnel-FETs", *Solid-State Electronics* Vol. 88, pp. 49-53 (2013).
46. M.G. Pala and D. Esseni, "Interface Traps in InAs Nanowire Tunnel-FETs and MOSFETs—Part I : Model Description and Single Trap Analysis in Tunnel-FETs", *IEEE Trans. Electron Devices*, vol. 60, pp. 2795 - 2801 (2013).
47. D. Esseni and M.G. Pala, "Interface Traps in InAs Nanowire Tunnel FETs and MOSFETs—Part II : Comparative Analysis and Trap-Induced Variability", *IEEE Trans. Electron Devices*, vol. 60, pp. 2802 - 2807 (2013).

48. S. Brocard, M.G. Pala and D. Esseni, "Large On-Current Enhancement in Hetero-Junction Tunnel-FETs via Molar Fraction Grading", *IEEE-Electron Device Letters*, vol. 35, pp. 184-186 (2014).
49. M.G. Pala and S. Brocard, "Exploiting hetero-junctions to improve the performance of III-V nanowire Tunnel-FETs", *IEEE-Journal of Electron Device Society*, vol. 3, pp. 115-121 (2015).
50. P. Liu, F. Martins, B. Hackens, L. Desplanque, X. Wallart, M.G. Pala, S. Huant, V. Bayot and H. Sellier, "Formation of quantum dots in the potential fluctuations of InGaAs nanowires controlled by scanning gate microscopy", *Physical Review B*, vol. 91, p. 075313 (2015).
51. M.G. Pala and A. Cresti, "Increase of self-heating effects in nanodevices induced by surface roughness: a full-quantum study", *Journal of Applied Physics*, vol. 117, p. 084313 (2015).
52. D. Esseni, M.G. Pala and T. Rollo, "Essential Physics of the OFF-State Current in Nanoscale MOSFETs and Tunnel FETs" *IEEE Trans. Electron Devices*, vol. 62, pp. 3084-3091 (2015).
53. J. Cao, M.G. Pala, A. Cresti and D. Esseni, "Quantum simulation of a heterojunction vertical tunnel FET based on 2D transition metal dichalcogenides", *Solid-state Electronics*, vol. 116, pp. 1-7 (2016).
54. J. Cao, D. Logoteta, S. Özkaya, B. Biel, A. Cresti, M. Pala, D. Esseni, "Operation and Design of van der Waals Tunnel Transistors: A 3-D Quantum Transport Study", *IEEE Trans. Electron Devices*, vol. 63, pp. 4388-4394 (2016).
55. M.G. Pala, C. Grillet, J. Cao, D. Logoteta, A. Cresti, D. Esseni, "Impact of inelastic phonon scattering in the OFF state of Tunnel-field-effect transistors", *J. Comp. Elec.*, vol. 15, pp. 1240-1247 (2016).
56. C. Grillet, D. Logoteta, A. Cresti and M. G. Pala, "Assessment of the electrical performance of short channel InAs and strained Si nanowire FETs", *IEEE Trans. Electron Devices*, vol. 64, pp. 2425-2431 (2017).
57. D. Esseni, M. Pala, et al., "A Review of Selected Topics in Physics Based Modelling of Small Slope Transistors based on Band-to-Band-Tunnelling", *Semiconductor Science and Technology*, vol. 32 (8), p. 083005 (2017).
58. J. Cao, D. Logoteta, M.G. Pala, A. Cresti, "Impact of momentum mismatch on 2D van der Waals tunnel field-effect transistors", *Journal of Physics D: Applied Physics* vol. 51 (5), p. 055102 (2017).
59. D. Logoteta, N. Cavassilas, A. Cresti, M.G. Pala, M. Bescond, "Impact of the gate and insulator geometrical model on the static performance and variability of ultra-scaled silicon nanowire FETs", *IEEE Trans. Electron Devices* vol. 65 (2), pp. 424-430 (2018).
60. S. Toussaint, F. Martins, S. Faniel, M. Pala, L. Desplanque, X. Wallart, et al., "On the origins of transport inefficiencies in mesoscopic networks", *Scientific reports* vol. 8 (1), p. 3017 (2018).
61. M.G. Pala and D. Esseni, "Full-band quantum simulation of electron devices with the pseudopotential method: Theory, implementation, and applications", *Physical Review B* vol. 97 (12), p. 125310 (2018).
