1. **Bio sketch**

Nicola Marzari holds the chair of Theory and Simulation of Materials at the École Polytechnique Fédérale de Lausanne (Switzerland), where he is also the director of the National Centre for Competence in Research on Computational Design and Discovery of Novel Materials of the Swiss National Science Foundation (NCCR MARVEL, a 12-year effort started in 2014 involving more than 30 principal investigators), and the head of the Laboratory for Materials Simulations at the Paul Scherrer Institut (Villigen, Switzerland). He holds an Excellence Chair at the University of Bremen (Germany).

Previous tenured appointments include the Toyota Chair for Materials Processing at the Massachusetts Institute of Technology (US) and the first Statutory Chair of Materials Modelling at the University of Oxford (UK), where he was also the director of the Materials Modelling Laboratory. He is a past Chairperson and Trustee of the Psi-k Charity and Board of Trustees. He has a PhD in Physics from the University of Cambridge (UK) and a Laurea in Physics from the University of Trieste (Italy).

His research is dedicated to the development and application of first-principles simulations to understand, predict, and design the properties and performance of novel materials and devices. Core interests during the years have been on materials discovery, electronic-structure theory, first-principles electrochemistry, and electronic and thermal transport, with applications dedicated to materials for energy, functional materials, 2D materials, and materials and devices for information-and-communications technologies.

2. **Personal information**

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https://scholar.google.com/citations?hl=en&user=YjHKNAUAAAAJ&view_op=list_works&sortby=pubdate

3. **Employment history including current positions**

Head, Laboratory for Materials Simulations, Paul Scherrer Institut	Jul 2021 - onwards
Director, MARVEL National Centre on Computational Design and Discovery, SNSF	May 2014 - onwards
Chair, Theory and Simulation of Materials, EPFL	Sep 2011 - onwards
Statutory Chair of Materials Modeling, University of Oxford	Feb 2010 - Aug 2011
Director, Materials Modeling Laboratory, University of Oxford	Feb 2010 - Aug 2011
Toyota Chair of Materials Processing, DMSE, MIT	Jul 2009 - Jan 2011
Associate Professor with tenure, DMSE, MIT	Jul 2007 - Jan 2011
Associate Professor without tenure, DMSE, MIT	Jul 2005 - Jun 2007
AMAX Assistant Professor, DMSE, MIT	Aug 2001 - Jun 2005
Research Staff, Department of Chemistry, Princeton University	Sep 1999 - Aug 2001
Research Faculty, George Mason University and Naval Research Laboratory	Sep 1998 - Aug 1999

4. Education

Department of Physics, Rutgers University, NSF Postdoctoral Fellow	Apr 1996 - Aug 1998
Advisor: *Prof David Vanderbilt*	
University of Cambridge, UK, PhD in Physics, EU HCM Fellow	Apr 1993 - Mar 1996
Advisor: *Prof Michael C. Payne*	
University of Trieste, Italy, Laurea in Physics, summa cum laude	Oct 1992
Advisors: *Prof Alfonso Baldereschi* and *Prof Stefano Baroni*	

5. Other relevant appointments

Scientific Advisory Board, Italian Institute of Technology	Jan 2024 - onwards
Scientific Council, National Research Council (Italy)	Feb 2022 - onwards
Editorial Board, PRX Energy (American Physical Society)	Dec 2021 - onwards
Chair, Scientific Advisory Board, DOE MICCoM (U. of Chicago)	May 2020 - onwards
Senior Editor, Scientific Data (Nature Publishing Group)	Apr 2019 - onwards
U Bremen Excellence Chair (Dept. of Physics, Dept. of Mechanical Engineering)	Jan 2019 - onwards
Scientific Advisory Board, Villum Center for the Science of Sustainable Fuels and Chemicals (Denmark)	Aug 2016 - onwards
Chair, Psi-k Charity and Board of Trustees (UK)	Jan 2018 - Dec 2020
Scientific Advisory Board, Department of Materials, Imperial College (UK)	Sep 2011 - Aug 2022
Trustee, Psi-k Charity (UK)	Jan 2011 - Dec 2023
Chair, CCP9 (Collab. Comp. Project, Electronic Structure of Condensed Matter, UK)	Feb 2010 - Aug 2011

