

Paolo Restuccia

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Research Experience and Education

- Oct 2026
(officially appointed) **Fixed-term Researcher in Tenure Track**
Dipartimento di Fisica e Astronomia, Università di Bologna, Italy
Activity: Advancing materials for tribology applications by *in silico* experiments based on machine learning molecular dynamics
- Aug 2022 – Sep 2026 **RTD-A (Junior Assistant Professor)**
Dipartimento di Fisica e Astronomia, Università di Bologna, Italy
Activity: Coordination and support of *ab initio* and machine learning-based molecular dynamics simulations to investigate the adhesion and friction properties of lubricant additives within metallic interfaces, as well as the catalytic reactions leading to carbon nanotube formation over iron nanoparticles at the atomistic scale
- Feb 2019 – Apr 2022 **PostDoc Research Associate**
Department of Chemistry, Imperial College London, UK
Activity: Development of a theoretical model for corrosion scale formation through *ab initio* simulations. Creation of a machine learning-based predictive model for the adsorption and catalytic properties of molecule-surface systems from *ab initio* databases
- Feb 2017 – Feb 2019 **PostDoc Research Associate**
Dipartimento FIM, Università di Modena e Reggio Emilia, Italy
Activity: Performing static and dynamics *ab initio* and multiscale simulations of layered materials and lubricant additives to uncover the microscopic mechanisms governing their tribological behaviour. Development of a computational workflow for materials design aimed at surface and interface optimization
- Jan 2014 – Dec 2016 **PhD in Physics and Nanoscience**
Dipartimento FIM, Università di Modena e Reggio Emilia, Italy
Thesis title: *Multiscale modelling of tribological systems: adsorbed monolayer and carbon-based materials*
- Nov 2013 – Jan 2014 **Research Fellow**
CNR Istituto di Nanoscienze S3, Italy
Activity: Molecular dynamics simulations based on *ab initio*-derived potentials to understand the atomistic mechanisms of xenon slippage over gold and graphene surfaces
- Oct 2010 – Apr 2013 **Master Degree in Physics** Final mark: 110 (out of 110)
Università di Modena e Reggio Emilia, Italy
Thesis Title: *Friction phenomena in the sliding of molecular layers between metallic surfaces*

Sep 2007 – Oct 2010 **Bachelor Degree in Physics** Final mark: 110 cum laude (out of 110)
Università di Modena e Reggio Emilia, Italy
Thesis Title: *Plasmonic interaction in the Ag/MgO system*

Participation in National and International Research groups

- Oct 2025 – : Team member of the EIC Pathfinder Challenged project MOJITO as support in coordinating WP4 (PI: Dr. Diego Marazza)
- Aug 2022 – Oct 2025: Team member of the ERC Consolidator Grant “SLIDE” project as support in coordinating the activities involving molecular dynamics simulations (PI: Prof. Clelia Righi)
- Feb 2019 – Apr 2022: Team member of the bp-ICAM 56 project as PostDoc Research Associate (PI: Prof. Nicholas Harrison)
- Jan 2014 – Feb 2019: Member of the Tribogy Research Group at the University of Modena (Coordinator: Dr. Clelia Righi)

Oral presentations at Conferences

- 8th Multiscale Materials Modeling Conference, Dijon, France (2016)
- 10th European Solid Mechanics Conference, Bologna, Italy (2018)
- 45th Leeds-Lyon Symposium on Tribology, Leeds, UK (2018)
- Materials.it, Bologna, Italy (2018)
- MM-Hub++ Conference, virtual (2021)
- BP-ICAM Annual Conference, virtual (2021)
- EMMC18, Oxford, UK (2022)
- 48th Leeds-Lyon Symposium on Tribology, Leeds, UK (2023)
- [CMT@Brixen](#) 2024, Brixen, Italy (2024)
- 49th Leeds-Lyon Symposium on Tribology, Lyon, France (2024)

National Scientific Qualification (Abilitazione scientifica nazionale)

