

M. Clelia Righi

Personal information

Citizenship Italian

Marital status Married, two daughters

Address Department of Physics, Informatics and Mathematics University of Modena and Reggio Emilia, Via Campi 213/a, 41125 Modena

E-mail mcrighi@unimore.it

Orcid <http://orcid.org/0000-0001-5115-5801>

University web page <http://personale.unimore.it/rubrica/dettaglio/mcrighi>

Personal web page www.tribchem.it

Education

2004 PhD in Physics University of Modena and Reggio Emilia
Thesis: "First-principles Study on SiC Homoepitaxy"
Mark: Excellent

1998 Laurea Degree in Physics University of Modena and Reggio Emilia
Thesis: "Density Functional Theory in the Hubbard Model"
Mark: 110/110 *cum laude*

Attended international schools on computational methods in condensed matter

1. "Tutorial on **high-throughput computations**: general methods and applications using AiiDA" EPFL, Lausanne, June 22-24, 2016.
2. "**Python** Syntax", a CINECA SCAI Course, Modena 20-22 January 2016.
3. "Dynamic **QM / MM** simulations with adaptive quantum zones" ICTP, Trieste, Feb. 18-21 2013.
4. "Tutorial on **molecular dynamics simulations** in condensed matter and molecular physics" CECAM, Lyon, May 13-17, 2008.
5. "Introduction to the **C language** for scientific programming" CINECA, Bologna, November 13-14, 2006.
6. "Tutorial on **kinetic Monte Carlo**, from phase transition and crystal growth to econophysics" CECAM, Lyon, October, 14-17 2002.
7. "Application of **density functional theory** in condensed matter physics chemistry, engineering and biology" Fritz-Haber-Institute, Berlin July 23 - August 1, 2001.
8. "Introduction to **Fortran 90**" CINECA, Bologna 4-5 November 1999.
9. "VIII summer school of **parallel computing**" CINECA, Bologna September 13-24, 1999.

Career History

My research is in the field of **computational materials physics**, with focus on chemical/physical processes at **surfaces and interfaces**, recently on **adhesion, friction and tribochemistry**. It was initially conducted at the International School for Advanced Studies (SISSA) in Trieste, later at the R&D Labs of Tetra Pak SPA, CNR Institute of Nanoscience and University of Modena and Reggio Emilia (UNIMORE). More specifically:

Mar 2019 - Present	Associate Professor at UNIMORE.
Mar 2016 - Apr 2019	Assistant Professor at UNIMORE.
Dec 2014 - Feb 2016	Senior Researcher, CNR Institute of Nanoscience (CNR-NANO)
Sept 2012 - Nov 2014	Researcher, CNR-NANO
Jan. 2004 - July 2012	Post-doctoral Research Assistant, CNR-NANO and UNIMORE
Jan. 2001- Mar 2004	PhD fellow (fellowship awarded by the Italian Ministry), UNIMORE
Apr. 2000 - Dec. 2001	Research staff member at Tetra Pak, Division of Modena, Italy
Jan. 1999 - Mar 2000	Research fellow at SISSA, Trieste, Italy
Visiting stays	Imperial College, London. July – Aug 2018 and 2019 Institute for Molecules & Materials, Radboud University, Nijmegen, Dec. 2011 – Mar. 2012
Two maternity leaves	Date of birth of the first daughter 26/11/08 Date of birth of the second daughter 18/04/2011

Esteem Factors

National Scientific Habilitation	- Full Professor in Theoretical Physics of Matter (Sector 02/B2) since Aug. 2018 - Associate Professor in Theoretical Physics of Matter (Sector 02/B2) since Apr. 2017
Formal attribution of functions at international institutions	- Academic Visitor at Imperial College since June 2017 - Scientific Advisor for the industry Total Sa. Since June 2016.
Member of Editorial Boards	- Scientific Report , Springer Nature publishing Group, ISSN 2045-2322. - Lubricants , MDPI AG, ISSN 2075-4442. - Lubrication Science , Wiley, ISSN:0954-0075. - Coatings , MDPI AG, ISSN 2075-4442.

