

Guido Fratesi

CURRICULUM VITAE

INFORMAZIONI PERSONALI (NON INSERIRE INDIRIZZO PRIVATO E TELEFONO FISSO O CELLULARE)

COGNOME	FRATESI
NOME	GUIDO
DATA DI NASCITA	28 / 09 / 1978

Table of Contents

1 Education.....	2
2 Research positions held.....	2
3 Scientific output.....	3
3.1 Overview of the scientific production.....	3
3.2 Publications.....	4
3.3 Conferences and seminars.....	13
3.4 Software development.....	18
4 Coordination of research activities.....	19
5 Other scientific and organizational responsibilities.....	20
6 Research grants.....	21
7 Scientific collaborations.....	23
8 Teaching activities.....	24
8.1 Institutional courses at Universities.....	24
8.2 Supervision of students.....	25
8.3 Software tutorials.....	28
9 Evaluation of research activities.....	29

1 Education

- 2005: **Ph.D. in Physics** at the International School for Advanced Studies (SISSA), Trieste, Italy (cum laude)
Supervisor: Prof. Stefano de Gironcoli. Dissertation date: 24/10/2005. Thesis title: “Low temperature methane-to-methanol conversion on transition metal surfaces”.
Published online at: <http://hdl.handle.net/20.500.11767/4087> .
- 2002: **Master in Physics** (“Laurea quadriennale”) at the Università degli Studi di Milano-Bicocca, Milano, Italy (110/110 cum laude)
Supervisor: Prof. Gian Paolo Brivio. Dissertation date: 11/04/2002. Thesis title: “Effetti a molti corpi nel jellium semi-infinito” (Many-body effects in semi-infinite jellium).
- 1997: **High-school diploma** at Liceo Scientifico E. Medi, Senigallia, Italy (60/60).

2 Research positions held

Associate Professor (3 years):

- Since 31/03/2020
Dipartimento di Fisica, Università degli Studi di Milano
Italian scientific sectors:
SSD: FIS/03 (Fisica della Materia);
SC: 02/B2 (Fisica Teorica della Materia)

Fixed-term University researcher (RTD) (6 years total):

(*Ricercatore a tempo determinato*”, art. 24, comma 3 lettera b, Legge n. 240/2010)

- 31/03/2017 – 30/03/2020
Dipartimento di Fisica, Università degli Studi di Milano
Italian scientific sectors:
SSD: FIS/03 (Fisica della Materia);
SC: 02/B2 (Fisica Teorica della Materia)

(*Ricercatore a tempo determinato*”, art. 24, comma 3 lettera a, Legge n. 240/2010)

- 20/12/2013 – 19/12/2016
Dipartimento di Fisica, Università degli Studi di Milano
Italian scientific sectors:
SSD: FIS/03 (Fisica della Materia);
SC: 02/B2 (Fisica Teorica della Materia)

Post-doctoral research contracts (ca 7.5 years total):

(*“Assegni di ricerca”*, art. 22, Legge n. 240/2010)

- 01/05/2012 – 19/12/2013
Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca

- 01/07/2011 – 30/04/2012
Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca

(“Assegni di ricerca”, art. 51, comma 6, Legge n. 449/1997)

- 01/03/2009 – 28/02/2011
Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca
- 01/03/2007 – 28/02/2009
Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca
- 01/03/2006 – 28/02/2007
Dipartimento di Fisica, Università degli Studi di Milano

Other appointments for research collaborations:

GF also reports shorter appointments for research activities in collaboration with: Scuola Internazionale Superiore di Studi Avanzati, Trieste (2005); Università di Milano-Bicocca (2006, 2011, 2012); Università degli Studi di Milano (2011); National Research Council (CNR, 2010).

