

Research Profile **Alessio Gagliardi**



Personal data

Name Alessio Gagliardi, Prof. Dr.
Date/place of birth 1978-10-31, Rome, Italy
Address Technische Universität München, Karlstrasse 45-47, 80333 Munich, Germany
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Academic education / degrees

2007 PhD degree from the Paderborn University
(Theoretical Modeling and Simulation of Electron-Phonon Scattering Processes in Molecular Electronic Devices)

2004–2007 PhD student at the Paderborn University

2003 Diploma degree from the University of Rome "Tor Vergata"
(Modelli di Trasporto di Carica in Dispositivi Elettronici Molecolari; Charge Transport Models in Molecular Electronic Devices)

1997–2003 Engineering studies at the University of Rome "Tor Vergata"

Professional career

Since 2020 Associate Professor at the Technische Universität München, Germany

Since 2014 Tenure Track Assistant Professor at the Technische Universität München, Germany

2008-2014 Post-doc at the University of Rome "Tor Vergata", Italy

2007–2008 Post-doc at the University of Bremen, Germany

Research interests

Finite element based semi-classical transport modeling (development and applications)

Kinetic Monte Carlo (development and applications)

Atomistic modeling and quantum transport (development and application)

Nanostructured photovoltaic devices

Nanoelectronics

Thermodynamics at the nanoscale

Machine learning

Electrochemical systems

10 most important publications

1. B Garlyyev, K Kratzl, M Rück, J Michalička, J Fichtner, J M. Macak, T Kratky, S Günther, M Cokoja, A Bandarenka, **A Gagliardi**, R. A. Fischer; *How small: selecting the optimal size of Pt nanoparticles for enhanced oxygen electro-reduction mass activity*, *Angewandte Chemie*, 58, 9596-9600 (2019).
2. W Kaiser, **A Gagliardi**; *Kinetic Monte Carlo Study of the Role of the Energetic Disorder on the Open-Circuit Voltage in Polymer/Fullerene Solar Cells*, *Journal of physical chemistry letters*, 10 (20), 6097-61041 (2019).
3. J Lederer, W Kaiser, A Mattoni, **A Gagliardi**, *Machine Learning–Based Charge Transport Computation for Pentacene*, *Adv. Theory Simul.*, 180013 (2018).
4. M Rück, A Bandarenka, F Calle-Vallejo, **A Gagliardi**, *Oxygen Reduction Reaction: Rapid Prediction of Mass Activity of Nanostructured Platinum Electrocatalysts*, *The journal of physical chemistry letters*, 9 (15), 4463-4468 (2018)
5. **Gagliardi A.**; Abate A.; *Mesoporous Electron Selective Contacts Enhance the Tolerance to Interfacial Ions Accumulation in Perovskite Solar Cells*; *ACS Energy Letters* **12** 1-20 (2017).
6. Albes T.; **Gagliardi, A.**; *Charge Pair Separation Dynamics in Organic Bulk-Heterojunction Solar Cells*; *Advanced Theory and Simulations* 1800032 (2018).
7. **Gagliardi A.**; Auf der Maur M.; Gentilini D.; Di Fonzo F.; Abrusci A.; Snaith H.J.; Divitini G.; Ducati C.; Di Carlo A.; *The real TiO₂/HTM interface of solid-state dye solar cells: role of trapped states from a multiscale modelling perspective Nanoscale*; *Nanoscale* **7** 1136 (2015).
8. Schulze G.; Franke K. J.; **Gagliardi A.**; Romano G.; Lin C.S.; Rosa A.L.; Niehaus T. A.; Frauenheim Th.; Di Carlo A.; Pecchia A.; Pascual J.I.; *Resonant Electron Heating and Molecular Phonon Cooling in Single C60 Junctions*; *Physical Review Letter* **100** 136801 (2008).
9. **Gagliardi A.**; Solomon G. C.; Pecchia A.; Frauenheim Th.; Di Carlo A.; Hush N. S.; Reimers J. R.; *A Priori Method for Propensity Rules for Inelastic Electron Tunneling Spectroscopy of Single-Molecule Conduction*; *Physical Review B* **75** 174306 (2007).
10. Solomon G. C.; **Gagliardi A.**; Pecchia A.; Frauenheim Th.; Di Carlo A.; Reimers J. R.; Hush N. S.; *Understanding the Inelastic Electron-Tunneling Spectra of Alkanedithiols on Gold*; *Journal of Chemical Physics* **124** 094704 (2006).

