

Paolo Restuccia

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Summary of Research Interest

My research activity is focused on friction and corrosion reduction, through analyses of chemical and physical processes occurring at surfaces and interfaces. I have performed these studies with state-of-the-arts computational materials science approaches, namely static and dynamics first-principles simulations, classical Molecular Dynamics and Quantum Mechanics/Molecular Mechanics multi-scale approach. I have also developed workflows for high-throughput calculations to study relevant figures of merit in the adhesion and sliding of homogenous interfaces and molecular dissociation of molecules over substrates. I have recently developed a machine learning approach in the prediction of molecular adsorption and study the properties of metal-metal adhesion through high throughput calculations.

Research Experience and Education

- Aug 2022 – present **Junior Assistant Professor** in *Computational tribology*
Dipartimento di Fisica e Astronomia, Università di Bologna, Italy
- Feb 2019 – Apr 2022 **PostDoc Research Assistant** in *Computational corrosion*
Department of Chemistry, Imperial College London, UK
- Feb 2017 – Feb 2019 **PostDoc Research Assistant** in *Computational tribology*
Dipartimento FIM, Università di Modena e Reggio Emilia, Italy
- Jan 2014 – Dec 2016 **PhD in Physics and Nanoscience**
Dipartimento FIM, Università di Modena e Reggio Emilia, Italy
Project title: “*Multiscale modelling of tribological systems*”
- Nov 2013 – Jan 2014 **Temporary Research Fellow**
CNR Istituto di Nanoscienze S3, Italy
- 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*

Oral and Poster Presentations at Conference

- Poster presentation, 611. WE-Heraeus-Seminar, Bad Honnef, Germany (2016)
- Poster presentation, Gordon Research Conference: Tribology, Lewiston, USA (2016)
- Oral presentation, 8th Multiscale Materials Modeling Conference, Dijon, France (2016)
- Oral presentation, 10th European Solid Mechanics Conference, Bologna, Italy (2018)
- Oral presentation, 45th Leeds-Lyon Symposium on Tribology, Leeds, UK (2018)

- Oral presentation, Materials.it, Bologna, Italy (2018)
- Poster presentation, BP-ICAM Annual Conference, Manchester, UK (2019)
- Oral presentation, MM-Hub++ Conference, virtual (2021)
- Oral presentation, BP-ICAM Annual Conference, virtual (2021)
- Oral presentation, EMMC18, Oxford, UK (2022)

Supervision and Teaching

- 2021-2022: Lecture and Marking for the Master Degree course in Nanomaterials at Imperial College
- MSSC 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
- 2019-2020: Supervision of two Bachelor thesis projects at Imperial College
- 2017-2018: Supervision of one Master thesis project at Università di Modena e Reggio Emilia
- 2013-2018: Exercise tutoring activity for Chemistry and Engineering Bachelor Degree students at Università di Modena e Reggio Emilia

Funding Secured

- HPC-Europa3 travel grant for visiting Imperial College London in 2019
- Principal Investigator in two Iskra B and three Iskra C projects to access CINECA HPC resources
- Principal Investigator in an EuroHPC Benchmark Access

Industrial Collaborations

- Collaborations with Toyota (2014–2016) and Total (2016–2018) to study coatings for friction reduction, and with BP (2019–2022) to study corrosion reduction in pipelines

Member of Editorial Journal Office and Conference Committee

- Editorial Office: Guest Editor for the Special Issue First-Principles Simulation–Nano-Theory on *Crystal*, MDPI AG, ISSN 2073-4352
- Conference Scientific Committee: MSSC 2021 - Ab initio Modelling in Solid State Chemistry, London, UK (2021)

Personal Skills

- Languages: Italian (mother tongue), English (advanced), French and Spanish (beginner)
- Advanced knowledge of C, C++, Fortran and Python code programming
- Attended courses in MPI and OpenMP parallel code programming

List of Publications

- S. Peeters, G. Losi, P. Restuccia, M.C. Righi, *Applied Surface Science* **606**, 154880 (2022)
- P.V. Antonov, P. Restuccia, M.C. Righi, J.W.M. *Nanoscale Advances* **4**, 4175 (2022)
- P. Restuccia, E.A. Ahmad, N.M. Harrison, *Physical Chemistry Chemical Physics* **24**, 16545 (2022)
- K. Kousar, M. Dowhyj, M.S. Walczak, T. Ljungdahl, A. Wetzal, H. Oskarsson, A. Walton, P. Restuccia, N.M. Harrison, R. Lindsay, *Faraday Discussions* **236**, 374 (2022)
- G. Losi, M. Cutini, P. Restuccia, M.C. Righi, *Journal of Nanostructure in Chemistry*, in press (2022)
- P. Restuccia, *Crystals* **11**, 855 (2021)

- K. Kousar, M.S. Walczak, T. Ljungdahl, A. Wetzel, H. Oskarsson, P. Restuccia, E.A. Ahmad, N.M. Harrison, R. Lindsay, *Corrosion Science* **180**, 109195 (2021)
- S. Peeters, P. Restuccia, S. Loehlé, B. Thiebaut, M.C. Righi, *Journal of Physical Chemistry C*, **124**, 13688 (2020)
- P. Restuccia, M. Ferrario, M.C. Righi, *Computational Materials Science* **173**, 109400 (2020)
- G. Losi, P. Restuccia, M.C. Righi, *2D Materials* **7**, 025033 (2020)
- P. Restuccia, M. Ferrario, M.C. Righi, *Carbon* **156**, 93 (2020)
- S. Peeters, P. Restuccia, S. Loehlé, B. Thiebaut, M.C. Righi, *Journal of Physical Chemistry A* **123**, 7007 (2019)
- M. Schulzendorf, A. Hinaut, M. Kisiel, R. Jöhr, R. Pawlak, P. Restuccia, E. Meyer, M.C. Righi, T. Glatzel, *ACS Nano* **13**, 5485 (2019)
- G. Fatti, P. Restuccia, C. Calandra, M.C. Righi, *Journal of Physical Chemistry C* **122**, 28105 (2018)
- P. Restuccia, G. Levita, M. Wolloch, G. Losi, G. Fatti, M. Ferrario, M.C. Righi, *Computational Materials Science* **154**, 517 (2018)
- M. Wolloch, G. Levita, P. Restuccia, and M.C. Righi, *Physical Review Letters* **121**, 026804 (2018)
- P. Nicolini, R. Capozza, P. Restuccia, T. Polcar, *ACS Applied Materials and Interfaces* **10**, 8937 (2018)
- D. Marchetto, P. Restuccia, A. Ballestrazzi, M.C. Righi, A. Rota, S. Valeri, *Carbon* **116**, 375 (2017)
- P. Restuccia, M. Ferrario, P.L. Silvestrelli, G. Mistura, M.C. Righi, *Physical Chemistry Chemical Physics* **18**, 28997 (2016)
- G. Levita, P. Restuccia, and M.C. Righi, *Carbon* **107**, 878 (2016)
- P. Restuccia and M.C. Righi, *Carbon* **106**, 118 (2016)

In total, I published 21 papers, seven as first-named author. Full details of all publications at <https://orcid.org/0000-0002-0419-723X>