3 Scientific output





3.1 Overview of the scientific production

- **H index: 19** (Source: Web of Science, July 22nd 2023)
- **N. of citations: >24'000** (Source: Web of Science, July 22nd 2023)
- **82 research articles** published on international peer-reviewed journals with Impact Factor
- **3 book chapters**
- **4 conference papers**
- **6 international conferences organized / co-organized**
- **7 invited talks** at international conferences and workshops
- **38 oral presentations** at international conferences and workshops
- **20 invited seminars** at research institutes / Universities

“Abilitazione Scientifica Nazionale” (ASN): GF holds the National Scientific Qualification for **Full professors** in the sector 02/B2 (ASN I fascia, DM 602 29/07/2016). The qualification is valid from 11/11/2020 to 11/11/2029. All three numerical criteria are satisfied.



BANDO D.D. 2175/2018
SETTORE CONCORSUALE 02/B2
FISICA TEORICA DELLA MATERIA
CANDIDATO: FRATESI Guido - FASCIA: I

Informazioni Indicatori 	
Soglia di riferimento: 02/B2	
Indicatore 1: 25 - Indicatore 2: 648 - Indicatore 3: 14	
Indicatori del candidato:	
Indicatore 1: 55	
Indicatore 2: 14209	
Indicatore 3: 16	

3.2 Publications

Publications on peer-reviewed journals with Impact Factor

- 82) S. Achilli, D.S. Dhungana, F. Orlando, C. Grazianetti, C. Martella, A. Molle, and G. Fratesi
“Crystal phase engineering of silicene by Sn-modified Ag(111)”
Nanoscale 15, 10845 (2023)
ISSN: 2040-3372, URL and DOI: <http://dx.doi.org/10.1039/D3NR01581E>
Role of GF: Last and co-corresponding author
- 81) F. Goto, G. Perozzi, A. Calloni, G. Albani, G. Fratesi, S. Achilli, L. Duò, M. Finazzi, F. Ciccacci, G. Bussetti
“Oxygen contribution to the magnetic response of ultrathin Fe/Ni multilayers grown on Fe-p(1 × 1)O”
Appl. Surf. Sci. 606, 154735 (2022)
ISSN: 0169-4332, URL and DOI: <http://dx.doi.org/10.1016/j.apsusc.2022.154735>
Role of GF: First theoretical author
- 80) G. Albani, L. Schio, F. Goto, A. Calloni, A. Orbelli Biroli, A. Bossi, F. Melone, S. Achilli, G. Fratesi, C. Zucchetti, L. Floreano, and G. Bussetti
“Ordered assembly of non-planar vanadyl-tetraphenylporphyrins on ultra-thin iron oxide”
Phys. Chem. Chem. Phys. 24, 17077 (2022)
ISSN: 1463-9084, URL and DOI: <http://dx.doi.org/10.1039/D1CP05914A>
- 79) A. Baby, G. Marcaud, Y.J. Dappe, M. D'Angelo, J. Cantin, M. Silly, and G. Fratesi
“Phthalocyanine reactivity and interaction on the 6H-SiC(0001)-(3×3) surface by core-level experiments and simulations”
Phys. Chem. Chem. Phys. 24, 14937 (2022)
ISSN: 1463-9084, URL and DOI: <http://dx.doi.org/10.1039/D2CP00750A>
Role of GF: Last and co-corresponding author
- 78) S. Achilli, F. Tumino, A. Rabia, A. Orbelli Biroli, A. Li Bassi, A. Bossi, N. Manini, G. Onida, G. Fratesi, and C.S. Casari
“Steric hindrance in the on-surface synthesis of diethynyl-linked anthracene polymers”
Phys. Chem. Chem. Phys. 24, 13616 (2022)
ISSN: 1463-9084, URL and DOI: <http://dx.doi.org/10.1039/D2CP00730D>
- 77) S. Achilli, A. Milani, G. Fratesi, F. Tumino, N. Manini, G. Onida, and C.S. Casari
“Graphdiynes interacting with metal surfaces: first-principles electronic and vibrational properties”
2D Materials 8, 044014 (2021)
ISSN: 2053-1583, URL and DOI: <http://dx.doi.org/10.1088/2053-1583/ac26ad>
- 76) D.S. Dhungana, C. Grazianetti, C. Martella, S. Achilli, G. Fratesi, and A. Molle
“Two-Dimensional Silicene–Stanene Heterostructures by Epitaxy”
Adv. Funct. Mater. 31, 2102797 (2021)
ISSN: 1616-3028, URL and DOI: <http://dx.doi.org/10.1002/adfm.202102797>
Role of GF: Co-corresponding author
- 75) S. Achilli, N.H. Le, G. Fratesi, N. Manini, G. Onida, M. Turchetti, G. Ferrari, T. Shinada, T. Tanii, and E. Prati
“Position-Controlled Functionalization of Vacancies in Silicon by Single-Ion Implanted Germanium Atoms”
Adv. Funct. Mater. 31, 2011175 (2021)
ISSN: 1616-3028, URL and DOI: <http://dx.doi.org/10.1002/adfm.202011175>
- 74) P.-C. Lin, R. Villarreal, S. Achilli, H. Bana, M.N. Nair, A. Tejeda, K. Verguts, S. De Gendt, M. Auge, H. Hofsäss, S. De Feyter, G. Di Santo, L. Petaccia, S. Brems, G. Fratesi, and L.M.C. Pereira
“Doping Graphene with Substitutional Mn”
ACS Nano 15, 5449 (2021)
ISSN: 1936-086X, URL and DOI: <http://dx.doi.org/10.1021/acsnano.1c00139>
- 73) F. Orlando, G. Fratesi, G. Onida, and S. Achilli
“Tailoring the magnetic ordering of the Cr4O5/Fe(001) surface via a controlled adsorption of C60 organic molecules”
Phys. Chem. Chem. Phys. 23, 7948 (2021)
ISSN: 2053-1583, URL and DOI: <http://dx.doi.org/10.1039/d0cp05848c>