62. C. Grillet, A. Cresti, M.G. Pala, "Vertical GaSb/AlSb/InAs Heterojunction Tunnel-FETs: A Full Quantum Study", *IEEE-Transactions on Electron Devices* vol. 65 (7), pp. 3038-3044 (2018).
63. J. Cao, J. Park, F. Triozon, M. Pala, A. Cresti, "Simulation of 2D material-based tunnel field-effect transistors : planar vs. vertical architectures", *ISTE Open Science* vol. 1 (2018). DOI: 10.21494/ISTE.OP.2018.0222.
64. J. Choukroun, M. Pala, S. Fang, E. Kaxiras, P. Dollfus, "High performance tunnel field effect transistors based on in-plane transition metal dichalcogenide heterojunctions", *Nanotechnology* vol. 30 (2), p. 025201 (2019).
65. D. Logoteta, M.G. Pala, J. Choukroun, P. Dollfus, G. Iannaccone, "A Steep-Slope MoS₂-Nanoribbon MOSFET Based on an Intrinsic Cold-Contact Effect", *IEEE Electron Device Letters* vol. 40 (9), pp. 1550-1553 (2019).
66. M. G. Pala, D. Esseni, "Quantum transport models based on NEGF and empirical pseudopotentials for accurate modeling of nanoscale electron devices", *Journal of Applied Physics* vol. 126 (5), p. 055703 (2019).
67. M.G. Pala, P. Giannozzi, D. Esseni, "Unit cell restricted Bloch functions basis for first-principle transport models: Theory and application", *Physical Review B* vol. 102 (4), p. 045410 (2020).
68. A. M'foukh, M.G. Pala, D. Esseni, "Full-Band Quantum Transport of Heterojunction Electron Devices with Empirical Pseudopotentials", *IEEE Transactions on Electron Devices* vol. 67, pp. 5662 – 5668 (2020).
69. D. Logoteta, J. Cao, M. Pala, P. Dollfus, Y. Lee, G. Iannaccone, "Cold-source paradigm for steep-slope transistors based on van der Waals heterojunctions", *Physical Review Research* vol. 2 (4), p. 043286 (2021)
70. C. Ernandes, et al., "Indirect to direct band gap crossover in two-dimensional WS₂(1-x)Se_{2x} alloys", *npj 2D Materials and Applications* vol. 5, n. 7 (2021).
71. J. Cao, Y. Wu, H. Zhang, D. Logoteta, S. Zhang, M. Pala, "Dissipative transport and phonon scattering suppression via valley engineering in single-layer antimonene and arsenene field-effect transistors" *npj 2D Materials and Applications* vol. 5, n. 59 (2021).
72. L. Khalil, et al., "Electronic band gap of van der Waals α -As₂Te₃ crystals", *Applied Physics Letters* vol. 119 (4), p. 043103 (2021).
73. C. Ernandes, et al., "Strain and Spin-Orbit Coupling Engineering in Twisted WS₂/Graphene Heterobilayer", *Nanomaterials* vol. 11 (11), p. 2921 (2021).
74. T. Cazimajou, M. Pala, J. Saint-Martin, R. Helleboid, J. Grebot, D. Rideau, P. Dollfus, "Quenching Statistics of Silicon Single Photon Avalanche Diodes", *IEEE Journal of the Electron Devices Society* vol. 9, pp. 1098-1102 (2021).
75. D. Pierucci, et al., "Evidence for highly p-type doping and type II band alignment in large scale monolayer WSe₂/Se-terminated GaAs heterojunction grown by molecular beam epitaxy", *Nanoscale* vol. 14 (15), pp. 5859-5868 (2021).
76. Y. Shao, M. Pala, D. Esseni, J. del Alamo, "Scaling of GaSb/InAs Vertical Nanowire Esaki Diodes Down to Sub-10-nm Diameter", *IEEE Transactions on Electron Devices* vol. 69 (4), pp. 2188-2195 (2022).
77. A. M'foukh, J. Saint-Martin, P. Dollfus, M. Pala, "Phonon-assisted transport in van der Waals heterostructure tunnel devices", *Solid-State Electronics* vol. 194, p. 108344 (2022).

78. P. Dollfus, J. Saint-Martin, T. Cazimajou, R. Helleboid, A. Pilotto, D. Rideau, M. Pala, "Avalanche breakdown and quenching in Ge SPAD using 3D Monte Carlo simulation", *Solid-State Electronics* vol. 194, p. 108361 (2022).
