

CURRICULUM VITAE ET STUDIORUM

Prof. Dr. GiovanniMaria Piccini



Personal data: Born in Udine (I), 10/10/1986

Present Position: Associate Professor

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[ORCID](#), [Google Scholar](#), [Scoups](#)

EDUCATION

- 2015 – PhD (*Doctor rerum naturalium*), Theoretical & Physical Chemistry (funded by VCI Kekulé Mobility Fellowship), Humboldt-Universität zu Berlin, DE, Grade: Summa cum Laude (with honors)
- 2010 – M.Sc. in Chemistry, Università degli studi di Trieste, I
- 2010 – Master M2, Theoretical Chemistry (funded by Leonardo scholarship and HPC-Europa2 project), Groningen University, NL
- 2008 – Master M1, Theoretical Chemistry, Groningen University, NL & Katholieke Universiteit Leuven, B

PREVIOUS POSITIONS AND FELLOSHIPS

- 11/2022 to 12/2023 – Juniorprofessor for Modeling & Simulation in Catalysis, RWTH Aachen University, DE
- 01/2021 to 10/2022 – Staff Scientist, Pacific Northwest National Laboratory (PNNL), USA
- 01/2016 to 12/2020 – Postdoc, Chemistry & Applied Biosciences, ETH Zurich, CH
- 04/2015 to 12/2016 – Postdoc, Chemistry, Humboldt-Universität, Berlin, DE

BRIEF DESCRIPTION OF THE RESEARCH ACTIVITY

Research involves the development and application of advanced quantum chemical molecular simulation methods combined with machine learning techniques to investigate chemical reactivity, with a particular focus on various catalytic processes. The scope includes exploring intersecting lines across heterogeneous, homogeneous, enzymatic, and supramolecular catalysis.

FUNDING AND PROJECTS

- 2023 – Seed funding for new external professors, €15,000, UNIMORE, I
- 2022-2023 – Explorative Research Space grant, €80,000, RWTH Aachen U., DE
- 2022-2023 – Computational grant, 1.5M hours/processor, RWTH Aachen U., DE
- 2022-2025 – Special Tenure track, Fuel Science Center, €215,000, RWTH Aachen U., DE
- 2022-2025 – Core funding for tenure track, €356,000, RWTH Aachen U., DE
- 2022 – Internal grant, €126,000, PNNL, USA
- 2021 – Internal grant, €115,000, PNNL, USA
- 2020 – Computing production grant, 100,000 Node hours, CSCS, CH
- 2012-2015 – 3-year computing production grant, 500,000 Node hours, HLRN, DE
- 2011-2014 – VCI Kekulé Mobility Fellowship, €90,000, Humboldt U., DE
- 2010 – Max Planck PhD Fellowship, €7,200, Humboldt U., DE
- 2010 – HPC-Europa2 fellowship, €5,000, SARA, NL
- 2010 – Leonardo fellowship, €2,500, Groningen U., NL

MAJOR COLLABORATIONS

- Prof. K. Tiefenbacher, Supramolecular catalysis, U. of Basel, CH
- Prof. J. Lercher, Zeolites biomass catalysis, TU Munich, DE & PNNL, USA
- Prof. T. Wiegand, NMR proton mobility in catalysts, RWTH Aachen, DE
- Prof. U. Simon, Transport in zeolite catalysts, RWTH Aachen, DE
- Prof. F. Santoro, Synthetic retinas simulation, RWTH Aachen, DE
- Prof. P. Carloni, COVID-19 drug screening, Forschungszentrum Jülich, DE
- Prof. M. Pavone, CO₂ photocatalytic reduction, U. of Naples Federico II, IT