- 72) A. Rabia, F. Tumino, A. Milani, V. Russo, A. Li Bassi, N. Bassi, A. Lucotti, S. Achilli, G. Fratesi, N. Manini, G. Onida, Q. Sun, W. Xu, and C.S. Casari
 “Structural, Electronic, and Vibrational Properties of a Two-Dimensional Graphdiyne-like Carbon Nanonetwork Synthesized on Au(111): Implications for the Engineering of sp-sp² Carbon Nanostructures”
 ACS Applied Nano Materials 3, 12178 (2020)
 ISSN: 2574-0970, URL and DOI: <http://dx.doi.org/10.1021/acsanm.0c02665>
- 71) G. Fratesi, S. Achilli, A. Ugolotti, A. Lodesani, A. Picone, A. Brambilla, L. Floreano, A. Calloni, and G. Bussetti
 “Nontrivial central-atom dependence in the adsorption of M-TPP molecules (M = Co, Ni, Zn) on Fe(001)-p(1x1)O”
 Appl. Surf. Sci. 530, 147085 (2020)
 ISSN: 0169-4332, URL and DOI: <http://dx.doi.org/10.1016/j.apsusc.2020.147085>
 Role of GF: First author
- 70) A. Ugolotti, G. P. Brivio, and G. Fratesi
 “Coverage-dependent electronic and optical properties of H- or F-passivated Si/Ag(111) from first principles”
 Phys. Rev. B 101, 195413 (2020)
 ISSN: 2469-9950, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.101.195413>
 Role of GF: Last author
- 69) R. Costantini, L. Colazzo, L. Batini, M. Stredansky, M.S.G. Mohammed, S. Achilli, L. Floreano, G. Fratesi, D.G. De Oteyza, and A. Cossaro
 “Keto-enol tautomerization drives the self-assembly of leucoquinizarin on Au(111)”
 Chem. Commun., 56, 2833 (2020)
 ISSN: 1359-7345, URL and DOI: <http://dx.doi.org/10.1039/c9cc09915h>
- 68) F. Otto, T. Kirchhuebel, A. Baby, F. Sojka, G. Fratesi, T. Fritz, and R. Forker
 “High Potassium Concentrations Nested in Epitaxial Monolayers of a Flexible Lander-Type Molecule on Ag(111)”
 J. Phys. Chem. C 124, 4114 (2020)
 ISSN: 1932-7455, URL and DOI: <http://dx.doi.org/10.1021/acs.jpcc.9b10560>
- 67) A. Calloni, M.S. Jagadeesh, G. Bussetti, G. Fratesi, S. Achilli, A. Picone, A. Lodesani, A. Brambilla, C. Goletti, F. Ciccacci, L. Duò, M. Finazzi, A. Goldoni, A. Verdini, and L. Floreano
 “Cobalt atoms drive the anchoring of Co-TPP molecules to the oxygen-passivated Fe(001) surface”
 Appl. Surf. Sci. 505, 144213 (2020)
 ISSN: 0169-4332, URL and DOI: <http://dx.doi.org/10.1016/j.apsusc.2019.144213>
 Role of GF: First theoretical author
- 66) A. Rabia, F. Tumino, A. Milani, V. Russo, A. Li Bassi, S. Achilli, G. Fratesi, G. Onida, N. Manini, Q. Sun, W. Xu, and C. S. Casari
 “Scanning tunneling microscopy and Raman spectroscopy of polymeric sp-sp² carbon atomic wires synthesized on the Au(111) surface”
 Nanoscale 11, 18191 (2019)
 ISSN: 2040-3372, URL and DOI: <http://dx.doi.org/10.1039/C9NR06552K>
- 65) A. Brambilla, A. Picone, S. Achilli, G. Fratesi, A. Lodesani, A. Calloni, G. Bussetti, M. Zani, M. Finazzi, L. Duò, and F. Ciccacci
 “Effects of the introduction of a chromium oxide monolayer at the C₆₀/Fe(001) interface”
 J. Appl. Phys. 125, 142907 (2019)
 ISSN: 0021-8979 / 1089-7550, URL and DOI: <http://dx.doi.org/10.1063/1.5075531>
- 64) M. Ferri, G. Fratesi, G. Onida, and A. Debernardi
 “Ab initio study of the structural, electronic, magnetic, and optical properties of silicene nanoribbons”
 Phys. Rev. B 99, 085414 (2019)
 ISSN: 1098-0121, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.99.085414>
- 63) G. Fratesi, S. Achilli, N. Manini, G. Onida, A. Baby, A. Ravikumar, A. Ugolotti, G.P. Brivio, A. Milani, and C.S. Casari
 “Fingerprints of sp¹ Hybridized C in the near-edge X-ray absorption spectra of surface-grown materials”
 Materials 11, 2556 (2018)
 ISSN: 1996-1944, URL and DOI: <http://dx.doi.org/10.3390/ma11122556>
 Role of GF: First author
- 62) M. Ferri, G. Fratesi, G. Onida, and A. Debernardi
 “Optical properties of shortest-width zig-zag silicene nano-ribbons: Effects of local fields”