79. D. Lizzit, P. Khakbaz, F. Driussi, M. Pala, D. Esseni, "A study of metal-MoS₂ contacts by using an in-house developed ab-initio transport simulator", *Solid-State Electronics* vol. 194, p. 108365 (2022).
80. R. Helleboid, D. Rideau, J. Grebot, I. Nicholson, N. Moussy, O. Saxod, J. Saint-Martin, M. Pala, P. Dollfus, "Modeling of SPAD avalanche breakdown probability and jitter tail with field lines", *Solid-State Electronics* vol. 194, p. 108376 (2022).
81. R. Helleboid et al., "Comprehensive Modeling and Characterization of Photon Detection Efficiency and Jitter Tail in Advanced SPAD Devices", *IEEE Journal of the Electron Devices Society* vol. 10, pp. 584 - 592 (2022).
82. L. Khalil et al., " α -As₂Te₃ as a platform for the exploration of the electronic band structure of single layer β -tellurene", *Physical Review B* vol. 106 (12), p. 125152 (2022).
83. A. Pilotto, P. Dollfus, J. Saint-Martin, M. Pala, "Full Quantum Simulation of Shockley-Read-Hall Recombination in p-i-n and Tunnel Diodes", *Solid-State Electronics* vol. 198, p. 108469 (2022).
84. R. Helleboid, et al., "A Fokker–Planck-based Monte Carlo method for electronic transport and avalanche simulation in single-photon avalanche diodes", *J. Phys. D: Appl. Phys.* Vol. 55, p. 505102 (2022).
85. L. Khalil et al., "Hybridization and localized flat band in the WSe₂/MoSe₂ heterobilayer", *Nanotechnology* vol. 34 p. 045702 (2022).
86. J. Zribi et al., "Unidirectional Rashba spin splitting in single layer WS₂ (1-x) Se_{2x} alloy", *Nanotechnology* vol. 34 (7), p. 075705 (2022).
87. V.-T. Tran, T.-T. Vu, P. Dollfus, J. Saint-Martin, M. Pala, "Thermal conductance of twisted-layer graphite nanofibers", *Carbon* vol. 204, pp. 601-611 (2023).
88. D. Lizzit, P. Khakbaz, F. Driussi, M. Pala, D. Esseni, "Ohmic Behavior in Metal Contacts to n/p-Type Transition-Metal Dichalcogenides: Schottky versus Tunneling Barrier Trade-off", *ACS Appl. Nano Mater.* Vol. 6, pp. 5737-5746 (2023).
89. A. Mahmoudi, et al., "Electronic properties of rhombohedrally stacked bilayer obtained by chemical vapor deposition", *Physical Review B* vol. 108 (4), p. 045417 (2023).
90. G. Kremer et al., "Direct observation of highly anisotropic electronic and optical nature in indium telluride", *Physical Review Materials* vol. 7 (7), p. 074601 (2023).
91. G. Kremer et al., "Quantum Confinement and Electronic Structure at the Surface of van der Waals Ferroelectric α -In₂Se₃", *ACS nano* vol. 17 (19), pp. 18924–18931 (2023).
92. M. Bouaziz et al., "Intrinsic defects and mid-gap states in quasi-one-dimensional indium telluride", *Physical Review Research* vol. 5 (3), p. 033152 (2023).
93. A. M'foukh, J. Saint-Martin, P. Dollfus, M. Pala, "Ab-initio simulation of dissipative transport in tunnel devices based on heterostructures of 2D materials", *Journal of Computational Electronics* vol. 22 (5), pp. 1257-1263 (2023).
94. A. Mahmoudi, et al., "Quasi van der Waals Epitaxy of Rhombohedral-Stacked Bilayer WSe₂ on GaP(111) Heterostructure", *ACS nano* vol. 17, pp. 21307-21316 (2023).
95. D. Lizzit, M. Pala, F. Driussi, D. Esseni, "Reinterpreting Low Resistance in Sb–MoS Ohmic Contacts by Means of Ab Initio Transport Simulations", *IEEE Transactions on Electron Devices* Vol. 71, pp. 3301-3306 (2024).
96. A. Chiout, et al., "High Strain Engineering of a Suspended WSSe Monolayer Membrane by Indentation and Measured by Tip-Enhanced Photoluminescence", *Advanced Optical Materials* vol. 12 (14), p. 2302369 (2024).