- Dec 2023 – present: Qualification for Associate Professorship in Theoretical Physics of Matter (Sector 02/B2)

Teaching

- 2026 – present: Lecturer and Marking for the Bachelor Degree in Industrial Chemistry and Technologies of Materials (course in Physics) at Università di Bologna (academic year 2025/2026)
- 2025 – present: Lecturer and Marking for the Bachelor Degree in Materials Science (course in Materials for Energy) at Università di Bologna (academic year 2025/2026)
- 2025 – present: Lecturer for the Professional Master programme in High Performance and Quantum Computing (course in Materials Modelling and Design) at Università di Bologna (academic years 2024/2025 and 2025/2026)
- 2024–2026: Lecturer in Computational Materials for the PhD courses in Physics (academic years from 2023/2024 to 2025/2026) and Nanoscience for Medicine and the Environment (academic year 2024/2025 and 2025/2026) at Università di Bologna
- 2023–2025: Lecturer and Marking for the Bachelor Degree in Natural Sciences (course in Physics) at Università di Bologna (academic years 2023/2024 and 2024/2025)
- 2021–2022: Lecture and Marking for the Master Degree course in Nanomaterials at Imperial College

- MSc 2020–2022 (CRYSTAL17 School): Tutoring on Magnetic Properties
- 2019–2022: Computational Lab, Math and Solid, Liquid and Interfaces exercise tutoring activity for Chemistry Bachelor Degree students at Imperial College
- 2013–2018: Exercise tutoring activity for Chemistry and Engineering Bachelor Degree students (course in Physics) at Università di Modena e Reggio Emilia

Supervision

- 2023 – present: Co-supervision of one PhD, four Master and two Bachelor thesis projects at Università di Bologna
- 2019–2020: Co-supervision of two Bachelor thesis projects at Imperial College
- 2017–2018: Co-supervision of one Master thesis project at Università di Modena e Reggio Emilia

Institutional activities

- 2025: Member of the PhD admission committee – 41st cycle, academic year 2025/2026 at Università di Bologna, Department DIFA
- 2025 – present: Member of the OPH Computing Cluster Management Committee at Università di Bologna, Department DIFA

Funding Secured

- 2025: PI of the EuroHPC AI for Science and Collaborative project “Towards a sustainable lime production through machine learning molecular dynamics simulations”. HPC budget: 2.399.040 CPU-h (HPC resources at CINECA, Italy)
- 2025: “Bando Strutture” from University of Bologna – Co-author and team member in the proposal selected to fund the Department's Summer School organization. Total budget: €20k
- 2025: EIC Pathfinder Challenges project MOJITO (Grant number: 101221957) – Co-author and Research Team Member: project writing and proposal development. Total budget: €2.2M
- 2025: Co-PI of the EuroHPC AI and Data-Intensive Applications project “Active Learning for Efficient and Scalable Dataset Creation for Large-Scale Atomistic simulations”. HPC budget: 1.600.000 CPU-h (HPC resources at CINECA, Italy)
- 2023: Co-PI of the EuroHPC Extreme Scale Access project “From methane and iron nanoparticles to “Turquoise” H₂ and carbon nanotubes: simulating the whole catalytic process inside a reactor”. HPC budget: 20.468.000 CPU-h (HPC resources at CINECA, Italy)
- 2023: PI of a Prace-ICEI project “High throughput screening of metal-semiconductor tribological properties”. HPC budget: 807.000 CPU-h (HPC resources at CINECA, Italy)
- 2019: HPC-Europa3 travel grant for visiting Imperial College London
- PI in three Iskra B and four Iskra C projects to access CINECA HPC resources, such as:
 - ◆ 2025: PI of the Iskra C project “Machine learning-based molecular dynamics of methyl thiolate tribology at confined copper interfaces”, HPC budget: 80.000 CPU-h
 - ◆ 2024: PI of the Iskra B project “Tribochemistry of graphene interacting with iron through ab initio molecular dynamics calculations”, HPC budget: 2.000.000 CPU-h
 - ◆ 2024: PI of the Iskra C project “Database for high throughput screening of metal-semiconductor tribological properties”, HPC budget: Cloud resources (ADACloud)
 - ◆ 2018: PI of the Iskra B project “Environmental Effect on Graphene and Graphite Lubricant Properties”, HPC budget: 875.000 CPU-h
 - ◆ 2017: PI of the Iskra B project “Tribochemistry of Graphene and MoS₂ Interacting With Water”, HPC budget: 800.000 CPU-h