61) A. Baby, H. Lin, A. Ravikumar, C. Bittencourt, H.A. Wegner, L. Floreano, A. Goldoni, and G. Fratesi
“Lattice Mismatch Drives Spatial Modulation of Corannulene Tilt on Ag(111)”
J. Phys. Chem. C 122, 10365 (2018)
ISSN: 1932-7447, URL and DOI: <http://dx.doi.org/10.1021/acs.jpcc.7b11581>
Role of GF: Last author and director of the research

60) A. Ravikumar, G. P. Brivio, and G. Fratesi
“Core Level Spectra of Organic Molecules Adsorbed on Graphene”
Materials 11, 518 (2018)
ISSN: 1996-1944, URL and DOI: <http://dx.doi.org/10.3390/ma11040518>
Role of GF: Last author and director of the research

59) A. Ravikumar, G. Kladnik, M. Müller, A. Cossaro, G. Bavdek, L. Patera, D. Sánchez-Portal, L. Venkataraman, A. Morgante, G. P. Brivio, D. Cvetko, and G. Fratesi
“Tuning ultrafast electron injection dynamics at organic-graphene/metal interfaces”
Nanoscale 10, 8014 (2018)
ISSN: 2040-3372, URL and DOI: <http://dx.doi.org/10.1039/C7NR08737C>
Role of GF: Last author and director of the research

