Curriculum Vitae

Personal Information and Contacts

NAME: **Alessio Gagliardi;**

DATE OF BIRTH: October 31, 1978;

NATIONALITY: Italian;

EMAIL: gagliardi@ing.uniroma2.it

Education and Training

◦ Doctor of Philosophy, Science 2004-2007
(With Honours, “mit Auszeichnung bestanden”)
Conferred on : 29 June , 2007;
Department of Physics The University of Paderborn (Germany).

◦ Master of Science (Honours), 28 October 2003
Department of Telecommunication Engineer
Università degli studi di Roma Tor Vergata, Rome (Italy).

◦ Bachelor of Science, (Honours), 1997-2001
Department of Telcommunication Engineer
Università degli studi di Roma Tor Vergata, Rome (Italy).

Professional Experiences

Tenure Track Assistant Professor 2014 - current
Department of Electrical Engineering and Information Technology
Technische Universität München (Germany).

Postdoctoral Fellow 2008 - 2013
Department of Electronic Engineer
Università degli studi di Roma Tor Vergata, Rome (Italy).

Postdoctoral Fellow 2007 - 2008
Bremen Center for Computational Material Science (BCCMS)
University of Bremen, Bremen (Germany).

PhD Student 2004 - 2007
Department of Physics
University of Paderborn, Paderborn (Germany).

Responsibilities:

- designing and conducting research projects (theory);
- preparing papers for publication and reports for grants and invention disclosure;

- supervising undergraduate students and assisting graduate students;
- Assistant lecturer (Optoelectronic devices course);

Skills & Expertises

RESEARCH INTERESTS:

- Molecular electronics, charge transport and dissipation in nanoscale devices;
- Many-body corrections (GW, TDDFT) to simulate transport in quantum systems;
- Photovoltaic devices (Dye Solar cells, polymeric cells, small molecule cells);
- Organic memories (resistive bistable memories);
- Connection between information theory and statistical mechanics;
- Smart grids.

LANGUAGES: Italian (Native), English (Advanced level), German (Basic level).

PROGRAMMING: C++, Fortran90, Maple, Matlab, Office, Windows, Linux, Shell scripting, Latex.

INDUSTRIAL SPIN-OFF:
Part of the TiberLAB project and developer of the TiberCAD software (module Dye Solar Cells/ Transport in Organic and disordered semiconductors), www.tibercad.org.

PRESS
"*Il Simulatore per le celle del futuro*" *(The Simulator for future cells)*, PV Technology, Year 4, N° 1/2011, January-March.

CONFERENCE PRESENTATIONS: 16 oral presentations, 8 poster presentations.

CONFERENCE ORGANIZER: Organizer of the CECAM meeting "*Titania for all seasons: Multifunctionality of an undercover semiconductor*", September 6-10, 2010, Bremen, Germany.

LECTURES

5. *"Dye Solar Cells: Open Issues"*
Department of Condensed Matter Physics, Università degli studi di Roma Tor Vergata,
Rome, Italy (2010).

4. *"Seminario sul Fotovoltaico" (A lecture about photovoltaics)*
Department of Condensed Matter Physics, Università degli studi di Roma Tor Vergata,
Rome, Italy (2010)

3. *"gDFTB: a Non-equilibrium Green function method to characterize electron-phonon interaction in nanoscale systems "*
Department of Theoretical Physics, The University of Bremen (BCCMS),
Bremen, Germany (2007)

2. *"Theoretical modeling and simulation of electron-phonon scattering processes in molecular electronic devices"*
Department of Material Science, Technische Universitaet Dresden,
Dresden, Germany (2007).

1. *"Electron transport in molecular devices"*
School of Chemistry, The University of Sydney,
Sydney, Australia (2005).

INVITED TALKS
Invited Lecture "Nanotechnology Summer School" (20-23/09/2011)
"Simulation of Dissipation in Nano-Junctions: A Non-Equilibrium Green's Function method".
University of Trieste, Trieste, Italy.

Invited Speaker "International Conference on Simulation of Organic Electronics and Photovoltaics" (10-14/06/2012),
SimOEP12, Oliva (Spain).

Funding ID

Post Doc Grant (2 years long) from European Project HYMEC. Started: 1st of June 2012 (expiring 31st of May 2014).

List of Publications

Refereed Journal Articles (total citations: 506):

[26] J. Lykkebo, **A. Gagliardi**, A. Pecchia, G. C. Solomon, *"Strong Overtones Modes in Inelastic Electron Tunneling Spectroscopy with Cross-Conjugated Molecules: a Prediction from Theory"*, **ACS Nano**, 7 (10), 9183-9194 (2013).