TEACHING ACTIVITIES

- 2025 – Lecturer, Physical Chemistry – Exercises, UNIMORE, Italy
- 2024 – Lecturer, Physical Chemistry of Catalysis, UNIMORE, Italy
- 2024 – Lecturer, Physical Chemistry of Natural Systems, UNIMORE, Italy
- 2023 – Lecturer, Molecular Dynamics & Nanostructured Catalysts, RWTH Aachen, Germany
- 2022-2023 – Lecturer, Heterogeneous & Environmental Catalysis, RWTH Aachen, Germany
- 2022 – Lecturer, Enhanced Sampling, University of Milano Bicocca, Italy
- 2020 – Lecturer, Rare Events (postponed), University of Roma Tor Vergata, Italy
- 2012-2015 – Organizer/Lecturer, Molecular Modelling Lab, Humboldt University, Berlin, Germany
- 2008-2010 – Tutor, Physical Chemistry Lab, University of Trieste, Italy

SUPERVISION OF PhD STUDENTS AND POSTDOCTORAL FELLOWS

- 2024 – present 1 PhD Students UNIMORE, Italy
- 2023 – present 3 PhD Students RWTH Aachen U., DE
- 2020 – 2022 1 Postdoc Forschungszentrum Jülich & ETH Zurich & RWTH Aachen University, DE/CH
- 2017 – 2021 1 PhD Student ETH Zurich, CH
- 2018 – 2021 2 Visiting PhD Students, University of Calabria & University of Naples Federico II, visiting at ETH Zurich, IT/CH

ACADEMIC DUTIES

- 2024 – present, Member of the committee for the evaluation of the defense rules of the PhD Program and Course in "Models and Methods for Material and Environmental Sciences", UNIMORE, Italy
- 2025 – present, Chair of the "Commissione Paritetica Docenti-Studenti" of the "Green and sustainable chemistry" bachelor, UNIMORE, Italy
- 2024 – present Member of PhD Program and Course in "Models and Methods for Material and Environmental Sciences", UNIMORE, Italy
- 2024 – Member and organizer of the high-school dissemination activity for the "Green and sustainable chemistry" bachelor, UNIMORE, Italy
- 2022 – present Member of various PhD committees in Germany and Italy
- 2022 – 2023 Advisory Board Member, Fuel Science Center Cluster, RWTH Aachen Univ., DE
- 2021 – 2022 Organizer, Review Group, Molecular Foundations, PNNL, USA
- 2016 – 2021 Manager & Spokesperson for the HPC Facilities of the Parrinello Group, CSCS & ETH "Euler" Cluster, CH

AWARDS

- 2018 – Ewald Wicke Prize, German Bunsen Society for Physical Chemistry, DE
- 2016 – Fischer-Nernst Prize for the best PhD thesis in chemistry, Humboldt U., DE
- 2015 – Student award, 65th Lindau Nobel Laureate Meeting, DE
- Abilitazione Scientifica Nazionale 2021/2023 – associate professor, sector: 03/A2, validity: dal 31/01/2022 to 31/01/2033
- Abilitazione Scientifica Nazionale 2021/2023 – associate professor, sector: 03/B1, validity: dal 01/02/2022 to 01/02/2033

MEMBERSHIPS AND APPOINTMENTS

- 2025 - present – Member, American Chemical Society, USA
- 2024 - present – Member, Società Chimica Italiana (SCI), IT
- 2018 - present – Co-Founder, PLUMED Consortium, International
- 2018 - present – Member, German Bunsen Society for Physical Chemistry (DBG), DE
- 2022 - 2023 – Member & Principal Investigator, Fuel Science Center, RWTH Aachen, DE
- 2017-2022 – Member, Swiss Chem. Society (SCS), CH
- 2019-2021 – Swiss Member, COST Action 18234, COST
- 2010-2012 – Member, Società Chimica Italiana (SCI), IT

ORGANISATION OF SCIENTIFIC MEETINGS AND SCHOOLS

- 2025 – Organizer, ACS Symposium on Enhanced Sampling Simulations, San Diego, USA
- 2024 – Organizer, CECAM Workshop on Catalytic Operando Simulations, Genoa, Italy
- 2022 – Organizer, CECAM Workshop on Machine Learning in Molecular Dynamics, Pisa, Italy
- 2011 – Organizer, Workshop at Schloss Ringberg, Max Planck Society, Germany