Organizer	<ul style="list-style-type: none"> - CECAM workshop “Molecular Mechanisms of Tribochemistry” 27-29 January 2020, Lausanne. - Kick-off meeting of a project with TOTAL with the participation of the Rector of the University of Modena and Reggio Emilia and Directors of the Total Industry. January 2018 - Series of seminars “Research in Physics at Unimore” for the undergraduate students of Unimore. Dec. 2017.
Technology transfer	<ul style="list-style-type: none"> - Training of researchers seconded from the industry to work at Unimore under my supervision: 1) Seiji Kajita, <i>Toyota Central R&D Labs</i> (April 2014 – April 2016). 2) Sophie Loehle, <i>Total Marketing Services</i> (Sept. 2014 – Sept. 2016).
Peer-Review	<ul style="list-style-type: none"> - Reviewer of Projects: for Israel Science Foundation (ISF), Austrian funding program (FWF), HPC international projects PRACE, HPC national projects ISCRA. - Reviewer for scientific journals: Science, Physical Review Letters, Europhysics Letters, Applied Physics Letters, Physical Review B, Journal of Applied Physics, ACS Applied Materials & Interfaces, Nanoscale, Carbon, Reviews of Modern Physics, Journal of Physics D: Applied Physics, Journal of Physics: Condensed Matter, Scientific Reports, etc..
Third Mission activity	<ul style="list-style-type: none"> - Presentation of my research activity at the “European Research Night”, Modena, Sept. 2017 and 2018. - Presentation of my research activity at “University Orientation”, an initiative for the high schools of Modena. Mar. 2017 and 2018 - Invited presentation at the initiative “We make STEM” organized within the national project Women@Work - Organization of a computational laboratory for high school students in visit at Unimore. June 2018 and 2017.
Institutional responsibilities	<ul style="list-style-type: none"> - Member of the Council of the PhD school in Physics and Nanoscience at Unimore. - Member of the committees for the Research and Third Mission at the Department of Physics, Informatics and Mathematics at the Unimore.
Highlights	<ul style="list-style-type: none"> - Publication “<i>Altering the Properties of Graphene on Cu(111) by Intercalation of Alkali Halides</i>” on ACS Nano, in press (2019) https://www.dropbox.com/s/mzxc5ugeztdkw4/Grafene%20Righi.pdf?dl=0 - Publication “Interfacial Charge Density and Its Connection to Adhesion and Frictional Forces” M. Wolloch, G. Levita, P. Restuccia, and M. C. Righi, Phys. Rev. Lett. 121, 026804 (2018) http://www.magazine.unimore.it/site/home/notizie/articolo820044153.html - Collaboration with Total http://www.magazine.unimore.it/site/home/avvisi/articolo820041805.html https://www.dropbox.com/s/2aukgojurd60cr2/Dossier%20Clelia%20Righi.pdf?dl=0 - Collaboration with Toyota

<https://www.dropbox.com/s/2dmlu16f87vc4sb/il-gruppo-toyota-stringe-una-collaborazione-con-il-fim.pdf?dl=0>

- Publication “Onset of frictional slip by domain nucleation in adsorbed monolayers” M. Reguzzoni, M. Ferrario, S. Zapperi, and M.C. Righi, PNAS 107, 1311 (2010): <https://www.pnas.org/content/107/4/1257>
http://www.lescienze.it/news/2010/02/03/news/un_modello_a_scala_atmica_dell_attrito-557184/; http://www.cnr.it/sitocnr/Highlights_view.html?id=239&id_edizione=3;
<http://www.incamper.org/public/numeri/135/67.pdf>

Teaching

The focus of my teaching activity is in Physics and Computational Material Science at all levels of studies (Bachelor, Master and PhD). Specifically:

- Lecturer at the University of Modena and Reggio Emilia, courses:
 - “**NanoMechanics**”, for degree in Physics, from a.y. 2019/2020, 32 hours per year.
 - “**Physics**”, for degree in Electronic Engineering, since a.y. 2016/17, 108 hours per year.
- Lecturer for the PhD school in “Physics and Nanoscience”, University of Modena and Reggio Emilia, course: “**(Nano)Tribology and materials to reduce friction**”.
- Lecturer of Exercises Courses at the Physics Department, University of Modena and Reggio Emilia, exercises courses in:
 - “**Laboratory of computational Physics**”, a.y. 2007/08 and 2006/07.
 - “**Solid state physics**” academic year 2005/06
 - “**Mechanics**” academic years 2002/03 and 2001/02