97. M. Bouaziz, et al., "Anisotropic flat band and charge density wave in quasi-one-dimensional indium telluride", *Physical Review B* Vol. 110 (4), p. 045441 (2024).
98. A. Mahmoudi, et al., "Distinguishing different stackings in WSe₂ bilayers grown using chemical vapor deposition", *Physical Review B* Vol. 110 (16), p. 165418 (2024).
99. Y. Shao, M. Pala, H. Tang, B. Wang, J. Li, D. Esseni, J.A. del Alamo, "Scaled vertical-nanowire heterojunction tunnelling transistors with extreme quantum confinement", *Nature Electronics*, (2024) DOI: <https://doi.org/10.1038/s41928-024-01279-w>

Proceedings in peer-reviewed international conferences

1. G. Iannaccone, M. Macucci, P. Coli, G. Curatola, G. Fiori, M. Gattobigio, M. Pala, "Towards nanotechnology computer aided design: the NANOTCAD project, 1-st IEEE Conference on Nanotechnology", p. 117 (2001).
2. P. Allegrini, G. Aquino, M. Bologna, P. Grigolini, M. Ignaccolo, M.G. Pala, L. Palatella, A. Rosa, and B.J. West, "Decoherence, Wave-Function Collapses, Non-Ordinary Statistical Mechanics and the Second Principle", *AIP Conf. Proc.* 643, p. 72 (2002).
3. G. Iannaccone, M. Burghard, P. Coli, G. Curatola, P. Delaney, G. Fiori, A. Forchel, J. Greer, F. Heinz, H. Kosina, M. Macucci, M. Nedjalkov, M.G. Pala, S. Reitzenstein, A. Schenk, A. Schliemann, R. Sordan, L. Worschech, "NANOT-CAD Project: Nanotechnology Computer Aided Design", *Phantoms Newsletter* 14, p. 4 (2003).
4. M.G. Pala, G. Iannaccone, M. Macucci, and G. Marola, "Modelling the effects of dephasing on mesoscopic noise", *Proc. of SPIE Int. Soc. Opt. Eng.* 5472, p. 51 (2004).
5. G. Fiori, M.G. Pala, G. Iannaccone, "Three-dimensional simulation of single electron transistors", 4-th IEEE Conference on Nanotechnology, p. 337 (2004).
6. G. Scappucci, M.G. Pala et al., "Ballistic transport in strained-Si cavities: experiment and theory", 4-th IEEE Conference on Nanotechnology, p. 92 (2004).

7. L. Clavelier, M.G. Pala et al., "Fully Depleted Germanium p-MOSFETs with High-K and Metal Gate Fabricated on 200mm GeOI Substrates", Silicon Nanoelectronics Workshop (SNW) 2005, p. 18 (2005).
8. L. Bonci, M. Macucci, G. Iannaccone, M.G. Pala, "Numerical study of weak localization effects in disordered cavities", Nonequilibrium Carrier Dynamics in Semiconductors Proceedings 110, p. 55 (2006).
9. S. Poli, M.G. Pala, T. Poiroux et al., "Size dependence of surface roughness limited mobility in silicon nanowire FETs", IEEE- Silicon Nanoelectronics Workshop (SNW) 2008, p. 141 (2008).
10. S. Poli and M.G. Pala, "Full-quantum investigation of low-field mobility in short channel silicon nanowire FETs", SISPAD 2009, p. 285 (2009).
11. C. Buran, M.G. Pala, M. Mouis, S. Poli, Full-3D real-space treatment of surface roughness in double gate MOSFETs, ULIS 2009, p. 47 (2009).
12. E. Buccafurri, R. Clerc, F. Calmon, M. Pala, A. Poncet, G. Ghibaudo, "Intrinsic cut off frequency of Si and GaAs based Resonant Tunneling Diodes", 10th ULIS, p. 91 (2009).
13. E. Buccafurri, R. Clerc, F. Calmon, M. Pala, A. Poncet, G. Ghibaudo, "Challenges and prospects of RF oscillators using silicon resonant tunneling diodes", ESSDERC 2009, p. 220 (2009).
14. M. Bescond, M. Lannoo, L. Raymond, F. Michelini, M.G. Pala, Influence of Ionized Impurities in Silicon Nanowire MOS Transistors, 13th IWCE, p. 137 (2009).