EDITORIAL ACTIVITIES

- 2024 – Member of the Editorial Advisory Board of *ACS Journal of Chemical Theory and Computation*
- 2021 - Chief Editor - *Frontiers in Catalysis*, Topic: Modelling Heterogeneous Catalytic Materials, *Frontiers Journal*

REVIEWER ACTIVITIES

- 2025 - Grant Reviewer – European Research Council (ERC – Starting Grant), EU
- 2023 - Grant Reviewer - Alexander von Humboldt-Stiftung, DE
- 2023 - Grant Reviewer - NWO Open Comp. Domain Science - M, NL
- 2020 - Grant Reviewer - ACS Petroleum Research Fund, USA
- 2014 - present - Article Reviewer (>15 articles/year), Multiple Int. Journals: wide-spectrum scientific journals (*Nature comm.*), general chemistry (*J. Am. Chem. Soc*, *ACS Omega*), physical and theoretical chemistry (*J. Phys. Chem. Lett.*, *J. Phys. Chem.*, *J Chem. Theory and Comput.*, *Int. J. Quant. Chem.*) and catalysis (*J. Catal.*)

OUTREACH AND DISSEMINATION

- Guest contributor on the radio program *Baobab* for Swiss Italian Radio (RSI – Rete 3), Lugano (CH).
- Dissemination article on fake scientific news published on *Chiedi le Prove* (Italian edition of *Ask for Evidence*): [Read the article](#).
- Organizer and participant in high school outreach activities promoting the Green and Sustainable Chemistry bachelor's program at UNIMORE, Mantua (Italy).
- Organizer of the scientific aperitif "Una chimica per il futuro", focused on chemistry and sustainability challenges, Mantua (Italy).

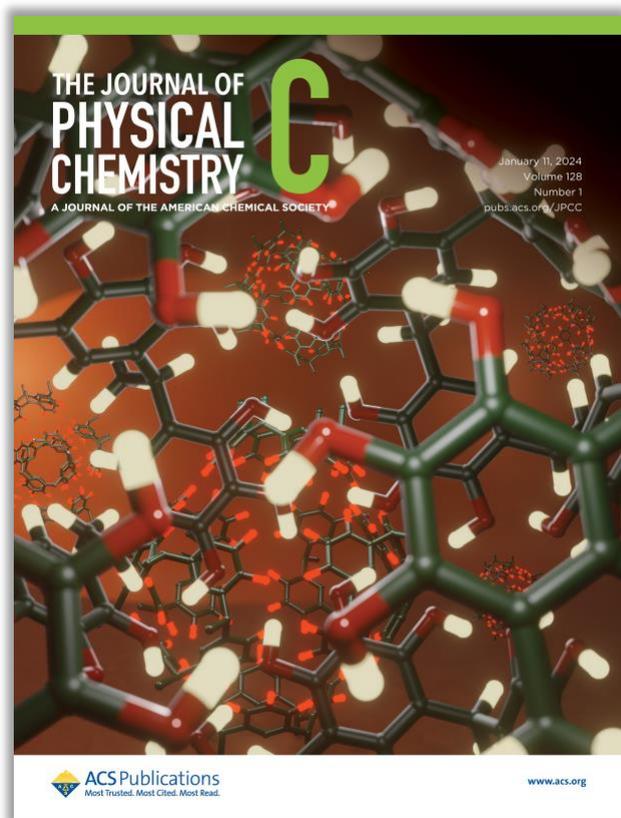
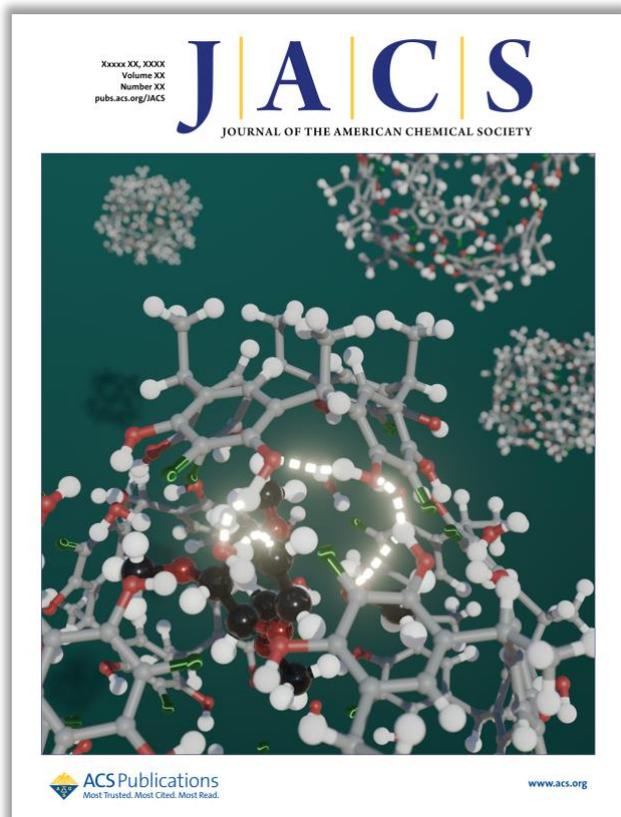
BIBLIOMETRICS AND CITATIONS