58) M. Müller, D. Sánchez-Portal, H. Lin, G. P. Brivio, A. Selloni, and G. Fratesi
“Effect of Structural Fluctuations on Elastic Lifetimes of Adsorbate States: Isonicotinic Acid on Rutile(110)”
J. Phys. Chem. C 122, 7575 (2018)
ISSN: 1932-7447, URL and DOI: <http://dx.doi.org/10.1021/acs.jpcc.7b12821>
Role of GF: Last author and co-corresponding author

57) A. Brambilla, A. Picone, D. Giannotti, A. Calloni, G. Berti, G. Bussetti, S. Achilli, G. Fratesi, M. I. Trioni, G. Vinai, P. Torelli, G. Panaccione, L. Duò, M. Finazzi, and F. Ciccacci
“Enhanced Magnetic Hybridization of a Spinterface through Insertion of a Two-Dimensional Magnetic Oxide Layer”
Nano Lett. 17, 7440 (2017)
ISSN: 1530-6984, URL and DOI: <http://dx.doi.org/10.1021/acs.nanolett.7b03314>

56) E. Molteni, G. Fratesi, G. Cappellini, and G. Onida
“Optical Properties of Free and Si(001)-Adsorbed Pyrimidinic Nucleobases”
Physica Status Solidi (B) 1700497 (2017)
ISSN: 0370-1972, URL and DOI: <http://dx.doi.org/10.1002/pssb.201700497>

55) P. Giannozzi, O. Andreussi, T. Brumme, O. Bunau, M.B. Nardelli, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, M. Cococcioni, N. Colonna, I. Carnimeo, A.D. Corso, S. de Gironcoli, P. Delugas, R.A.D. Jr, A. Ferretti, A. Floris, G. Fratesi, G. Fugallo, R. Gebauer, U. Gerstmann, F. Giustino, T. Gorni, J. Jia, M. Kawamura, H.-Y. Ko, A. Kokalj, E. Küçükbenli, M. Lazzeri, M. Marsili, N. Marzari, F. Mauri, N.L. Nguyen, H.-V. Nguyen, A. Otero-de-la-Roza, L. Paulatto, S. Poncè, D. Rocca, R. Sabatini, B. Santra, M. Schlipf, A.P. Seitsonen, A. Smogunov, I. Timrov, T. Thonhauser, P. Umari, N. Vast, X. Wu, and S. Baroni
“Advanced capabilities for materials modelling with Quantum ESPRESSO”
J. Phys.: Condens. Matter 29, 465901 (2017)
ISSN: 0953-8984, URL and DOI: <http://dx.doi.org/10.1088/1361-648X/aa8f79>

54) A. Ugolotti, S. S. Harivyasi, A. Baby, M. Dominguez, A. L. Pinardi, M. F. López, J. A. Martín-Gago, G. Fratesi, L. Floreano, and G. P. Brivio
“Chemisorption of Pentacene on Pt(111) with a Little Molecular Distortion”
J. Phys. Chem. C 121, 22797 (2017)
ISSN: 1932-7447, URL and DOI: <http://dx.doi.org/10.1021/acs.jpcc.7b06555>

53) A. Baby, M. Gruenewald, C. Zwick, F. Otto, R. Forker, G. van Straaten, M. Franke, B. Stadtmueller, C. Kumpf, G. P. Brivio, G. Fratesi, T. Fritz, and E. Zofer
“Fully Atomistic Understanding of the Electronic and Optical Properties of a Prototypical Doped Charge-Transfer Interface”
ACS Nano 11, 10495 (2017)
ISSN: 1936-0851, URL and DOI: <http://dx.doi.org/10.1021/acs.nano.7b05828>
Role of GF: Co-corresponding author

52) A. Calloni, G. Fratesi, S. Achilli, G. Berti, G. Bussetti, A. Picone, A. Brambilla, P. Folegati, F. Ciccacci, and L.