Supervision

20 Researchers, PostDoc, PhD and MSc Degree Students supervised.

Position	Name	Research Topic / Thesis	Period
Researcher from the Industry	Sophie Loehlé @Total	Computational design of lubricant additives	2014-2016
Researcher from the Industry	Seiji Kajita @Toyota Centrals R&D Labs	Doped DLC, <i>ab initio</i> Green’s function simulations of tribochemistry	2014-2016
Post Doc (Marie Curie fellow)	Alessandra Ciniero	Tribo-charging phenomena for energy harvesting	2017-2019
Post Doc	Michael Wolloch	High Throughput calculations of interfaces	2017-2019
Post Doc	Paolo Restuccia	QM/MM simulations of tribological interfaces	2017-2019
Post Doc	Marcello Rosini	Kinetic Monte Carlo simulations of materials growth	2009-2010

PhD	Carlos Latorre @Imperial College	Multi-scale simulations of tribological materials	2018-2021
PhD	Losi Gabriele	Computational design of materials to reduce friction	2018-2021
PhD	Stefan Peeters	Reactions activated by mechanical stresses	2017-2020
PhD	Giulio Fatti	Multiscale simulations of tribology phenomena	2016-2019
PhD	Paolo Restuccia	"Multiscale modelling of tribological systems: adsorbed monolayer and carbon-based materials"	2014-2017
PhD	Marco Reguzzoni	"Fundamental Mechanisms of Friction in Adsorbed Layers and Graphene Films by Atomistic Simulations"	2010-2013
PhD	Giovanna Zilibotti	"Tribochemistry of diamond by ab initio calculations"	2009-2012
Master	Davide Delle Ave	"Load effect on shear strength of materials. A high throughput approach"	2019
Master	Gabriele Losi	"Phosphorene a possible solid lubricant: an <i>ab initio</i> comparative study with MoS ₂ and graphene"	2018
Master	Omar Manelli	"Ab initio study of water adsorption at the (001) surface of diamond"	2009
Master	Marco Reguzzoni	"Onset of frictional slip in adsorbed monolayers"	2008
Master	Giovanna Zilibotti	"Adesion and friction of diamond interfaces in the presence of adsorbates"	2008

Contracts with industries

1. Coordinator of a research contract with **Total Marketing and Services**, Puteaux, FR, for the study of lubricant additives (24 months, on-going).
2. Coordinator of a research contract with **Toyota Central R&D Labs.**, Nagakute, Japan, for the development of a computational method to simulate tribochemical reactions (2016 - 2019).
3. Coordinator of a two-years research contract with **Toyota Central R&D Labs.**, Nagakute, Japan, for training on computational methods for tribochemistry (2014 - 2016).
4. Coordinator of two-years research contract with **Total SA**, France, for training and research on lubricant additives (2014 -2016).

5. Coordinator of three-year research contract with **Total SA**, France for the study of the mechanism of action of phosphide and sulphide in terms of reactions and friction (2012 – 2015).

Competitive research projects

1. Grant for the **CECAM workshop** “*Molecular Mechanisms of Tribochemistry and Lubrication*” in program for Jan 2020.
2. Coordinator of the project of the **Emilia Romagna Region** “*Education to research*”. Grant: **three-year PhD scholarship** (AA 2018/19 – 2020/21).
3. Coordinator of the projects “*Describing tribochemical phenomena*” and **HPC-Europa3** Transnational Access programme (April 2018 – on-going).
4. Supervisor of a **Marie Curie Individual Fellowship** (Call H2020-MSCA-IF-2017).
5. Coordinator of **Mobility Action Projects 2017-2018** within the Program for the Scientific and Cultural Collaboration of the University of Modena and Reggio Emilia with foreigner Universities.
6. Coordinator of the project for Basic Research **MIUR-FFABR** (law 11/12/16, n. 232, art.1).
7. Coordinator of the project **Fondo di Ateneo per la Ricerca** (FAR) “Understanding tribological phenomena in solid lubricants” (a.a. 2016-17).
8. Coordinator of the European Project “Ab initio molecular dynamics simulations of iron lubrication”, 16th Preparatory Access call, Partnership for Advance Computing in Europe (**PRACE**). (2018)
9. Coordinator of the Task *Computational protocol for friction and tribochemistry* within the **MaX, European Center of Excellence (H2020, 2015-2017)**.
10. Coordinator of **EU DEISA Extreme Computing Initiative** (DECI Call5 2009) “*Ab initio investigation of tribochemical reactions*”.
11. Coordinator of **9 HPC-ISCRA** projects on tribochemistry granted by CINECA, Bologna Italy.
12. Coordinator of **6 INFM Supercomputing** projects granted by CINECA, Bologna, Italy

