Paolo Restuccia

Flat 2, 10 Batoum Gardens, London W6 7QD, UK
Telephone: +44 7464 665281 Email: p.restuccia@imperial.ac.uk

Summary of Research Interest

My research activity is focused on corrosion and friction 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.

Research Experience and Education

Feb 2019 – present **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: adsorbed monolayer and carbon-based materials*"

Nov 2013 – Jan 2014 **Temporary Research Fellow**
CNR Istituto di Nanoscienze S3, Italy
Research project: *Atomistic simulations in nanostructure*

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*

Selected Publications

- ☐ K. Kousar, M. S. Walczak, T. Ljungdahl, A. Wetzel, H. Oskarsson, P. Restuccia, E. A. Ahmad, N. M. Harrison, R. Lindsay, *Corrosion inhibition of carbon steel in hydrochloric acid: Elucidating the performance of an imidazoline-based surfactant*, Corrosion Science **180**, 109195 (2021)
- ☐ P. Restuccia, M. Ferrario, M. C. Righi, *Monitoring water and oxygen splitting at graphene edges and folds: Insights into the lubricity of graphitic materials,* Carbon **156**, 93-103 (2020)

- ☐ M. Wolloch, G. Levita, P. Restuccia, and M. C. Righi, *Interfacial charge density and its connection to adhesion and frictional forces*, Physical Review Letters **121**, 026804 (2018)
- ☐ G. Levita, P. Restuccia, and M. C. Righi, *Graphene and MoS2 interacting with water: A comparison by ab initio calculations,* Carbon **107**, 878 (2016)
- ☐ P. Restuccia and M. C. Righi, *Tribochemistry of graphene on iron and its possible role in lubrication of steel*, Carbon **106**, 118 (2016)

In total, sixteen papers published, six as first-named author. Full details of all publications at https://orcid.org/0000-0002-0419-723X

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)

Supervision and Teaching

- ☐ 2021: Lecture and Marking for the MRes course in Nanomaterials at Imperial College London
- ☐ MSSC 2020: Tutoring on Magnetic Properties
- ☐ 2019-present: Computational laboratory and Math exercise tutoring activity for Chemistry Bachelor Degree students at Imperial College London
- ☐ 2019-2020: Supervision of two UROP projects at Imperial College
- ☐ 2017-2018: Supervision of one MRes 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 Iscra B and three Iscra C projects to access CINECA High Performance Computing resources

Industrial Collaborations

- ☐ Collaborations with Toyota (2014–2016) and Total (2016–2018) to study coatings for friction reduction, and with BP (2019–Present) 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 an OpenMP parallel code programming