- ◆ 2017: PI of the Iscra C project “Graphene and MoS2 tribo-dynamics with water”, HPC budget: 100.000 CPU-h
- ◆ 2016: PI of the Iscra C project “Ab Initio Investigation of Graphene and Molybdenum Disulfide Lubricity in the Presence of Water Molecules”, HPC budget: 1.000.000 CPU-h
- ◆ 2014: PI of the Iscra C project “First Principles and Molecular Dynamics Simulations of Graphene on Fe(110) for Tribological Applications”, HPC budget: 1.000.000 CPU-h

Industrial Collaborations

- Served as project team member in industrial collaborations with Toyota (2014–2016), Total (2014–2018), BP (2019–2022) and TotalEnergies (2022–present)

Member of Editorial Journal Office and Conference Committee

- 2026: Conference Scientific Committee: FEMT Summer School – Future Energy Materials and Technology, Bologna, Italy
- 2023 – present: Editorial Office: Topical Advisory Panel Member and Guest Editor for the Special Issue “2D Materials in Tribology” on *Lubricants*, MDPI AG, ISSN 2075-4442
- 2021 – present: Editorial Office: Topical Advisory Panel Member and Guest Editor for the Special Issue “First Principles Simulation–Nano-Theory” on *Crystal*, MDPI AG, ISSN 2073-4352
- 2021: Conference Scientific Committee: MSSC 2021 - Ab initio Modelling in Solid State Chemistry, London, UK

Computational and Personal Skills

- Advanced knowledge of C, C++, Fortran and Python code programming
- Experience in MPI and OpenMP parallel code programming
- Advanced knowledge in scientific computational suites like Quantum ESPRESSO, LAMMPS, DeePMD, DP-GEN and MACE
- Languages: Italian (mother tongue), English (advanced), French and Spanish (beginner)

List of Publications

A star symbol (*) indicates the manuscript in which I am corresponding author. Up-to-date SCOPUS bibliometric indices: h-index 18; total citations 1078.

1. P. Restuccia, E. Pedretti, F. Benini, S. Loehlé, M.C. Righi, *Applied Surface Science* **733**, 166599 (2026)
2. M. Montebelli, P. Restuccia*, M.C. Righi, *Materials & Design* **259**, 114898 (2025)
3. F. Benini, P. Restuccia, E. Pedretti, M.C. Righi, *ACS Appl. Nano Mater.* **8**, 14103 (2025)
4. A. Rosenkranz, B. Wang, D. Zambrano, J.M. Henríquez, J.Y. Aguilar-Hurtado, E. Marquis, P. Restuccia, B.C. Wyatt, M.C. Righi, B. Anasori, *Mater. Today Nano* **25**, 100464 (2024)
5. F. Benini, P. Restuccia, M.C. Righi, *Appl. Surf. Sci.* **642**, 158419 (2024)
6. E. Pedretti, P. Restuccia, M.C. Righi, *Comput. Phys. Comm.* **291**, 108827 (2023)
7. G. Losi, M. Cutini, P. Restuccia, M.C. Righi, *J. Nanostructure Chem.* **13**, 497 (2023)
8. F. Benini, N. Bassoli, P. Restuccia, M. Ferrario, M.C. Righi, *Molecules* **28**, 3570 (2023)
9. P. Restuccia, G. Losi, O. Chehaimi, M. Marsili, M.C. Righi, *ACS Appl. Mater. Interfaces* **15**, 19624 (2023)
10. C. de Tomas, S. Alabidun, L. Chater, M.T. Darby, F. Raffone, P. Restuccia, H. Au, M.M. Titirici, C.S. Cucinotta, M. Crespo-Ribadenyra, *J. Phys. Energy* **5**, 024006 (2023)
11. S. Peeters, G. Losi, P. Restuccia, M.C. Righi, *Appl. Surf. Sci.* **606**, 154880 (2022)
12. P.V. Antonov, P. Restuccia, M.C. Righi, J.W.M. Frenken, *Nanoscale Adv.* **4**, 4175 (2022)
13. P. Restuccia*, E.A. Ahmad, N.M. Harrison, *Phys. Chem. Chem. Phys.* **24**, 16545 (2022)