[25] R. Tagliaferro, D. Gentilini, S. Mastroianni, A. Zampetti, **A. Gagliardi**, T. M. Brown, A. Reale, A. Di Carlo, *"Integrated Tandem Dye Solar Cells"*, **RSC Advances**, 3 (43), 20273-20280 (2013).

[24] P. Deak, B. Aradi, **A. Gagliardi**, H. A. Huy, G. Penazzi, B. Yan, T. Wehling, T. Frauenheim, *"The possibility of a field effect transistor based on Dirac-particles in semiconducting anatase-TiO2 nanowires"*, **Nano letters,** 13, 1073-1079 (2013).

[23] **A. Gagliardi**, D. Gentilini, A. Di Carlo, *"Charge transport in Solid-state Dye-Sensitized Solar cells"*, **The Journal of Physical Chemistry C**, 116 (45), 23882-23889 (2012).

[22] **A. Gagliardi**, A. Di Carlo, *"Innovative structure for dye solar cells"*, **Optical and Quantum Electronics**, 44 (3-5), 141-147 (2012).

[21] D. Gentilini, **A. Gagliardi**, A. Di Carlo, "*Dye solar cells efficiency maps: a parametric study"*, **Optical and Quantum Electronics,** 44 (3-5), 155-160 (2012).

[20] D. Gentilini, **A. Gagliardi**, M. Auf der Maur, L. Vesce, D. D'Ercole, T.M. Brown, A. Di Carlo, *"Correlation between cell performance and physical transport parameters in dye solar cells"*, **The Journal of Physical Chemistry C,** 116 (1), 1151-1157 (2012).

[19] **A. Gagliardi**, M. A. der Maur, D. Gentilini, A. Di Carlo, *"Simulation of dye solar cells: through and beyond one dimension"*, **Journal of computational electronics**, 10 (4), 424-436 (2012).

[18] **A. Gagliardi**, A. Di Carlo, *"Generalization of thermodynamic potentials including information"*, **Physica A: Statistical Mechanics and its Applications,** 391, 6337-6341 (2012).

[17] **A. Gagliardi**, M. Auf der Maur, A. Di Carlo, "*Theoretical Investigation of a Dye Solar Cell Wrapped Around an Optical Fiber*", IEEE Journal of Quantum Electronics, 47, 1214 (2011).

[16] M. Auf der Maur, **A. Gagliardi**, A. Di Carlo, "*Physics based simulation of dye solar cells*", **Optical and Quantum Electronics**, 1-7 (2011).

[15] G. Romano, **A. Gagliardi**, A Pecchia, A Di Carlo, "*Heating and Cooling mechanisms in single-molecule junctions*", **Physical Review B**, 81, 115438 (2010).

[14] D. Gentilini, D. D'Ercole, A. Gagliardi, A. Brunetti, A. Reale, T. Brown, A. Di Carlo, "*Analysis and simulation of incident photon to current efficiency in dye sensitized solar cells*", **Superlattices and Microstructures**, 47, 192 (2010).

[13] **A. Gagliardi**, S. Mastroianni, D. Gentilini, F. Giordano, A. Reale, T. Brown, A. Di Carlo, "*Multiscale Modelling of Dye Sensitized Solar Cell and Comparison with Experimental Data*", **IEEE Journal of Selected Topics in Quantum Electronics**, 16, 1611 (2010).

[12] **A. Gagliardi**, G. Romano, A. Pecchia, A. Di Carlo, "*Simulation of Inelastic Scattering in Molecular Junctions: Application to Inelastic Electron Tunneling Spectroscopy and Dissipation Effects*", **Journal of Computational and Theoretical Nanoscience**, 7, 2512 (2010).

[11] **A. Gagliardi**, M. Auf der Maur, D. Gentilini, A. Di Carlo, "*Modeling of Dye sensitized solar cells using a finite element method*", **Journal of Computational Electronics**, 8, 398 (2009).

[10] **A. Gagliardi**, G. Romano, A. Pecchia, A. Di Carlo, Th. Frauenheim, T. A. Niehaus, "*Electron-phonon scattering in molecular electronics: from inelastic electron tunnelling spectroscopy to heating effects*", **New Journal of Physics**, 10, 065020 (2008).

[9] G. Schulze, K. J. Franke, **A. Gagliardi**, G. Romano, C. Lin, A. Da Rosa, T. A. Niehaus, Th. Frauenheim, A. Di Carlo, A. Pecchia, J. I. Pascual, "*Resonant Electron Heating and Molecular Phonon Cooling in Single C60 Junctions*". **Physical Review Letter**, 100, 136801 (2008).

[8] **A. Gagliardi**, G. C. Solomon, A. Pecchia, Th. Frauenheim, A. Di Carlo, N. S. Hush and J. R. Reimers, "*A Priori Method for Propensity Rules for Inelastic Electron Tunneling Spectroscopy of Single-Molecule Conduction*", **Physical Review B**, 75, 174306 (2007).