Invited presentations

1. Invited seminar at Bilkent University, Ankara Turkey. Title: *(nano)Tribology and materials to reduce friction*. May 15, 2019.
2. Invited presentation at *MRS Spring Meeting*, Phoenix Arizona April 22-26, 2019.
3. Invited to present at the CECAM workshop *Modeling tribology: friction and failure across scales*, EPFL Lausanne, January 28-30, 2019.
4. Invited talk at *Beilstein Nanotechnology Symposium 2018*, Potsdam, Germany, 2 – 4 October 2018.

5. Invited seminar at Imperial College, London. Title *Ab initio investigation of tribochemistry mechanisms in solid and boundary lubricants*, 2nd August 2018.
6. Invited talk at the conference *From Electron to Phase Transition*, Wien 4-6 April 2018.
7. Invited talk at the conference *255th ACS National Meeting & Exposition*, New Orleans, 18-22 March 2018.
8. Invited talk at *MaX International Conference 2018*, Trieste 29-31 January 2018.
9. Invited talk at the *Course on Industrial Tribology*, Brescia 6 November 2017.
10. Invited talk at the *64th AVS International Symposium*, Tampa, Florida, USA 29 Oct – 3 Nov 2017.
11. Invited talk at *Ecotrib Conference*, Ljubljana 7-9 June, 2017.
12. Invited seminar at the Physics Department, Basel University, Switzerland Title: “*Ab initio investigation of tribochemistry mechanisms in solid lubricants and nanotribology phenomena in adsorbed layers*” March 2017
13. Invited talk at the Lorentz Center Workshop *Micro/Nanoscale Models for Tribology (μ/n -Tribo-Models)*, Leiden, Holland 30 January – 3 February 2017.
14. Invited talk at the conference *Second International Workshop on Understanding and Controlling Nano and Mesoscale Friction*, Riga, Latvia July 4-7, 2016.
15. Invited talk at the conference *Mechanisms of Tribology*, Physikzentrum Bad Honnef, March 29 – April 1, 2016.
16. Invited talk at the conference *Tribochemistry Forum*, Nikko, Japan, September 13-15, 2015.
17. Invited talk at the *International Tribology Congress*, Tokyo, Japan, September 16-20, 2015.
18. Invited talk at the conference *Chemical Foundations of Tribology* 248th ACS National Meeting & Exposition, San Francisco, US, August 10-14, 2014.
19. Invited talk at the *Tribology Gordon Research Conference*, Boston, USA, July 20-25, 2014.
20. Invited talk at the *International Conference on Metallurgical Coatings and Thin Films*, San Diego, USA, April 28 - May 2, 2014.
21. Invited talk at the conference *TriboLyon 2013*, Lyon, France, September 4-6, 2013.
22. Invited to present at CECAM workshop *Materials chemomechanics at the atomic scale: modelling and experiments*, Lausanne, Switzerland, April 29 - May 2, 2013.
23. Invited talk at the ECI conference, *Advances in Lubrication: Linking Molecular, Meso and Machine scales*, Puntarenas, Costa Rica, January 8-13, 2012.
24. Invited seminar at the Institute for Molecules and Materials, Radboud University Nijmegen, The Netherlands. Title: “*Ab initio simulations of tribochemical reactions at diamond surfaces interacting with water*”. Dec. 2012
25. Invited seminar at CNR-S3, Modena. Title: “*Microscopic investigation of frictional behaviors in realistic systems*”. December 2010
26. Invited seminar at Physikalisches Institut, Georg-August-Universität Göttingen. Title: “*Combined ab initio and classical molecular dynamics simulations of the tribological properties of sliding monolayers*”. January 2008.

27. Invited seminar at Laboratoire de Tribologie et Dynamique des Systemes, Ecole Centrale de Lyon. Title: "*Tribological properties of adsorbed layers*". May 2007.
28. Invited talk at the XXII Conference on *Theoretical Physics and Condensed Matter*, April 2004, Fai della Paganella, Italia.
29. Invited seminar at the Physics Department, University of Modena and Reggio Emilia "*Stati di superficie ed affinita' elettronica negativa nel polietilene*". May 2002.