14. K. Kousar, M. Dowhyj, M.S. Walczak, T. Ljungdahl, A. Wetzel, H. Oskarsson, A. Walton, P. Restuccia, N.M. Harrison, R. Lindsay, Faraday Discuss. **236**, 374 (2022)
15. P. Restuccia, Crystals **11**, 855 (2021)
16. K. Kousar, M.S. Walczak, T. Ljungdahl, A. Wetzel, H. Oskarsson, P. Restuccia, E.A. Ahmad, N.M. Harrison, R. Lindsay, Corros. Sci. **180**, 109195 (2021)
17. S. Peeters, P. Restuccia, S. Loehlé, B. Thiebaut, M.C. Righi, J. Phys. Chem. C **124**, 13688 (2020)
18. P. Restuccia, M. Ferrario, M.C. Righi, Comput. Mater. Sci. **173**, 109400 (2020)
19. G. Losi, P. Restuccia, M.C. Righi, 2D Mater. **7**, 025033 (2020)
20. P. Restuccia, M. Ferrario, M.C. Righi, Carbon **156**, 93 (2020)
21. S. Peeters, P. Restuccia, S. Loehlé, B. Thiebaut, M.C. Righi, J. Phys. Chem. A **123**, 7007 (2019)
22. M. Schulzendorf, A. Hinaut, M. Kisiel, R. Jöhr, R. Pawlak, P. Restuccia, E. Meyer, M.C. Righi, T. Glatzel, ACS Nano **13**, 5485 (2019)
23. G. Fatti, P. Restuccia, C. Calandra, M.C. Righi, J. Phys. Chem. C **122**, 28105 (2018)
24. P. Restuccia, G. Levita, M. Wolloch, G. Losi, G. Fatti, M. Ferrario, M.C. Righi, Comput. Mater. Sci. **154**, 517 (2018)
25. M. Wolloch, G. Levita, P. Restuccia, and M.C. Righi, Phys. Rev. Lett. **121**, 026804 (2018)
26. P. Nicolini, R. Capozza, P. Restuccia, T. Polcar, ACS Appl. Mater. Interfaces. **10**, 8937 (2018)
27. D. Marchetto, P. Restuccia, A. Ballestrazzi, M.C. Righi, A. Rota, S. Valeri, Carbon **116**, 375 (2017)
28. P. Restuccia, M. Ferrario, P.L. Silvestrelli, G. Mistura, M.C. Righi, Phys. Chem. Chem. Phys. **18**, 28997 (2016)
29. G. Levita, P. Restuccia, M.C. Righi, Carbon **107**, 878 (2016)
30. P. Restuccia, M.C. Righi, Carbon **106**, 118 (2016)

Currently, two manuscripts are **submitted** to international journals:

- i. F. Barberini, A. Barile, P. Restuccia*, P. Atanasio, D. Passeri, D. Di Tommaso, R. Mazzaro, L. Pasquini, M.C. Righi, *Dopant Redox Stability as a Design Principle for Selective CO₂ Electroreduction on Cu*, Physical Chemistry Chemical Physics
- ii. F. Benini, P. Restuccia, S. Loehlé, Q. Arnoux, M.C. Righi, *Combined ab initio and experimental study of phosphorus-based anti-wear additives interacting with iron and iron oxide*, Materials Today Nano