Publication summary

Summary: **86** research publications (peer-reviewed), **3** other publications (not peer-reviewed).

Authorships: **18** first author publications (peer-reviewed).

Statistics: available from Google Scholar (26/10/2018): H-index: **21**, Number citations: **1318**.

Invited Conferences/Workshops since 2017 (60 oral contributions in total, 12 Invited):

- 1) PVTC , 24-28/4/2017, Marsillie, France
- 2) SSI-21, 19-23/6/2017, Padua, Italy.
- 3) Summer School ISOPHOS, 1-9/9/2017, Arbatax, Italy
- 4) Summer School Materials 4.0, 11-15/9/2017, Dresden, Germany
- 5) Winter School CNST, 18-20/12/2017, Bormio, Italy
- 6) NanoGe FallMeeting18, 22-26/10/2018, Torremolinos, Spain
- 7) SimOEP, 4-6/09/2018, Winterthur, Switzerland
- 8) "Novel Concepts and Elect. Phen. in Heterosyst.", 29-30/5/2018 Tutzing, Germany
- 9) QuantSol19 Winter School, 17-22/3/2019, Rauris, Austria
- 10) StatPhys

Organizer Conference NMEP (with NIM) (26-28/7/2017)

<http://www.nano-initiative-munich.de/events/nim-conference-nanostructured-functional-materials-for-sustainable-energy-provision/>

Memberships:

- 1) Past Member of the NIM (Nanosystem Initiative Munich) as group leader in the Nanosystems for Energy Conversion area.
- 2) IEEE Member.

Grants:

- 1) **DFG grant FflexCom:** The project is aimed to develop new flexible radio frequency devices based on carbon nanotubes to apply as RFID. Originally submitted with Prof. Lugli, since 1/1/2017 I am the only PI for both projects.
- 2) **European project COST Action MP1406 “MultiscaleSolar”:** The project is about funding travelling and collaboration visits among the group network to enhance joint research. The topic is simulation of third generation photovoltaics. I am one of the PI of the project.
- 3) **DFG grant Optimization of electrocatalysts for fuel cell applications without alloying: a joint theoretical and experimental study:** This project uses recent experimental discoveries and fundamental understanding of how one can increase the activity of the surface of pure Pt by at least the factor of 3.5-5 without any alloying to design active and more stable electrocatalysts for the oxygen reduction reaction. The key fact in this approach is that it is possible to increase the activity of e.g. Pt by controlling the atom coordination near to the ORR active sites. The aim of this project is to elucidate and implement “3D open” structures with the maximum density of active sites of right coordination, improved stability and local mass transport properties.
- 4) **IGSSE CONTROL:** Project in collaboration with Dr. Eva Herzig on the analysis of recombination and exciton dynamics in organic solar cells.
- 5) **Seed Project (in collaboration with Dr. Gregor Koblmüller, NIM):** a SEED project has been approved to investigate novel concepts for thermoelectric devices using nanowires.
- 6) **DAAD, PhD scholarship Mr. Mohammed Kashif:** simulation of tandem solar cells (organic and perovskite devices).
- 7) **DAAD, PhD scholarship Mr. Ajai Singh:** simulation of perovskite solar cells lead free.
- 8) **Airbus collaboration:** PhD scholarship to characterize large area multijunction solar cells for space applications (**industrial collaboration**).
- 9) **EU FET project LION-HEARTED:** application of organic nanoparticles optically activated for heart diseases.