Other contributions at conferences

1. "16th International Conference on Nanoscience and Nanotechnologies", Salonicco (Greece) 2-5 July 2019. Oral contribution.
2. "Ecotrib 2019: European conference on Tribology", 12-14 June 2019. Oral contribution.
3. "The 10th European Solid Mechanics Conference, Bologna 2-6 July 2018. Oral contribution.
4. "International Tribology Conference", Hiroshima (Japan), 31 Oct – 4 Nov. 2011. Oral contribution.
5. "MMM2010 Multiscale Materials Modeling", Freiburg (Germany), 4-8 Oct 2010. Oral contribution.
6. "ECOSS 27 European Conference on Surface Science", Groningen (the Netherlands), 29 Agosto - 3 Settembre 2010. Oral contribution.
7. "Ecole de Cargese 2010: Theoretical modeling & experimental simulation in tribology" Cargese, France, 22-26 (2010). Poster contribution.
8. "Diamond 2009", Athens (Greece), 6-10 Settembre 2009. Oral contribution.
9. "ECOSS, 26nd European Conference on Surface Science", Parma (Italy), 30 Aug.-4 Sept. 2009. Oral contribution.
10. "Multiscale approach to nanomechanics", CECAM, Lyon (France), 5-7 Feb. 2007. Poster contribution.
11. "Nanotribology meeting", Modena (Italia), 3-4 Nov. 2006. Poster contribution.
12. "5th ESF-Nanotribology Workshop", Antalya (Turkey), 23-27 Sept. 2006. Poster contribution.
13. "Gordon Research Conference on Tribology", Waterville (Maine, USA), 18-23 June 2006. Poster contribution.
14. "MRS Fall meeting", Boston (USA), 1-5 Dicembre 2003. Contributo orale.
15. "ECOSS, 22nd European Conference on Surface Science", Praha (Czech Republic), 7-12 Sept. 2003. Oral contribution.
16. "INFMeeting 2003", Genova (Italia), 23-25 Giugno 2003. Poster contribution.
17. "III SiC Workshop", Chivasso (Torino, Italia), 28-29 Marzo 2003. Poster contribution.
18. "Si Workshop 2003", Genova (Italia), Febbraio 2003. Oral contribution.
19. "XI International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods" ICTP, Trieste (Italia), 16-18 Jan. 2003. Poster contribution.
20. "INFMeeting 2002", Bari (Italia), 24-28 Giugno 2002. Contributo poster

21. "II National workshop on Silicon Carbide" CNR-MASPEC, Parma (Italia), 18-19 March 2002. Oral contribution.
22. "XXI Convegno Fisica teorica e struttura della materia", Fai della Paganella (Trento, Italia), 21-2 Marzo 2002. Poster contribution.
23. "Conference on Computational Physics", Aachen (Germany), 5-8 Sept. 2001. Poster contribution.
24. "INFMeeting 2001" Roma (Italia), 18-22 Giugno 2001. Poster contribution

Research interests

Multi-scale Approach to Material Function

I have experience in the computational study of materials function in multidisciplinary fields, particularly in: tribology, electronics, catalysis, and crystal growth. I have applied several (linked) methods to study the materials behaviour on different time and length scales. They include molecular dynamics (*ab initio*, classical and based on Green Functions), QM/MM, Transition-State methods, kinetic Monte Carlo.

Ab initio study of Surfaces/interfaces and High Throughput

I have experience in Density Functional Theory (DFT) calculations of structural and electronic properties of surfaces/interfaces, nanoscale systems such as graphene and other 2D materials, atoms/molecules-adsorption. Recently I developed a protocol to calculate the adhesive and shear strength of solid interfaces by first principles calculations and supervised its implementation as a workflow, based on the Aiiida platform, to apply it in a high throughput way.

Scientific publications

Author of two book chapters and 51 articles published in peer review journals and 4 additional papers under review, h-index 20. I have conceived and written most of the published works, as indicated by the position of my name in the author list and by the fact that I have been the corresponding author of almost all the publications. My work is published in major international journals in the fields of condensed matter physics, nanoscience, computational material science, physical chemistry, tribology and lubrication. The top publications include (in parenthesis the current journal impact factor): 1 ACS Nano (13.7), 1 PNAS (9.6), 5 Physical Review Letters (9.2), 5 Carbon (7.5), 1 Nanoscale (7.0), 6 Journal of Chemistry C (4.5), 10 Physical Review B (3.8), etc.