15. C. Buran, M.G. Pala, M. Mouis, S. Poli, "Full-3D real-space simulation of surface-roughness effects in double-gate MOSFETs", 13th IWCE, p. 309 (2009).
16. K. Rogdakis, E. Bano, M.G. Pala, S. Poli, K. Zekentes, "Backscattering coefficient in gate-all-around 3C-SiC nanowire FETs", 9-th IEEE Conference on Nanotechnology, p. 504 (2009).
17. F. Conzatti, M.G. Pala, D. Esseni, E. Bano and L. Selmi, "A Simulation Study of Strain Induced Performance Enhancements in InAs Nanowire Tunnel-FETs", IEDM 2011, p. 5.2.1 (2011).
18. F. Conzatti, M.G. Pala, D. Esseni, and E. Bano, "Investigation of localized versus uniform strain as a performance booster in InAs Tunnel-FETs", ULIS 2012, p. 183-186 (2012).
19. J. H. Choi, M. Pala, L. Latu-Romain, E. Bano, "Theoretical study of thermoelectric properties of SiC nanowires", Materials Science Forum, vol. 717-720, p. 561 (2012).
20. M.G. Pala, D. Esseni and F. Conzatti, "Impact of interface traps on the IV curves of InAs Tunnel-FETs and MOSFETs: a full quantum study", IEDM 2012, p. 6.6.1 (2012).
21. F. Martins, S. Faniel, M.G. Pala, et al., "Locating an individual quantum hall island inside a quantum ring", Proceedings of ICPS 2012, Vol. 1566 p. 299-300 (2013).
22. S. Brocard, M.G. Pala and D. Esseni, "Design Options for Hetero-Junction Tunnel FETs with High on Current and Steep Sub-VT Slope", IEDM 2013, p. 5.4.1 (2013).
23. M.G. Pala and D. Esseni, "Modeling the Influence of Interface Traps on the Transfer Characteristics of InAs Tunnel-FETs and Mosfets", ECS Transactions, vol. 61, pp. 237-251 (2014).
24. D. Esseni, M.G. Pala, A. Revelant, P. Palestri, L. Selmi, M.O. Li, G. Snider, D. Jena, H.G. Xing, "Challenges and Opportunities in the Design of Tunnel FETs: Materials, Device Architectures, and Defects", ECS Transactions, vol. 64, pp. 581-595 (2014).
25. M.G. Pala, A Cresti, "Quantum simulation of self-heating effects in rough Si nanowire FETs", Computational Electronics (IWCE), 2014 International Workshop on, p. 1-3 (2014)
26. B. De Salvo, P. Morin, M.G. Pala, et al., "A Mobility-enhancement strategy for sub-14nm power-efficient FDSOI technologies", IEDM 2014, p. 7.2.1 (2014).
27. J. Cao, M. Pala, A. Cresti and D. Esseni, "Quantum simulation of a heterojunction inter-layer Tunnel FET based on 2-D gapped crystals", Ultimate Integration on Silicon (EUROSUI-ULIS), pp. 245-248 (2015).
28. F.G. Pereira, M. Pala et al., "Modeling study of the mobility in FDSOI devices with a focus on near-spacer-region", Ultimate Integration on Silicon (EUROSUI-ULIS), pp. 49-52 (2015).
29. L. Lucci, J.-C. Barbe, M. Pala, "Full-quantum study of AlGaIn/GaN HEMTs with InAlN back-barrier", Simulation of Semiconductor Processes and Devices (SISPAD), pp. 128-131 (2015).
30. L. Lucci, J.-C. Barbe, M. Pala, "Electric performance of AlGaIn/GaN heterojunction devices: A full-quantum study", ESSDERC 2015, pp. 318-321 (2015).
31. D. Esseni, M. Pala, E. Gnani, E. Sangiorgi, "Influence of interface traps on the performance of Tunnel FETs", Energy Efficient Electronic Systems (E3S), (2015).
32. J. Cao, D. Logoteta, S. Ozkaya, B. Biel, A. Cresti, M. Pala, and D. Esseni, "A Computational Study of van der Waals Tunnel Transistors: Fundamental Aspects and Design Challenges", IEDM 2015, pp. 12.5.1-12.5.4 (2015).