6. Institutional responsibilities at EPFL

Member, EPFL SCITAS CoDir Committee	Sep 2018 - onwards
Chair, EPFL HPC CoPil Committee	Mar 2016 - Jun 2018
Member, EPFL HPC CoPil Committee	Oct 2011 - Feb 2016
Chair, EPFL ACCES Committee	Apr 2012 - Mar 2022
Member, EPFL Research Commission	Apr 2012 - Jun 2018

7. Recent research funding (active in 2021 or later; summarizes funding for PI at EPFL)

- Horizon Europe, *Developing New 2D Materials and Heterostructures for Printed Digital Devices* (2 postdocs 2023-26)
- EPFL *Energy-efficient carbon capture, utilisation and storage for a sustainable and circular economy* (1 postdoc 2023-25)
- SNSF/Belgium Weave, *In search of the electron-phonon gems* (1PhD 2023-27)
- Samsung GRO, *Electronic-structure of 2D heterostructures from the equivariant machine learning of Wannier Hamiltonians* (1 postdoc 2023-25)
- EPFL Quantum Science and Engineering, *Many-body neural simulations of quantum materials* (1 postdoc 2023-25)
- LUMI-G/CSCS (GPU time only, 1.3M node hours), *Turning up the heat on computational materials discovery: high-throughput screening of novel Li-ion cathodes at finite temperature* (2023-24)
- SNSF, *Accurate and efficient electronic-structure functionals for energies and spectra of materials* (2 postdocs and 2 PhD students, 2022-26)
- Horizon Europe MaX, *Centre of Excellence for e-Infrastructure – Materials Design at the Exascale* (@ UBremen), 2 postdocs (2023-26)

- H2020 EPFLeaders4impact, *A computational platform for the prediction and intensification of (electro)sorption processes applied to environmental services* (1 postdoc (40% contribution), 2023-2026)
- Solvay, *The microscopic structure of interfaces in solid-state batteries* (1 postdoc 2022-24)
- EPFL Platform, *Supporting the analysis of XPS data by quantum chemistry: making simulated photoelectron spectra routine* (1 postdoc 2022-23)
- BIG-MAP Stakeholders, *Autonomous robotic battery innovation platform (Aurora)* (1 postdoc 2022-23)
- NCCR Catalysis, *Development and open-access deployment of first-principles operando spectroscopies* (1 postdoc, 2022-24)
- PASC ETH, *Spectral properties of materials on accelerated architectures* (2 postdocs, 2021-24)
- EPFL/UM6P Excellence in Africa, *Embedded exact quantum dynamics for photocatalytic water splitting* (1 PhD student, 2021-26)
- Marie Skłodowska-Curie Postdoctoral Fellowship, *Thermoelectricity in metal-organic perovskites: recycling waste energy heat as electricity* (Lorenzo Monacelli, 2022-24)
- NCCR Catalysis, *Development and open-access deployment of first-principles operando spectroscopies* (1 postdoc, 2021-24)
- CSCS (CPU time only, 44.2M core hours/year), *Materials for energy* (2021-24)
- Bosch Research Foundation, *Workflow and algorithms for modeling strongly correlated electrons on a near-term quantum computer* (1 PhD student, 2020-24)
- H2020 NEP, *Nanoscience Foundries and Fine Analysis* (1 postdoc, 2020-25)
- H2020 DOME, *Digital Open Marketplace Ecosystem 4.0* (1 postdoc, 2020-24)
- H2020 OpenModel, *Integrated Open Access Materials Modelling Innovation Platform for Europe* (1 postdoc, 2020-24)
- H2020 BIG-MAP, *Battery Interface Genome – Materials Acceleration Platform* (2 postdocs, 2020-23)
- PRACE (CPU time only, 70.0M core hours), *The electronic-structure genome of materials* (2020-21)
- Samsung GRO, *The dielectric response of complex oxides* (1 postdoc, 2019-21)
- SNSF Sinergia, *Hydronics* (2 PhD students, 2020-24)
- University of Bremen, *Excellence Chair* (3 postdocs and 1 PhD students, 2019-23)
- H2020 Intersect, *Interoperable Material-to-Device simulation box for disruptive electronics* (2 postdocs, 2019-22)
- Solvay, *Design and Discovery of Novel Materials for Solid-State Batteries* (2 postdocs, 2019-21)
- Swissuniversities, *Materials Cloud* (1 postdoc, 2019-21)
- H2020, *Materials modelling marketplace for increased industrial innovation* (2 postdocs, 2018-22)
- Marie Skłodowska-Curie Postdoctoral Fellowship, *Spin-electron-phonon in 2D materials* (Samuel Poncé, 2019-21)
- SNSF, *Accurate and efficient electronic-structure functionals for energies and spectra of materials* (1 postdoc and 2 PhD students, 2018-22)
- H2020 EPFL Innovators, *Engineering novel quantum devices* (Francesco Libbi, 2018-22)
- PASC ETH, *Development and optimization of the domain-specific SIRIUS library* (2 postdocs, 2016-21)
- H2020 MaX, *Centre of Excellence for e-Infrastructure – Materials Design at the Exascale* (3 postdocs, 2015-18; 2019-21)
- SNSF NCCR MARVEL, *Computational design and discovery of novel materials*, 48.3M CHF in total, 2014-18, 2018-22, 2022-26

