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
2014-2019	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. H Michaels, M Rinderle, R Freitag, I Benesperi, T Edvinsson, R Socher, **A Gagliardi**, M Freitag; *Dye-sensitized solar cells under ambient light powering machine learning: towards autonomous smart sensors for the internet of things*, **CHEMICAL SCIENCE**, 11, 2895-2906 (2020).
2. 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).
3. M Rinderle, W Kaiser, A Mattoni, **A Gagliardi**; *Machine-Learned Charge Transfer Integrals for Multiscale Simulations in Organic Thin Films*, **Journal of Physical Chemistry C**, 124, 17733-17743 (2020).
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. 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).
6. M Rück, B Garlyyev, F Mayr, A S Bandarenka, **A Gagliardi**; *Oxygen Reduction Activities of Strained Platinum Core–Shell Electrocatalysts Predicted by Machine Learning*, **Journal of physical chemistry letters,** 11, 1773-1780 (2020).
7. 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).
8. J Lederer, W Kaiser, A Mattoni, **A Gagliardi,** *Machine Learning–Based Charge Transport Computation for Pentacene*, Adv. Theory Simul., 180013 (2018).
9. **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).
10. **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).

Publication summary

Summary: **95** research publications (peer-reviewed), **3** other publications (not peer-reviewed).
Statistics: available from Google Scholar (19/02/2021): H-index: **23**, Number citations: **1626**.

Invited Conferences/Workshops since 2017 **(65 oral contributions in total, 17 Invited):**

1) Summer School ISOPHOS, 1-9/9/2017, Arbatax, Italy
2) Summer School Materials 4.0, 11-15/9/2017, Dresden, Germany
3) Winter School CNST, 18-20/12/2017, Bormio, Italy
4) NanoGe FallMeeting18, 22-26/10/2018, Torremolinos, Spain
5) SimOEP, 4-6/09/2018, Winterthur, Switzerland
6) "Novel Concepts and Elect. Phen. in Heterosyst.", 29-30/5/2018 Tutzing, Germany
7) QuantSol19 Winter School, 17-22/3/2019, Rauris, Austria
8) nanoGe StabPero, 2-3/6/2020 online meetup, Spain
9) nanoGe ComPer, 8-9/9/2020 online meetup
10) SEPOMO, 29/9/2020 online meetup

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) Member of the e-conversion Cluster of Excellence

3) IEEE Member.

Grants:

1) DFG grant FflexCom: The project is aimed to develop new flexible radio frequancy 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 applicationswithout 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.
10) Ptj Forschungszentrum Jülich – **BMBF SOLAR-ERA (PrOperPhtoMiLe):** On the way of predicting the lifespan of perovskite photovoltaics: determination of acceleration factors in stability analysis through machine learning.

Research group:

1) Barbara Asam (secretary)

2) Obaiudur Rahaman (PostDoc)

3) Milan Harth (PhD)
4) Michael Rinderle (PhD)
5) Carmine Pellegrino (PhD)
6) Ajay Singh (PhD)
7) Kashif Hussain (PhD)
8) Manuel Gößwen (PhD)
9) Felix Mayr (PhD)
10) John Kouroudis

Past Members:
1) Tim Albes
2) Mohammed Darwish
3) Marlon Rück
4) Ahmed Mahmoud
5) Waldemar Kaiser