Curriculum Vitae

Personal Data

Title	Prof.
First name	Alessio
Name	Gagliardi
Current position	Associate prof.
Current institution(s)/site(s), country	School of Computation, Information and Technology, Department of Electrical Engineering, Technical University of Munich (TUM), Garching bei München, Germany
Identifiers/ORCID	0000-0002-3322-2190

Qualifications and Career

Stages	**Periods and Details**
B.Sc. in Telecommunication Engineering (cum laude)	1997-2000, University of Rome „Tor Vergata“, Italy
M.Sc. in Telecommunication Engineering (cum laude)	2000-2003, University of Rome „Tor Vergata“, Italy
Ph.D	2004-2007, Paderborn University, Germany. Field: Physics Advisor: Prof. Thomas Frauenheim. Thesis: Theoretical Modeling and Simulation of Electron-Phonon Scattering Processes in Molecular Electronic Devices.
Postdoctoral fellow	2007-2008, Dept. of Physics, Bremen University, Germany. Supervisor: Prof. Thomas Frauenheim. Topic: Molecular Electronics. 2008-2014, Dept. of Electrical Engineering, University of Rome “Tor Vergata”, Italy. Supervisor: Prof. Aldo Di Carlo. Topic: Simulation of organic and dye sensitized solar cells.
Professorship	2014-2019, Tenure Track Assistant Professor at the Technische Universität München, Germany 2020-current, Associate Professor at the Technische Universität München, Germany

Supplementary Career Information

NA

Activities in the Research System

- 2024-current – Founder and board member of the Atomistic Modeling Center (TUM) https://www.mdsi.tum.de/amc/startseite/
- 2014-current – Member of the Nanoelectronic Institute (TUM, Electrical Engineering).
- 2021-current – Core member of the Munich Data Science Institute (MDSI). TUM.
- 2022-current – Core member of the Munich Institute for Integrated Materials, Energy and Process Engineering (MEP). TUM.
- Since 2018, contributed to around 70 international conferences with oral talks (26 as Invited Speakers).
- 2016-current – Part of the TUM-Asia program between TUM and Singapore for teaching at the Singapore Institute of Technology (SIT) and Nanyang Technology University (NTU).

Supervision of Researchers in Early Career Phases

At TUM since 2014, PI Gagliardi has supervised around 100 MSc and Bc. dissertations, 7 PhD dissertations and 2 postdoctoral fellows. He his currently supervising 9 PhD students and 1 PostDoc.

Scientific Results

Category A

10 publications most relevant to the current proposal

Summary: **139** research publications (peer-reviewed), **1** Book Chapter.
Statistics: available from Google Scholar (24/10/2024): h-index: **30**, Number citations: **3241**

1. I Kouroudis, K T Tanko, M Karimipour, A Ben Ali, D K Kumar, V Sudhakar, R Kant Gupta, I Visoly-Fisher, M Lira-Cantu, A Gagliardi; Artificial Intelligence-Based, Wavelet-Aided Prediction of Long-Term Outdoor Performance of Perovskite Solar Cells; ACS Energy Letters, 9 (4), 1581-1586 (2024).

2. G A Siddiqui, J A Stebani, D Wragg, P S Koutsourelakis, A Casini, A Gagliardi; Application of Machine Learning Algorithms to Metadynamics for the Elucidation of the Binding Modes and Free Energy Landscape of Drug/Target Interactions: a Case Study; Chemistry–A European Journal, 29, (62), e202302375 (2023).

3. C Lampe, I Kouroudis, M Harth, S Martin, A Gagliardi, AS Urban; Rapid Data-Efficient Optimization of Perovskite Nanocrystal Syntheses through Machine Learning Algorithm Fusion; Advanced Materials, 2208772 (2023).

4. M Harth, L Vesce, I Kouroudis, M Stefanelli, A Di Carlo, A Gagliardi; Optoelectronic perovskite film characterization via machine vision; Solar Energy 262, 111840 (2023).

5. 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).

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. F Mayr, A Gagliardi; Global property prediction: a benchmark study on open-source, perovskite-like datasets; ACS omega 6 (19), 12722-12732 (2021).

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

9. 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).

10. 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).

Category B

Other academic output relevant to the current proposal

1. 2019-2024 – Member (PI) of the German Cluster of Excellence E-conversion (funded by the German Research Foundation, DFG). Cluster of 55 PIs in the Munich area (LMU and TUM Universities) on the development of renewable energies and materials.
2. 2021-2024: SOLAR-ERA.NET Cofund 2 (EU)/Ptj Forschungszentrum Jülich – BMBF, leader: M. Lira-Cantu from Catalan Institute of Nanoscience and Nanotechnology (ICN2) Spain, Consortium of 6 research groups from 5 countries, German coordinator: Prof. A. Gagliardi, “Towards Prediction of Operational Lifetime of Perovskite Photovoltaics: Acceleration Factors in Stability Study through Machine Learning (PrOPerPhotoMiLe)“.
3. 2020-2025: TUM Innovation Network, 10 PIs. Coordinator: Prof. Alessio Gagliardi and Prof. Angela Casini (TUM, Germany). Cooperation on electrochemistry and regenerative medicine using supramolecular materials powered by machine learning. “Artificial Intelligence Powered Multifunctional Material Design (ARTEMIS)”.
4. 2024-2028: EU-HORIZON-TMA-MSCA Doctoral Network project – PI and PhD candidate advisor, 19 participating institutions, coordinator: Prof. Paola Vivo (Tampere University, Finland), “Indoor photovoltaics: towards an energy- and climate-neutral world (MENTOR)”.

Academic Distinctions

- 2024 – Nominated for the international “ENI: Energy Frontiers” award.
- 2014-2019 – Member of the Cluster of Excellence Nano Initiative Munich (NIM).

Other Information

Alessio Gagliardi´s research interests include the development and application of numerical models integrated with data-driven methods for the simulation of nanostructured devices. His focus is on new solar cells (organic semiconductors, dye sensitized and perovskite), electrochemical systems (fuel cells, batteries) and organic semiconductor materials. The development of new models ranges from the nanoscale (Density Functional Theory, Quantum Green Functions) through the mesoscale (Kinetic Monte Carlo) to the macroscopic scale (drift diffusion, continuum models). He is also a developer of TiberCAD and the gDFTB software. Machine learning methods include generative and non-generative architectures for structure-to-property prediction, numerical models acceleration and integration of simulations with experimental data.