Publications

Publication summary

Summary: 86 research publications (peer-reviewed), 3 other publications (not peer-reviewed).

Authorships: 18 first author publications; 23 last author (supervisor) publications; (peer-reviewed).

Statistics: available from Google Scholar (1/5/2019): H-index: 21, Number citations: 1318.

Publications (68) [no proceedings]:

[68] K Hussain, W Kaiser, **A Gagliardi**; *Effect of Polymer Morphology in Dilute Donor Organic Solar Cells*, **J. Phys. Chem. C**, (accepted 2020).

[67] C Pellegrino, **A Gagliardi**, C G Zimmermann; *Annual Energy Harvesting of Passively Cooled Hybrid Thermoelectric Generator-Concentrator Photovoltaic Modules* **IEEE Journal of Photovoltaics**, 9 (6), 1661-1667 (2019).

[66] W Kaiser, **A Gagliardi**; *Kinetic Monte Carlo Study of the Role of the Energetic Disorder on the Open-Circuit Voltage in Polymer/Fullerene Solar Cells*, **Journal of physical chemistry letters**, 10 (20), 6097-61041 (2019).

[65] C Pellegrino, **A Gagliardi**, C G Zimmermann; *Differences between the Effects of Proton and Electron Radiation-Induced Defects on the dark current in GaAs Solar Cells*, **Progress in Photovoltaics: Research and Application**, 27 (5), 379-390 (2019).

[64] J Stanley, F Mayr, **A Gagliardi**; *Machine Learning Stability and Bandgaps of Lead-Free Perovskites for Photovoltaics*, *Advanced Theory and Simulations* 3 (1), 1900178 (2020).

[63] M Darwish, **A Gagliardi**; *A Drift-Diffusion Simulation Model for Organic Field Effect Transistors: On the Importance of the Gaussian Density of States and Traps*, **Journal of Physics D: Applied Physics**, 53 (10), 105102 (2019).

[62] A. Singh, E. Radicchi, S. Fantacci, F. De Angelis, **A. Gagliardi**; *Interface Electrostatics of Solid-State Dye-Sensitized Solar Cells: A joint Drift-Diffusion and Density Functional Theory Study*, **J. Phys. Chem. C**, 123 (24), 14955-14963 (2019).

[61] M Rück, A Bandarenka, F Calle-Vallejo, **A Gagliardi**; *Fast Identification of Optimal Pure Platinum Nanoparticle Shapes and Sizes for Efficient Oxygen Electroreduction*, **Nanoscale Advances** 1 (8), 2901-2909 (2019).

[60] B Garlyyev, K Kratzl, M Rück, J Michalička, J Fichtner, J M. Macak, T Kratky, S Günther, M Cokoja, A Bandarenka, **A Gagliardi**, R. A. Fischer; *How small: selecting the optimal size of Pt nanoparticles for enhanced oxygen electro-reduction mass activity*, **Angewandte Chemie**, 58, 9596-9600 (2019).

[59] M Speckbacher, M Rinderle, W Kaiser, E Osman, D Chryssikos, A Cattani-Scholz, J M. Gibbs, **A Gagliardi**, M Tornow; *Directed Assembly of Nanoparticle Threshold Selector Arrays*, **Advanced Electronic Materials**, 5(7) 1900098 (2019).

[58] A. Singh, **A. Gagliardi**; *Efficiency of all-perovskite two-terminal tandem solar cells: A drift-diffusion study*, **Solar Energy**, 187, 39-46 (2019).

[57] M Darwish, H Boysan, C Liewald, B Nickel, **A Gagliardi**; *A resistor network simulation model for laser-scanning photo-current microscopy to quantify low conductance regions in organic thin films*, **Organic Electronics**, 62, 474-480 (2018).

[56] **A Gagliardi**, S Wang, T Albes, *Simulation of charge Carrier mobility unbalance in organic solar cells*, **Organic Electronics**, 59, 171-176 (2018).