Duò

“Combined spectroscopic and ab initio investigation of monolayer-range Cr oxides on Fe(001): The effect of ordered vacancy superstructure”

Phys. Rev. B 96, 085427 (2017)

ISSN: 1098-0121, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.96.085427>

Role of GF: First theoretical author

51) E. Molteni, G. Cappellini, G. Onida, and G. Fratesi

“Optical properties of organically functionalized silicon surfaces: Uracil-like nucleobases on Si(001)”

Phys. Rev. B 95, 075437 (2017)

ISSN: 1098-0121, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.95.075437>

Role of GF: Last author

50) P.M. Sheverdyaeva, S.Kr. Mahatha, P. Moras, L. Petaccia, G. Fratesi, G. Onida, and C. Carbone

“Electronic States of Silicene Allotropes on Ag(111)”

ACS Nano 11, 975 (2017)

ISSN: 1936-0851, URL and DOI: <http://dx.doi.org/10.1021/acsnano.6b07593>

Role of GF: First theoretical author

49) A. Calloni, G. Berti, G. Bussetti, G. Fratesi, M. Finazzi, F. Ciccacci, and L. Duò

“Electronic structure and magnetism of strained bcc phases across the fcc to bcc transition in ultrathin Fe films”

Phys. Rev. B 94, 195155 (2016)

ISSN: 1098-0121, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.94.195155>

Role of GF: Sole theoretical author

48) D. Cvetko, G. Fratesi, G. Kladnik, A. Cossaro, G.P. Brivio, L. Venkataraman, and A. Morgante

“Ultrafast electron injection into photo-excited organic molecules”

Phys. Chem. Chem. Phys. 18, 22140 (2016)

ISSN: 1463-9084, URL and DOI: <http://dx.doi.org/10.1039/C6CP04099C>

Role of GF: Co-corresponding author; first theoretical author

47) G. Di Filippo, F.O. Schumann, S. Patil, Z. Wei, G. Stefani, G. Fratesi, M.I. Trioni, J. Kirschner

“Electron coincidence studies of sulfur-overlayers on Cu(001) and Ni(001) surfaces”

J. Electron. Spectrosc. Relat. Phenom. 211, 32 (2016)

ISSN: 0368-2048, URL and DOI: <http://dx.doi.org/10.1016/j.elspec.2016.06.002>

46) D. Giofrè, D. Ceresoli, G. Fratesi, and M.I. Trioni

“Electronic transport in B-N substituted bilayer graphene nanojunctions”

Phys. Rev. B 93, 205420 (2016)

ISSN: 1098-0121, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.93.205420>

45) A. Ravikumar, A. Baby, H. Lin, G.P. Brivio, and G. Fratesi

“Femtomagnetism in graphene induced by core level excitation of organic adsorbates”

Scientific Reports 6, 24603 (2016)

ISSN: 2045-2322, URL and DOI: <http://dx.doi.org/10.1038/srep24603>

Role of GF: Last author and director of the research

44) H. Lin, G. Fratesi, S. Selçuk, G.P. Brivio, and A. Selloni

“Effects of Thermal Fluctuations on the Structure, Level Alignment, and Absorption Spectrum of Dye-Sensitized TiO₂: A Comparative Study of Catechol and Isonicotinic Acid on the Anatase (101) and Rutile (110) Surfaces”

J. Phys. Chem. C, 120, 3899 (2016)

ISSN: 1932-7447, URL and DOI: <http://dx.doi.org/10.1021/acs.jpcc.5b11885>

43) C. Zwick, A. Baby, M. Gruenewald, E. Verwüster, O.T. Hofmann, R. Forker, G. Fratesi, G.P. Brivio, E. Zojer, and T. Fritz

“Complex Stoichiometry Dependent Reordering of 3,4,9,10-Perylene Tetracarboxylic Dianhydride on Ag(111) upon K Intercalation”

ACS Nano 10, 2365 (2015)

ISSN: 1936-0851, URL and DOI: <http://dx.doi.org/10.1021/acsnano.5b07145>

42) A. Baby, H. Lin, G.P. Brivio, L. Floreano, and G. Fratesi

“Core-level spectra and molecular deformation in adsorption: V-shaped pentacene on Al(001)”

Beilstein J. Nanotechnol. 6, 2242 (2015)