[7] **A. Gagliardi**, Th. A. Niehaus, Th. Frauenheim, A. Pecchia and A. Di Carlo, "*Quasiparticle Correction for Electronic Transport in Molecular Wires*", **Journal of Computational Electronics**, 6, 345 (2007).

[6] J. R. Reimers, G. C. Solomon, **A. Gagliardi**, A. Bilic, N. S. Hush, Th. Frauenheim, A. Di Carlo and A. Pecchia, "*The Green's Function Density-Functional Tight-Binding (gDFTB) Method for Molecular-Electronic Conduction*", **Journal of Physical Chemistry A**, 111, 5692 (2007).

[5] F. Sacconi, M.P. Persson, M. Povolotskyi, L. Latessa, A. Pecchia, **A. Gagliardi**, A. Balint, T. Fraunheim, A. Di Carlo, *"Electronic and transport properties of silicon nanowires"*, **Journal of Computational Electronics**, 6 (1-3), 329-333 (2007).

[4] G. C. Solomon, **A. Gagliardi**, A. Pecchia, Th. Frauenheim, A. Di Carlo, J. R. Reimers and N. S. Hush**, "***Understanding the Inelastic Electron-Tunneling Spectra of Alkanedithiols on Gold*", **Journal of Chemical Physics**, 124, 094704 (2006).

[3] G. C. Solomon, **A. Gagliardi**, A. Pecchia, Th. Frauenheim, A. Di Carlo, J. R. Reimers and N. S. Hush, "*Molecular Origins of Conduction Channels Observed in Shot-Noise Measurements*", **Nano Letters**, 6, 2431 (2006).

[2] G. C. Solomon, **A. Gagliardi**, A. Pecchia, Th. Frauenheim, A. Di Carlo, J. R. Reimers and N. S. Hush, "*The Symmetry of Single Molecule Conduction"*, **Journal of Chemical Physics**, 125, 184702 (2006).

[1] A. Pecchia, A. Di Carlo, **A. Gagliardi**, S. Sanna, Th. Frauenheim, R. Gutierrez, "*Incoherent Electron-Phonon Scattering in Octanethiols"*, **Nano Letters**, 4, 2109 (2004) .

Proceedings:

[7] F. Santoni, **A. Gagliardi**, A. Di Carlo, *"Simulation of space charge limited organic non volatile memory elements"*, **MRS Proceedings** 1430 (1) (2012).

[6] **A. Gagliardi**, D. Gentilini, F. Giordano, M. Auf der Maur, A. Di Carlo. "*Analysis of changes in efficiency by simulating dye-sensitized solar cells varying the characteristics of* TiO_2*"*. **Proceedings of SPIE 7597**, 75970A (2010).

[5] **A. Gagliardi**, M. Auf der Maur, A. Pecchia, A. Di Carlo. "*Dye Solar Cell Simulations Using Finite Element Method"*. **IWCE09: 13th International Workshop on Computational Electronics,** pp. 1-4 (2009).

[4] A. Pecchia, G. Romano, **A. Gagliardi**, T. Frauenheim, A. Di Carlo, "*Heat dissipation and non-equilibrium phonon distributions in molecular devices"*, **Journal of Computational Electronics**, 6 (1), 335-339 (2007).

[3] A. Pecchia, **A. Gagliardi**, G. C. Solomon, A. Di Carlo, T Frauenheim, JR Reimers, "*Incoherent tunneling and heat dissipation in molecular bridges"*, **Journal of Physics: Conference Series**, 35, 349 (2006).

[2] **A. Gagliardi**, G. C. Solomon, A. Pecchia, A. Di Carlo, T. Frauenheim, J. R. Reimers, N. S. Hush, *Simulation of Inelastic Tunneling in Molecular Bridges*. **Non-Equilibrium Carrier Dynamics in Semiconductor**, 110, Editor M. Saraniti and U.Ravaioli, Publisher Springer, (2006).

[1] A. Pecchia, A. Di Carlo, **A. Gagliardi**, T. A. Niehaus, T. Frauenheim, "*Atomistic Simulation of Electronic Transport in Organic Nanostructures: Electron-Phonon and Electron-Electron Interactions"*, **Journal of Computational Electronics**, 4, 79 (2005).

Book Chapters:

[1] A. Pecchia, L. Latessa, **A. Gagliardi**, Th. Frauenheim, A. Di Carlo. "*The gDFTB Tool for Molecular Electronics in Molecular and Nano Electronics: Analysis, Design and Simulation*", Vol. 17, Editor J. Seminario, Publisher Elsevier, (2006).