Book Chapters

1. M. C. Righi, Title of the Chapter: *Understanding the Tribochemistry of Lubricant Additives by Ab initio Calculations: The Case of Phosphites*. Book title: *Advanced Analytical Methods in Tribology*, ed. da M. I. De Barros Bouquet e M. Dinwiebel, Springer Nature (2018).
2. D. Ceresoli, M.C. Righi, E. Tosatti, S. Scandolo, G. Santoro, and S. Serra, Title of the Chapter: *Electron-hole Trapping and Self-Trapping in Polyethylene*. Book title: *Festschrift in Honor of F. Bassani*, ed. da G. Grosso, G. Larocca e M.P. Tosi, Scuola Normale Superiore, Pisa, (2001).

Published papers

1. Stefan Peeters, Paolo Restuccia, Sophie Loehl'e, Benoit Thiebaut, and M. C. Righi *Characterization of Molybdenum Dithiocarbamates by First Principles Calculations* J. Phys. Chem A, in printing (2019).
2. M. Schulzendorf, A. Hinaut, M. Kisiel, R. Jöhr, R. Pawlak, P. Restuccia, E. Meyer, M. C. Righi, T. Glatzel, "Altering the Properties of Graphene on Cu(111) by Intercalation of Alkali Halides", *ACS Nano*, 13, 5, 5485 (2019).
3. G. Fatti, M. C. Righi, D. Dini, and A. Ciniero *First-Principles Insights into the Structural and Electronic Properties of Polytetrafluoroethylene in Its High-Pressure Phase (Form III)* J. Phys. Chem. C, 123, 6250 (2019).
4. G. Fatti, P. Restuccia, C. Calandra and M. C. Righi, *Phosphorus adsorption on Fe(110): An ab initio comparative study of iron passivation by different adsorbates* J. Phys. Chem. C, 122, 28105 (2018).
5. M. Wolloch, G. Levita, P. Restuccia, and M. C. Righi, *Interfacial charge densities and their connection to adhesion and frictional forces*, in printing *Physical Review Letters* (2018).
6. P. Restuccia, G. Levita, M. Wolloch, G. Losi, M. Ferrario and M. C. Righi, *Ideal adhesive and shear strengths of solid interfaces: A high throughput ab initio approach*, *Computational Materials Science*, 154, 517 (2018).
7. S. Lohele' and M. C. Righi, *Ab Initio Molecular Dynamics Simulation of Tribochemical Reactions Involving Phosphorus Additives at Sliding Iron Interfaces*, *Lubricants* 6, 31 (2018).
8. G. Levita, S. Kajita, and M. C. Righi, *Water adsorption on diamond (111) surfaces: an ab initio study* *Carbon* 127, 533 (2018).
9. S. Lohele' and M. C. Righi, *First principles study of organophosphorus additives in boundary lubrication conditions: effects of hydrocarbon chain length*, *Lubrication science*. *Lubrication Science* 29, 485 (2017).