ISSN: 2190-4286, URL and DOI: <http://dx.doi.org/10.3762/bjnano.6.230>

Role of GF: Last author and director of the research

41) E. Cinquanta, G. Fratesi, S. dal Conte, C. Grazianetti, F. Scotognella, S. Stagira, C. Vozzi, G. Onida, and A. Molle
“Optical response and ultrafast carrier dynamics of the silicene-silver interface”

Phys. Rev. B 92, 165427 (2015)

ISSN: 1098-0121, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.92.165427>

Role of GF: Co-corresponding author; first theoretical author

40) M. Riva, A. Picone, D. Giannotti, A. Brambilla, G. Fratesi, G. Bussetti, L. Duò, F. Ciccacci, and M. Finazzi
“Mesoscopic organization of cobalt thin films on clean and oxygen-saturated Fe(001) surfaces”

Phys. Rev. B 92, 115434 (2015)

ISSN: 1098-0121, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.92.115434>

Role of GF: Sole theoretical author

39) A. Baby, G. Fratesi, S.R. Vaidya, L.L. Patera, C. Africh, L. Floreano, and G.P. Brivio
“Anchoring and Bending of Pentacene on Aluminum (001)”

J. Phys. Chem. C 119, 3624 (2015)

ISSN: 1932-7447, URL and DOI: <http://dx.doi.org/10.1021/jp512337y>

38) G. Di Filippo, M.I. Trioni, G. Fratesi, F. Schumann, Z. Wei, C.-H. Li, L. Behnke, S. Patil, J. Kirschner, and G. Stefani
“The LVV Auger line shape of sulfur on copper studied by Auger photoelectron coincidence spectroscopy”

J. Phys.-Condens. Matter 27, 085003 (2015)

ISSN: 0953-8984, URL and DOI: <http://dx.doi.org/10.1088/0953-8984/27/8/085003>

37) V. Lanzilotto, G. Lovat, G. Fratesi, G. Bavdek, G.P. Brivio, and L. Floreano
“TiO₂(110) Charge Donation to an Extended π -Conjugated Molecule”

J. Phys. Chem. Lett. 6, 308 (2015)

ISSN: 1948-7185, URL and DOI: <http://dx.doi.org/10.1021/jz502523u>

Role of GF: First theoretical author

36) H. Lin, G. Fratesi, and G.P. Brivio

“Graphene magnetism induced by covalent adsorption of aromatic radicals”

Phys. Chem. Chem. Phys 17, 2210 (2015)

ISSN: 1463-9084, URL and DOI: <http://dx.doi.org/10.1039/C4CP04476B>

35) M. Caputo, M. Panighel, L. Petaccia, C. Struzzi, V. Alijani, M. Coreno, M. de Simone, G. Fratesi, G. Di Santo, and A. Goldoni

“Metallic picene/C60 heterojunctions and the effect of potassium doping”

Phys. Rev. B 90, 201401 (2014)

ISSN: 1098-0121, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.90.201401>

Role of GF: Sole theoretical author

34) A. Picone, M. Riva, G. Fratesi, A. Brambilla, G. Bussetti, M. Finazzi, L. Duò, and F. Ciccacci
“Enhanced Atom Mobility on the Surface of a Metastable Film”

Phys. Rev. Lett. 113, 046102 (2014)

ISSN: 1079-7114, URL and DOI: <http://dx.doi.org/10.1103/PhysRevLett.113.046102>

Role of GF: Sole theoretical author

33) F. Sirotti, N. Beaulieu, A. Bendounan, M. G. Silly, C. Chauvet, G. Malinowski, G. Fratesi, V. Vénier, and G. Onida

“Multiphoton k-resolved photoemission from gold surface states with 800-nm femtosecond laser pulses”

Phys. Rev. B 90, 035401 (2014)

ISSN: 1098-0121, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.90.035401>

Role of GF: First theoretical author

32) G. Fratesi, V. Lanzilotto, S. Stranges, M. Alagia, G. P. Brivio, and L. Floreano

“High resolution NEXAFS of perylene and PTCDI: a surface science approach to molecular orbital analysis”