8. Supervision of junior researchers at EPFL (PhDs first, then postdocs, including following employment)

For a full list of former group members see http://theossrv1.epfl.ch/Main/People. **PhDs at EPFL:** Daniele Dragoni, U. of Milano Bicocca (PhD 2011-2016), Andrea Cepellotti, UC Berkeley (PhD 2011-2016), Anand Chandrasekaran, Georgia Tech (PhD 2011-2016), Gianluca Prandini, EPFL (PhD 2014-2019), Leonid Kahle, EPFL (PhD 2015-2019), Matthieu Mottet, IBM (PhD 2015-2019), Pablo Piaggi, Princeton U. (PhD 2015-2019), Antimo Marrazzo, EPFL (PhD

2015-2019), Michele Simoncelli, EPFL (PhD 2016-2021), Mohammad Tohidivahdat (PhD 2017-2022), Riccardo de Gennaro (PhD 2018-2022), Francesco Libbi, Harvard U. (PhD 2018-2022), Norma Rivano, Harvard U. (PhD 2018-2022), Tommaso Chiarotti, EPFL (PhD 2018-2023), Luca Binci, UC Berkeley (PhD 2019-2023), Junfeng Qiao (2019-to date), Chiara Cignarella (2020-to date), Fatemeh Haddadi (Feb 2020-to date), Austin Zadoks (Oct 2020-to date), Changpeng Lin (Oct 2020-to date), Mario Caserta (Nov 2020-to date), Marija Stojcovich (Jan 2021-to date), Enrico Di Lucente (Mar 2021-to date), Alessandro Carbone (Oct 2021-to date), Andrea Fedrigucci (Dec 2021-to date), Tushar Thakur (July 2022-to date), Aleksandr Poliukhin (Aug 2022-to date), Guoyuan Liu (Apr 2023-to date), Luca Righetti (Sep 2023-to date), Matteo Quinzi (Jan 2024-to date) **Postdocs at EPFL:** David D. O' Regan, Trinity College Dublin (2011-13), Giovanni Borghi, University of Modena and Reggio Emilia (2012-15), Giovanni Pizzi, PSI (2012-2022), Emine Kucukbenli, SISSA (2012-14), Ngoc Linh Nguyen, U. of Chicago (2012-17), Marco Gibertini, University of Geneva (2013-18), Riccardo Sabatini, Craig Venter Institute (2013), Matteo Cococcioni, U. of Pavia (2013-2018), Ivano Castelli, Copenhagen U. (2014-15), Oliviero Andreussi, UNT (2015-17), Nicolas Mounet, CERN (2015-18), Nicola Colonna, PSI (2014-19), Aris Marcolongo, IBM (2015-17), Martin Uhrin, DTU (2015-2019), James Moraes de Almeida, U. Sao Paulo (2015-17), Spyros Zoupanos, Ioanian University (2015-29), Iurii Timrov (2016-to date), Davide Campi, University of Milano Bicocca (2016-20), Thibault Sohier, CNRS (2016-19), Nicolas Hoermann, TU Munich (2016-19), Fernando Gargiulo, ENEL (2016-17), Sebastiaan Huber, NCCR Catalysis (2016-2020), Robert Baldock, Google (2016-19), Giuliana Materzanini, UC Louvain (2017-2021), Francesco Nattino, Amsterdam eScience (2017-19), Conrad Johnston, Queen Mary University (2018-19), Marco Vanzini, College Champittet (2018-2021), Casper Anderson, SINTEF (2018-2021), Daniele Tomerini (2019-20), Loris Ercole, Microsoft Research (2019-2022), Francisco Ramirez (2019-2023), Sokseiha Muy (2019-2023), Michele Kotiuga (2019-2023), Du Dou (2019-2022), Simon Adorf, Nvidia (2019-2022), Francesco Aquilante (2019-2022), Edward Linscott (2019-to date), Samuel Poncé, UC Louvain (2019-2021), Antimo Marrazzo, University of Trieste (former PhD, 2019-20), Leonid Kahle, IBM (former PhD, 2020), Davide Grassano, CECAM (2020-2024), Marnick Bercx, PSI (2020-2023), Christopher Sewell (2020-2023), Flaviano Jose dos Santos, PSI (2020-2022), Giovanna Lani (2020-to date), Michele Simoncelli, University of Cambridge (former PhD, 2021), Martin Uhrin, U. of Grenoble (2021-2023), Louis Ponet (2021-to date), Jusong Yu, PSI (2021-2022), Lorenzo Monacelli, U. of Roma La Sapienza (2022-2023), Mouyi Weng (2022-to date), Giannis Savva (2022-to date), Riccardo De Gennaro (former PhD, 2022-2023), Francesco Libbi, Harvard U. (former PhD, 2022-2023), Giovanni Cistaro (2022-to date), Nicephore Bonnet (2023-to date), Tommaso Chiarotti (former PhD, 2023-to date).