Scopus	articles:	41	
	<i>h</i> -index:		22
	citations:		2246
Google Scholar	articles:	44	
	<i>h</i> -index:		24
	citations:		2770

PUBLICATION LIST

Please follow this [link](#)

COVER PAGES



INVITATIONS TO INTERNATIONAL CONFERENCES

KEYNOTE:

Towards Operando Simulations for Catalytic Processes through Integrated Enhanced Sampling and Machine Learning Techniques

XXVIII National Congress of Società Chimica Italiana
Milan (I, 2024)

Free energy sampling of catalytic processes at operando conditions

International Workshop on Multiscale Computational Design for Heterogeneous Functional Materials 2024
Naples (I, 2024)

INVITED:

Exploring Chemistry and Catalysis by Biasing Skewed Distributions via Deep Learning

Conference on Frontiers in Atomistic Simulations: from Physics to Chemistry and Biology
Trieste (I, 2025)

Dynamic effects in zeolites catalysis at operando conditions

CECAM workshop "Modelling supramolecular catalysis: Methods and Applications"
Varigotti (I, 2024)

Operando simulations of supramolecular capsule catalysis

CECAM workshop "Modelling supramolecular catalysis: Methods and Applications"
Paris (F, 2024)

Simulating Real Catalytic Systems at Operando Conditions

American Chemical Society – Fall meeting 2023
San Francisco (USA, 2023)

Enhancing Efficiency and Accuracy in Chemical Reactions Sampling

Swiss Chemical Society – 100 years of CASALE mini symposia
Virtual (CH, 2021)

Enhancing Efficiency and Accuracy in Chemical Reactions Sampling

CPMD Meeting 2019 - Pushing the Boundaries of Molecular Dynamics
Lausanne (CH, 2019)

Enhancing Efficiency and Accuracy in Chemical Reactions Sampling

CECAM workshop "Learning the Collective Variables of Biomolecular Processes"
Paris (F, 2019)

Enhancing Fluctuations along Kinetic Bottlenecks

Bunsentagung 2018 - Kinetics in the Real World,
Hannover (DE, 2018)

Accurate Ab Initio Free Energies of Surface Reactions from Anharmonic Vibrations

IMPRS Max Planck School Evaluation – Fritz Haber Institut
Berlin (DE, 2013)

CONTRIBUTED:

Overcoming Large Free Energy Barriers in Molecular Dynamics

Simulations of Realistic Catalytic Systems

Fuel Science Center International Conference 2023: from fuel to propulsion
Aachen (DE, 2023)

Atomistic simulations of catalytic confined environments from supramolecular systems to biomass conversion