- [55] M Rück, A Bandarenka, F Calle-Vallejo, **A Gagliardi**, *Oxygen Reduction Reaction: Rapid Prediction of Mass Activity of Nanostructured Platinum Electrocatalysts*, **The journal of physical chemistry letters**, 9 (15), 4463-4468 (2018).
- [54] T Albes, **A Gagliardi**, *Charge Pair Separation Dynamics in Organic Bulk-Heterojunction Solar Cells*, **Advanced Theory and Simulations**, 1 (7), 1800032 (2018).
- [53] W Kaiser, T Albes, **A Gagliardi**, *Charge carrier mobility of disordered organic semiconductors with correlated energetic and spatial disorder*, **Physical Chemistry Chemical Physics**, 20 (13), 8897-8908 (2018).
- [52] S Joshi, V Deep Bhatt, E Jaworska, A Michalska, K Maksymiuk, M Becherer, **A Gagliardi**, P Lugli, *Ambient Processed, Water-Stable, Aqueous-Gated sub 1 V n-type Carbon Nanotube Field Effect Transistor*, **Scientific Reports**, 8 (1), 11386 (2018).
- [51] T Albes, L Xu, J Wang, JWP Hsu, **A Gagliardi**, *Origin of Photocurrent in Fullerene-Based Solar Cells*, **The Journal of Physical Chemistry C**, 122 (27), 15140-15148 (2018).
- [50] W Kaiser, J Popp, M Rinderle, T Albes, **A Gagliardi**, *Generalized Kinetic Monte Carlo Framework for Organic Electronics*, **Algorithms**, 11 (4), 37 (2018).
- [49] M Auf der Maur, U Aeberhard, C David, **A Gagliardi**, *Multiscale Modeling of Photovoltaic Devices*, Hindawi Editorial International Journal of Photoenergy Volume 2018, Article ID 3065252, (2018).
- [48] J Lederer, W Kaiser, A Mattoni, **A Gagliardi**, *Machine Learning-Based Charge Transport Computation for Pentacene*, *Adv. Theory Simul.*, 180013 (2018).
- [47] J Popp, W Kaiser, **A Gagliardi**, *Impact of Phosphorescent Sensitizers and Morphology on the Photovoltaic Performance in Organic Solar Cells*, *Advanced Theory and Simulations*, 1800114 (2018).
- [46] C Pellegrino, **A Gagliardi**, C G Zimmermann, *Difference in space-charge recombination of proton and electron irradiated GaAs solar cells*, **Progress in Photovoltaics: Research and Application**, (accepted) (2018).
- [45] S. J. Sun, M. Mensik, P. Toman, **A. Gagliardi**, K. Kral, "Influence of acceptor on charge mobility in stacked π -conjugated polymers", **Chemical Physics**, 501, 8-14 (2018).
- [44] T. Albes, **A. Gagliardi**, "Influence of permittivity and energetic disorder on the spatial charge carrier distribution and recombination in organic bulk-heterojunctions", **Physical Chemistry Chemical Physics**, 19, 20974 (2017).
- [43] **A. Gagliardi**, A. Abate, "Mesoporous Electron Selective Contacts Enhance the Tolerance to Interfacial Ions Accumulation in Perovskite Solar Cells", **ACS Energy Letters**, 12, 1-20 (2017).
- [42] B. Weiler, T. Haeberle, **A. Gagliardi**, P. Lugli, "Kinetic monte carlo of transport processes in Al/AIOx/Au-layers: impact of defects", **AIP-Advances**, 6, 095112 (2016).
- [41] B. Weiler, **A. Gagliardi**, P. Lugli, "Kinetic monte carlo simulations of defects in anatase titanium dioxide", **Journal Physical Chemistry C**, 120, 10062-1007 (2016).
- [40] B. Weiler, R. Nagel, T. Albes, T. Haeberle, **A. Gagliardi**, Paolo Lugli, "Electrical and morphological characterization of transfer-printed Au/Ti/TiOx/p+-Si nano- and microstructures with plasma-grown titanium oxide layers", **Journal of Applied Physics**, 119, 145106 (2016).
- [39] J. Lykkebo, G. Romano, **A. Gagliardi**, A. Pecchia, G.C. Solomon, "Single-molecule electronics: Cooling individual vibrational modes by the tunneling current", **Journal of chemical physics**, 144 (11), 114310 (2016).
- [38] T. Albes, P. Lugli, **A. Gagliardi**, "Investigation of the Blend Morphology in Bulk-Heterojunction Organic Solar Cells", **IEEE Transactions on Nanotechnology**, 15, (2), 281-288 (2016).