43 members of the group have moved to faculty (33) and research positions worldwide, including MIT (Heather Kulik), Harvard University (Boris Kozinsky), Penn State (Ismaila Dabo, Mikael Rechtsmann), Imperial College (Arash Mostofi), King's College London (Francesca Baletto, Nicola Bonini), Trinity College Dublin (David O'Regan), EPFL (Michele Ceriotti, Philippe Schwaller), U. of Modena (M. Gibertini), SISSA (A. Marrazzo), U. of Roma La Sapienza (Lorenzo Monacelli), and Seoul National University (Cheol-Hwan Park); http://theossrv1.epfl.ch/Main/Mentoring. In particular, 5 former students or postdocs have been awarded the NSF CAREER Award: Matteo Cococcioni (U. of Minnesota), Ismaila Dabo (Penn State), Heather Kulik (MIT), Oliviero Andreussi (UNT), Xiaofeng Qian (Texas A&M).

9. Teaching Activities

Every Fall: Fundamentals of solid-state materials (4 credits, core MSc class)
Every (other) Spring: Atomistic and quantum simulations of materials (4 credits, elective MSc and PhD)

10. Invited talks and seminars

575 invited talks and seminars (up to Jan 2024), including 35 invited talks at the annual meetings of the:

- American Physical Society (9 in total: 03/99, 03/02, 03/06, 03/13, 03/15, 03/17, 03/19, 03/22, 03/24)

- Materials Research Society (18 in total: 12/04, 12/05, 12/07 (Bonini), 04/09 (2), 04/10, 04/11, 04/12, 04/14, 11/15, 03/16, 04/19, 04/20 (2, cancelled), 04/21 (3), 04/23)
- American Chemical Society (8 in total: 08/01, 04/02, 03/07 (Sit), 08/07 (Dabo), 04/14, 04/19 (2), 08/24)

11. <u>Memberships in panels, boards</u>

Board of Trustees: Psi-k (2011-2023; 2018-20 also Chairperson). *Scientific Advisory Boards:* Psi-k (2005-onwards); International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods (2007-2018); ASESMA African School on Electronic Structure Methods and Applications (2010-onwards), Department of Materials, Imperial College (2011-2022), Midwest Integrated Center for Computational Materials (2016-onwards; Chair from 2020), The Villum Center for the Science of Sustainable Fuels and Chemicals (2016-onwards). *Principal Founding Editor:* MRS Communications (2011-16, for Theory and Simulation of Materials). *Editorial Board:* Scientific Data (Nature Publishing Group, 2016 – onwards; from 2019 Senior Editor), Advanced Functional Materials (Wiley, 2018 – onwards), PRX Energy (APS, 2021 - onwards), IFIMAC (UAM Spain, 2022 - onwards), DIADEM (CNRS France, 2023 - onwards)

12. <u>Active memberships</u> APS (Lifetime member), ACS, MRS, Swiss Physical Society.