33. C. Grillet and M. Pala, "V_{DD} scaling of ultra-thin InAs MOSFETs: A full-quantum study", Ultimate Integration on Silicon (EUROSUI-ULIS) (2016).
34. G. Mugny, F.G. Pereira, D. Rideau, F. Triozon, Y.M. Niquet, M. Pala et al, "A study of diffusive transport in 14nm FDSOI MOSFET : NEGF versus QDD", ESSDERC 2016, pp. 424-427 (2016).
35. T. Cosnier, L. Lucci, A. Torres, M. Pala, "Local stress engineering for the optimization of p-GaN gate HEMTs power devices", Simulation of Semiconductor Processes and Devices (SISPAD), pp. 121-124 (2017).
36. M.G. Pala, O. Badami, D. Esseni, "NEGF based transport modelling with a full-band, pseudopotential Hamiltonian: Theory, implementation and full device simulations", IEEE International Electron Devices Meeting (IEDM), pp. 35.1. 1-35.1. 4 (2017)

37. D. Esseni, O. Badami, F. Driussi, D. Lizzit, M. Pala, et al., "New device concepts, transistor architectures and materials for high performance and energy efficient CMOS circuits in the forthcoming era of 3D integrated circuits", IEEE Electron Devices Technology and Manufacturing Conference (EDTM) pp. 236-238 (2018).
38. J. Choukroun, M. Pala, S. Fang, E. Kaxiras, P. Dollfus, "High performance WTe₂-MoS₂-in-plane heterojunction Tunnel Field Effect Transistors", ESSDERC 2018, pp. 42-45 (2018).
39. D. Rideau, G. Mugny, M. Pala, D. Esseni, "Inter-band coupling in Empirical Pseudopotential Method based bandstructure calculations of group IV and III-V nanostructures", Simulation of Semiconductor Processes and Devices (SISPAD), pp. 224-227 (2018).
40. M.G. Pala, O. Badami, D. Esseni, "Transport models based on NEGF and empirical pseudopotentials: a computationally viable method for self-consistent simulation of nanoscale devices", IEEE International Electron Devices Meeting (IEDM), pp. 33.1. 1-33.1. 4 (2018).
41. M. Pala, D. Esseni, "Full band quantum transport modelling with EP and NEGF methods; application to nanowire transistors", 2019 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), pp. 1-4 (2019). doi: 10.1109/SISPAD.2019.8870406.
42. N. D. Le, B. Davier, P. Dollfus, M. Pala, A. Bournel and J. Saint-Martin, "Full Band Monte Carlo simulation of phonon transfer at interfaces," 2020 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), pp. 27-30 (2020). doi: 10.23919/SISPAD49475.2020.9241629.
43. Y. Oussaiti et al., "Verilog-A model for avalanche dynamics and quenching in Single-Photon Avalanche Diodes," 2020 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), pp. 145-148, (2020). doi: 10.23919/SISPAD49475.2020.9241648.
44. M. Pala and D. Esseni, "Ab-initio quantum transport with a basis of unit-cell restricted Bloch functions and the NEGF formalism," 2020 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), pp. 3-6 (2020). doi: 10.23919/SISPAD49475.2020.9241641.
45. T. Cazimajou, M. Pala, J. Saint-Martin, D. Rideau, P. Dollfus, "Monte Carlo study of Single Photon Avalanche Diodes: quenching statistics", 21st International Workshop on Computational Nanotechnology (IWCN) 2021, p. 77 (2021).
46. A. M'foukh, M. Pala, "Ab initio quantum transport simulation of lateral heterostructures based on 2D materials: assessment of the coupling Hamiltonians", 21st International Workshop on Computational Nanotechnology (IWCN) 2021, p. 99 (2021).
47. D. Rideau et al., "Single Photon Avalanche Diode with Monte Carlo Simulations: PDP, Jitter and Quench Probability", 2021 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), (2021).
48. Y. Shao, M. Pala, D. Esseni, J. Del Alamo, "Sub-10-nm Diameter GaSb/InAs Vertical Nanowire Esaki Diodes with Ideal Scaling Behavior: Experiments and Simulations", IEEE International Electron Devices Meeting (IEDM) 2021, pp. 32.1.1-32.1.4 (2021).
49. D. Lizzit, P. Khakbaz, F. Driussi, M. Pala, D. Esseni, "Transport simulations unveil the Schottky versus Tunneling barrier trade-off in metalTMD contacts", IEEE International Electron Devices Meeting (IEDM) 2022, pp. 28.2.1-28.2.4 (2022).