- [37] F. Santoni, **A. Gagliardi**, M. Auf der Maur, A. Pecchia, S. Nau, S. Sax, E. J. W. List-Kratochvil, A. Di Carlo, "Modeling of Filamentary Conduction in Organic Thin Film Memories and Comparison With Experimental Data", **IEEE Nanotechnology**, 15, 60-69 (2016).
- [36] A. H. Fallahpour, D. Gentilini, **A. Gagliardi**, M. Auf der Maur, P. Lugli, A. Di Carlo, "Systematic Study of the PCE and Device Operation of Organic Tandem Solar Cells", **IEEE Journal of Photovoltaics**, 6 (1), 202-210 (2016).
- [35] A. Mahmoud, **A. Gagliardi**, P. Lugli, "Atomistic study of three-leg molecular devices", **Organic Electronics**, 24, 37-42 (2015).
- [34] A. Zampetti, A. H. Fallahpour, M. Dianetti, L. Salamandra, F. Santoni, **A. Gagliardi**, M. Auf der Maur, F. Brunetti, A. Reale, T. M. Brown, A. Di Carlo, "Influence of the interface material layers and semiconductor energetic disorder on the open circuit voltage in polymer solar cells", **Journal of Polymer Science Part B: Polymer Physics**, 53 (10), 690-699 (2015).
- [33] D. Gentilini, **A. Gagliardi**, A. A. Franco, F. Sauvage, A. Di Carlo, "A Drift-Diffusion Study on Charge Unbalancing Effects in Dye-Sensitized Solar Cells", **Journal of The Electrochemical Society**, 162 (10), H753-H758 (2015).
- [32] **A. Gagliardi**, M. Auf der Maur, D. Gentilini, F. di Fonzo, A. Abrusci, H. J. Snaith, G. Divitini, C. Ducati and A. Di Carlo, "Solid state Dye solar cells TiO₂/HTM real interface: role of trapped states from a multiscale modelling perspective", **Nanoscale**, 7, 1136 (2015).
- [31] S. Nau, C. Wolf, K. Popovic, A. Blümel, F. Santoni, **A. Gagliardi**, A. di Carlo, S. Sax and E. J. W. List-Kratochvil, "Inkjet-Printed Resistive Switching Memory Based on Organic Dielectric Materials: From Single Elements to Array Technology", **Advanced Electronic Materials**, 1, 1400003 (2015).
- [30] F. Santoni, **A. Gagliardi**, M. Auf der Maur, A. Di Carlo, "The relevance of correct injection model to simulate electrical properties of organic semiconductor", **Organic Electronics**, 15, 1557-1570 (2014).
- [29] A. Fallahpour, **A. Gagliardi**, D. Gentilini, A. Zampetti, F. Santoni, M. A. der Maur, A. Di Carlo, "Optoelectronic simulation and thickness optimization of energetically disordered organic solar cells", **Journal of Computational Electronics**, 1-10 (2014).
- [28] J Lykkebo, **A Gagliardi**, A Pecchia, GC Solomon, *IETS and quantum interference: Propensity rules in the presence of an interference feature*, **The Journal of chemical physics**, 141 (12), 124119 (2014).
- [27] A. H. Fallahpour, **A. Gagliardi**, F. Santoni, D. Gentilini, A. Zampetti, M. Auf der Maur, and A. Di Carlo, "Modeling and simulation of energetically disordered organic solar cells", **Journal of Applied Physics**, 116, 184502 (2014).
- [26] R. Tagliaferro, D. Gentilini, S. Mastroianni, A. Zampetti, **A. Gagliardi**, Th. M. Brown, A. Reale and A. Di Carlo, "Integrated Tandem Dye Solar Cells", **RCS Adv.**, 3, 20273-20280 (2013).
- [25] J. Lykkebo, **A. Gagliardi**, A. Pecchia, and G. C. Solomon, "Strong Overtones Mode Inelastic Electron Tunneling Spectroscopy with Cross-Conjugated Molecules: A Prediction from Theory", **ACS Nano**, 7, 9183-9194 (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).