Bunsentagung 2021

Regensburg – Virtual (DE, 2021)

Atomistic simulations of catalytic confined environments from supramolecular systems to biomass conversion

Swiss Chemical Society fall meeting

Lugano (CH, 2020)

Enhancing Efficiency and Accuracy in Chemical Reactions Sampling

Materials Simulations Days

Mainz (DE, 2019)

Accurate Ab Initio Free Energies of Surface Reactions from Anharmonic Vibrations

ACS Spring Meeting

San Diego (US, 2016) – Presented by J. Sauer

Accuratezza Chimica nel Calcolo di Energie Libere Ab Initio

CHITEL

Turin (I, 2015)

INVITED SEMINARS AT INTERNATIONAL INSTITUTIONS:

Exploring Chemistry and Catalysis by Biasing Skewed Distributions via Deep Learning

Conference on Frontiers in Atomistic Simulations: from Physics to Chemistry and Biology

Capri (I, 2025)

Free energy sampling of catalytic processes at *operando* conditions

International Centre for Theoretical Physics

Trieste (I, 2024)

Accelerating reactive events in molecular simulations

Università degli studi di Trieste

Trieste (I, 2023)

Accelerating reactive events in molecular simulations

RWTH Aachen University – Institute of Organic Chemistry

Aachen (DE, 2023)

Enhancing Fluctuations along Kinetic Bottlenecks – Sampling Reactive Events Catalysis

Università degli Studi di Milano Bicocca

Milan (I, 2022)

Simulating Catalysis in Confined Supramolecular Environments

Istituto Italiano di Tecnologia

Genoa (I, 2021)

Simulating Materials for Energy Conversion

Casale SA

Lugano (CH, 2021)

Simulating Materials for Sustainable Chemistry

Università della Svizzera italiana

Lugano (CH, 2021)

Enhancing Important Fluctuations along Kinetic Bottlenecks - Sampling Reactive Events in Catalysis

Ecole Normale Supérieure de Paris

Paris (F, 2020)

Enhancing Important Fluctuations in Chemical Reactions

Laboratoire de Physique et Chimie Théoriques

Nancy (F, 2020)

Simulating Reactive Events in Catalysis

Ecole Normale Supérieure de Lyon

Lyon (F, 2020)

Enhancing Important Fluctuations along Kinetic Bottlenecks

Institut Charles Gerhardt Montpellier

Montpellier (F, 2019)

Simulating the Acid-Base Equilibrium – from Solution to Catalysis

Humboldt-Universität zu Berlin

Berlin (DE, 2019)

Enhancing Important Fluctuations along Kinetic Bottlenecks - Sampling Reactive Events in Catalysis

Basel Universität

Basel (CH, 2019)

Efficiency and Accuracy in Chemical Reactions Sampling

Forschungszentrum Jülich

Jülich (DE, 2019)

Enhancing Fluctuations along Kinetic Bottlenecks

Humboldt-Universität zu Berlin

Berlin (DE, 2018)

Collective Variables from Local Fluctuations

EMPA Zurich

Zurich (CH, 2018)

Enhancing Fluctuations in Chemical Reactions

Humboldt-Universität zu Berlin

Berlin (DE, 2017)

Fischer-Nernst award ceremony

Humboldt-Universität zu Berlin

Berlin (DE, 2017)

Accurate Ab Initio Free Energies of Surface Reactions from Anharmonic Vibrations

IMPRS Max Planck School Evaluation – Fritz Haber Institut

Berlin (DE, 2013)

Ab Initio Molecular Dynamics of Surface Adsorption

Berlin-Brandenburg VCI Stipendiatentreffen

Berlin (DE, 2012)

Variational flooding for chemical kinetics

Università degli studi di Trieste

Trieste (I, 2016)

Modena, 22/03/2025



Handwritten signature of Gianni Morini. The signature is written in a cursive style. Above the signature, there is a large, hand-drawn oval shape. Inside this oval, there are three small dots arranged horizontally.