10. G. Levita and M. C. Righi, *Effects of water intercalation and tribochemistry on MoS₂ lubricity: an ab initio molecular dynamics investigation* ChemPhysChem, 18, 1475 (2017).
11. D Marchetto, P Restuccia, A Ballestrazzi, M. C. Righi, A Rota, S Valeri *Surface Passivation by graphene in the lubrication of iron: A comparison with bronze*, Carbon 116, 375 (2017).
12. Paolo Restuccia, Mauro Ferrario, Pier Luigi Sivistrelli, Giampaolo Mistura and Maria Clelia Righi, *Size-dependent commensurability and its possible role in determining the frictional behavior of adsorbed systems*, Phys.Chem.Chem.Phys., 18, 28997 (2016).
13. G. Levita, P. Restuccia and M. C. Righi *Graphene and MoS₂ interacting with water: a comparison by ab initio calculations* Carbon, 107, 878 (2016)
14. P. Restuccia and M. C. Righi *Tribochemistry of graphene on iron and its possible role in lubrication of steel* Carbon 106, 118 (2016).
15. M. C. Righi, G. Zilibotti, S. Corni, M. Ferrario, C. M. Bertoni, *First-Principle Molecular Dynamics of Sliding Diamond Surfaces: Tribochemical Reactions with Water and Load Effects*, Journal of Low Temperature Physics, Article in Press (2016).
16. M. C. Righi, S. Loehlé, M. I. De Barros Bouchet, S. Mambingo-Doumbe and J. M. Martin *A comparative study on the functionality of S- and P-based lubricant additives by combined first principles and experimental analysis* RSC Advances, 6, 47753 (2016).
17. S. Kajita and M. C. Righi, *A fundamental mechanism for carbon-film lubricity identified by means of ab initio molecular dynamics* Carbon, 103, 193 (2016).
18. S. Kajita and M. C. Righi *Insights into the tribochemistry of silicon-doped carbon based films by ab initio analysis of water/surface interactions*, Tribology Letters, 61, 17 (2016).
19. M. C. Righi, S. Loehle', M. I. de Barros Bouchet, D. Philippon and J. M. Martin *Trimethyl-phosphite dissociative adsorption on iron by combined first-principle calculations and XPS experiments*, RSC Advances 5, 101162 (2015).
20. G. Levita, E. Molinari, T. Polcar and M. C. Righi *First principles comparative study on interlayer adhesion and shear strength of transition metal dichalcogenides and graphene*, Phys. Rev. B, 92, 085434 (2015).
21. M. I. De Barros-Bouchet, M. C. Righi, D. Philippon, S. Mambingo-Doumbe, T. Le-Mogne, J. M. Martin and A. Buffet, *Tribochemistry of phosphorus additives: experiments and first-principles calculations*, RSC Advances 5, 49270 (2015).

22. M. Pierno, L. Bignardi, M.C. Righi, L. Bruschi, S. Gottardi, M. Stohr, P. Silvestrelli, P. Rudolf, and G. Mistura, *Thermolubricity of Xe monolayers on graphene*, 6, 8062 *Nanoscale* (2014).
23. G. Levita, A. Cavaleiro, E. Molinari, T. Polcar, and M. C. Righi, *Sliding properties of MoS₂ layers: Load and interlayer orientation effects*, *J. Phys. Chem. C* 118, 13809 (2014).
24. G. Zilibotti, S. Corni, M. C. Righi, *Load-induced confinement activates diamond lubrication by water*, *Phys. Rev. Letters* 111, 146101 (2013).
25. M. Reguzzoni, A. Fasolino, E. Molinari, M. C. Righi, *Frictional properties of multilayer graphene by ab initio and classical molecular dynamics calculations*, 5th World Tribology Congress, WTC 1, 744 (2013).
26. M. Reguzzoni, A. Fasolino, E. Molinari, M. C. Righi, *Potential energy surface for graphene on graphene: Ab initio derivation, analytical description, and microscopic interpretation*, *Phys. Rev. B* 86, 245434 (2012).
27. M. Reguzzoni, A. Fasolino, E. Molinari, M. C. Righi, *Friction by shear deformations in multilayer graphene*, *J. Phys. Chem. C* 116, 21104 (2012).
28. M. Reguzzoni, M. C. Righi, *Static friction by domain coalesce at critical size*, *Phys. Rev. B (RC)* 85, 201412 (2012).
29. M. I. De Barros-Bouchet, G. Zilibotti, C. Matta, M. C. Righi, L. Vandenbulcke, B. Vacher, J. M. Martin, *Friction of Diamond in Presence of Water Vapor and Hydrogen Gas. Coupling Gas Phase Lubrication and First Principles Studies*, *J. Phys. Chem. C* 116, 6966 (2012).
30. G. Zilibotti, S. Corni and M. C. Righi, *"The formation energy of dangling bonds on hydrogenated diamond surfaces: a first principle study"*, *Phys. Rev. B* 85, 033406 (2012).
31. G. Zilibotti and M. C. Righi, *"Ab Initio calculation of the adhesion and ideal shear strength of planar diamond interfaces with different atomic structure and hydrogen coverage"*, *Langmuir* 27, 6862 (2011).
32. G. Zilibotti, M. Ferrario, C. M. Bertoni and M. C. Righi, *Ab initio calculation of adhesion and potential corrugation of diamond (001) interfaces*, *Computer Physics Communications*, 182, 1796 (2011).
33. O. Manelli, S. Corni, and M. C. Righi, *Water adsorption on native and hydrogenated diamond (001) surfaces*, *J. Phys. Chem. C* 114, 7045 (2010).

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