Book Chapters (2):

[2] M. Auf der Maur, T. Albes, **A. Gagliardi**, Thin film solar cells, in "Handbook of Optoelectronic Device Modeling and Simulation: Laser, Modulators, Photodetectors and Solar Cells, and Numerical Methods (Volume 2)"; series in Optics and Optoelectronics, VIII. Solar Cells, 43 (2017). CRC Press, Taylor & Francis Group.

[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).

Proceedings (16):

[16] J. Stanley, **A. Gagliardi**, *Machine Learning Bandgaps of Inorganic Mixed Halide Perovskites*, 2018 IEEE 18th International Conference on Nanotechnology (IEEE-NANO), 1-2 (2018).

[15] J. Popp, W. Kaiser, **A. Gagliardi**, *Simulation of Enhanced Exciton Diffusion in Organic Solar Cells with Phosphorescent Sensitizers*, 2018 IEEE 18th International Conference on Nanotechnology (IEEE-NANO), 420-425 (2018).

[14] W. Kaiser, M. Rinderle, **A. Gagliardi**, *Impact of the Level and Orientation of Crystallinity on Charge Transport in Semi-Crystalline Organic Semiconductors*, 2018 IEEE 18th International Conference on Nanotechnology (IEEE-NANO), 420-425 (2018).

[13] T. Maister et al., *Program FFlexCom : High Frequency Flexible Bendable Electronics for Wireless Communication Systems*, International Conference on Microwaves, **Communications, Antennas and Electronic Systems, IEEE COMCAS 2017-11-13 - 2017-11-15**, Tel Aviv, Israel (2017).

[12] T. Albes, P. Lugli, **A. Gagliardi**, "Kinetic Monte Carlo simulations to Investigate The effects of interfaces in organic photovoltaic cells including a realistic blend morphology", **Simulation of Semiconductor Processes and Devices (SISPAD)**, 2015.

[11] A. Di Carlo, D. Gentilini, **A. Gagliardi**, "Simulation of solid-state dye solar cells based on organic and Perovskite sensitizers", **SPIE OPTO**, 935711-935711-7 (2015).

[10] **A. Gagliardi**, M. Auf der Maur, F. Di Fonzo, A. Abrusci, H. Snaith, G. Divitini, C. Ducati, A. Di Carlo, "Multiscale simulation of solid state dye sensitized solar cells including morphology effects", **Computational Electronics (IWCE)**, 2014 International Workshop on, 1-4 (2014).

[9] A. Mahmoud, **A. Gagliardi**, P. Lugli, "Theoretical Study on Conductance Switching of Single-Molecule Devices Nanotechnology" (**IEEE-NANO**), **2014 14th IEEE Conference on**, 1-4 (2014).

[8] G. Penazzi, P. Deak, B. Aradi, T. Wehling, **A. Gagliardi**, H. A. Huy, B. Yan, T. Frauenheim, "TiO₂ Nanowires as a Wide Bandgap Dirac Material: a numerical study of impurity scattering and Anderson disorder", **MRS Proceedings** 1659, mrsf13-1659 (2014).

- [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 TiO₂". **Proceedings of SPIE 7597**, 75970A (2010).
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