50. J. Park, M. Pala, J. Saint-Martin, "Full Band Monte Carlo Simulation of Thermal Transport Across Lateral Interface Between 2D Materials", 2023 Int. Conference on Simulation of Semiconductor Processes and Devices (SISPAD), (2023).
51. A. Pilotto, A. M'foukh, P. Dollfus, J. Saint-Martin, M. Pala, "Full-Band Quantum Simulations of Semiconductor Devices based on Empirical Pseudopotential Hamiltonians in the presence of Phonon Scattering and Non-Radiative Recombination", 2023 Int. Conference on Simulation of Semiconductor Processes and Devices (SISPAD), (2023).
52. R. Helleboid, J. Saint-Martin, M. Pala, et al., "Full-Band Monte Carlo Study of Hot Carriers for Advection-Diffusion Monte Carlo Simulations", 2023 Int. Conference on Simulation of Semiconductor Processes and Devices (SISPAD), (2023).

Invited talks at international conferences

1. M.G. Pala, G. Iannaccone, M. Macucci, and G. Marola, "Modeling the effects of dephasing on mesoscopic noise", SPIE International Symposium, Fluctuations and Noise, Maspalomas, Spain, 2004
2. M.G. Pala, "3D quantum transport simulations of Si Nanowires: impact of elastic and inelastic scattering", Nanosil Workshop 2009, Athens, Greece, 2009.
3. M.G. Pala, "Elastic and inelastic scattering in SiNWs, French-Ukrainian symposium and SemOI conference", Kiev, Ukraine, 2010.
4. M.G. Pala, "Quantum-mechanical modeling of advanced semiconductor devices", 4-th SINANO summer school, Bertinoro, Italy, 2010.
5. M.G. Pala, "Advanced transport simulations of nanodevices", 14-th MIGAS summer school, Autrans, France, 2011.
6. M.G. Pala, "Electron transport and phonons in disordered nanowires", Workshop on Phonons and Fluctuations, Paris, France, 2011.
7. M.G. Pala, "Challenges and opportunities in InAs Tunnel FETs: a simulation study", Sinano Workshop 2013, Bucharest, Romania, 2013.
8. M.G. Pala and D. Esseni, "Modeling the influence of interface traps on the transfer characteristics of InAs Tunnel-FETs and MOSFETs", 6th International Symposium on Dielectrics for Nanosystems in the 225th ECS meeting, Orlando USA, May 2014.

9. M. Pala et al., "Quantum simulation of mobility and current enhancement in sub-14nm strained SiGe FD-pMOSFETs", GRDi CNRS Mecano : Mechanical Issues for Advanced Electron Devices Workshop, Grenoble, France, June 2015.
10. M.G. Pala, "III-V Heterostructures and Transition Metal Dichalcogenides for Tunnel-FETs", Sinano Workshop 2015, Graz, Austria, 2015.
11. (Plenary) M. Pala, "Ab-initio quantum transport with a basis of unit-cell restricted Bloch functions and the NEGF formalism", SISPAD 2020, Kobe, Japon, 2020.
12. M. Pala, "Ab-initio quantum transport simulation of 2D-materials-based electron devices", Kick-off meeting of GDR Low-dimensionnal van der Waals Hetero-structures "Howdi", Paris, France, March 2021.
13. M. Pala, "Electron transport properties of van der Waals hetero-structures with ab-initio methods", Nano-TN 2022, Marrakech, Morocco, May 2022
14. M. Pala, "Frontiers in the atomistic simulation of nanoscale electron devices", EUROSOI-ULIS Conference 2022, Udine, Italy, May 2022.
15. M. Pala, "Quantum transport with plane-wave ab-initio Hamiltonians", CECAM Workshop on "Quantum Transport: From Nanoscopic to Microscopic Modelling", Zurich, Switzerland, July 2022.
16. M. Pala, "Quantum transport study of the electric resistance at the metal/TMD interface: Schottky vs tunneling barrier trade-off", Energy transfer at interfaces Workshop of GDR "NAME", Paris, France, July 2023.

Valorization

Development of several scientific codes for the numerical simulation of electronic transport in nanodevices capable of running in parallel on a cluster of CPUs, as well as on GPU architectures.