13. <u>Organization of conferences (27 in total)</u>

13th Annual Workshop on Electronic Structure Algorithms, Princeton (2001), NSF Summer School on Ab-initio Molecular Dynamics, University of Illinois Urbana-Champaign (2006), Conference Chairperson, 13th International Workshop on Computational Physics and Materials Science, ICTP Trieste (2007), Roberto Car 60th birthday symposium, ICTP Trieste (2007), CECAM Workshop and Tutorial on Maximally localized Wannier functions, Lyon (2007), Classical and Quantum Approaches in Molecular Modeling, IMA, University of Minnesota (2007), First East African School of Computational Materials Science, Addis Ababa (2008), NSF-ICMR Summer School on Quantum Simulations, UCSB Santa Barbara (2009), ICTP/Psi-k/CECAM College on Computational Nanoscience, ICTP Trieste (2010), CECAM Workshop on Electronic-structure challenges in materials modeling for energy applications, Lausanne (2010), CCP9/Psi-k/CECAM Biennial Graduate School on Electronic Structure Methods, Oxford (2011), DPG Symposium on Discovery of Novel Functional Materials, Regensburg (2013), Materials discovery from First-principles modeling, EUROMAT, Sevilla (2013), Symposium on Computational Materials Science, Africa MRS, Addis Ababa (2013), ICTP/Psi-k/CECAM Workshop on Total Energy and Forces, Lausanne (2014), Psi-k/CECAM Annual Research Conference, Rational Design of Functional Materials, Berlin (2015), Psi-k/CECAM Workshop on Automated Atomistic Simulations Lausanne (2015), Psi-k 2015 – Session on Materials Design, San Sebastian (2016), PASC16, Platform for Advanced Scientific Computing, Lausanne (2016), ASESMA 2016, Accra (2016), CECAM Lorenz OptiMaDe, ICTP/Psi-k/CECAM Advanced Workshop on High-performance and High-throughput Simulations using Quantum ESPRESSO, ICTP Trieste (2017), CECAM OptiMaDe (2018), CPMD2019 (2019), African MRS – Computational Materials Science (2020), Psi-k 2020 (chairperson, 2022, 1300+ in-person attendees), Psi-k CECAM Research Conference 2024 - Electronic-structure simulations for large-scale facilities: Opportunities, challenges, and roadmaps (2024).

14. <u>Prizes, awards, fellowships</u>

Clarivate Highly Cited Researcher (2018, 2019, 2023), PRACE HPC Excellence Award (2022), IBM Faculty Award (2018), Best Teacher, EPFL IMX (2018), Visiting Professor, U. La Sapienza (2017), Fellow, American Physical Society (2014), RP Feynman Chair of Nanoscience, U. of Addis Ababa (2008), Professeur Invité, Université Pierre et Marie Curie (2006). Among his group, Andrea Cepellotti was awarded the 2018 Nicholas Metropolis Award of the American Physical Society for outstanding doctoral thesis in computational physics and the 2017 EPFL IBM Prize; Giovanni Pizzi the 2020 Rodolphe and Renée Haenny Foundation Prize; Michele Simoncelli the 2020 Chorafas

Foundation Award, the 2022 EPFL Doctorate Award (for the top 2 or 3 PhDs across the entire University), and the 2023 Swiss Physical Society COMSOL Award for Computational Physics; Antimo Marrazzo the 2021 René Wasserman Award; Pablo Piaggi the 2021 EPFL IBM Prize; and 5 former group members (Matteo Cococcioni, Ismaila Dabo, Heather Kulik, Oliviero Andreussi, and Xiaofeng Qian) received in the US the NSF CAREER Award.