Phys. Chem. Chem. Phys. 16, 14834 (2014)

ISSN: 1463-9084, URL and DOI: <http://dx.doi.org/10.1039/C4CP01625D>

Role of GF: First author

31) G. Fratesi, C. Motta, M. I. Trioni, G. P. Brivio, and D. Sánchez-Portal

“Resonant Lifetime of Core-Excited Organic Adsorbates from First Principles”

J. Phys. Chem. C 118, 8775 (2014)

ISSN: 1932-7447, URL and DOI: <http://dx.doi.org/10.1021/jp500520k>

Role of GF: First author

30) F. Donati, G. Fratesi, L. Ning, A. Brambilla, M. I. Trioni, A. Li Bassi, C. S. Casari, and M. Passoni
“Electronic and magnetic properties of bulk Cr tips for scanning tunneling spectroscopy”

Phys. Rev. B 87, 235431 (2013)

ISSN: 1098-0121, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.87.235431>

Role of GF: First theoretical author

29) G. Fratesi, V. Lanzilotto, L. Floreano, and G. P. Brivio

“Azimuthal Dichroism in Near-Edge X-ray Absorption Fine Structure Spectra of Planar Molecules”

J. Phys. Chem. C 117, 6632 (2013)

ISSN: 1932-7447, URL and DOI: <http://dx.doi.org/10.1021/jp312569q>

Role of GF: First author

28) C. Motta, G. Fratesi, and M. I. Trioni

“Conductance calculation of hydrogen molecular junctions between Cu electrodes”

Phys. Rev. B 87, 075415 (2013)

ISSN: 1098-0121, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.87.075415>

27) A. Picone, G. Fratesi, M. Riva, G. Bussetti, A. Calloni, A. Brambilla, M. I. Trioni, L. Duò, F. Ciccacci, and M. Finazzi

“Self-organized chromium oxide monolayers on Fe(001)”

Phys. Rev. B 87, 085403 (2013)

ISSN: 1098-0121, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.87.085403>

Role of GF: Sole theoretical author

26) Y. Wang, M. Lingenfelder, S. Fabris, G. Fratesi, R. Ferrando, T. Classen, K. Kern, and G. Costantini

“Programming Hierarchical Supramolecular Nanostructures by Molecular Design”

J. Phys. Chem. C 117, 3440 (2013)

ISSN: 1932-7447, URL and DOI: <http://dx.doi.org/10.1021/jp309566s>

25) R. Gotter, G. Fratesi, R. A. Bartynski, F. Da Pieve, F. Offi, A. Ruocco, S. Ugenti, M. I. Trioni, G. P. Brivio, and G. Stefani

“Spin-Dependent On-Site Electron Correlations and Localization in Itinerant Ferromagnets”

Phys. Rev. Lett. 109, 126401 (2012)

ISSN: 1079-7114, URL and DOI: <http://dx.doi.org/10.1103/PhysRevLett.109.126401>

Role of GF: First theoretical author

24) G. Fratesi

“Depolarization and bonding in quasi-one-dimensional Na structures on Cu(001)”

Phys. Rev. B 84, 155424 (2011)

ISSN: 1098-0121, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.84.155424>

Role of GF: Single author

23) S. Achilli, G.P. Brivio, G. Fratesi, and M.I. Trioni

“Spin Polarized Metastable Helium De-excitation Processes on Metal Surfaces”

J. Phys. Chem. A 115, 8498 (2011)

ISSN: 1089-5639, URL and DOI: <http://dx.doi.org/10.1021/jp2005875>

22) V. Sirtori, P. L. Cavallotti, R. Rognoni, X. Xu, G. Zangari, G. Fratesi, M.I. Trioni, and M. Bernasconi

“Unusually Large Magnetic Anisotropy in Electrochemically Deposited Co-Rich Co–Pt Films”

ACS Appl. Mater. Interfaces 3, 1800 (2011)

ISSN: 1944-8244, URL and DOI: <http://dx.doi.org/10.1021/am200267u>

Role of GF: First theoretical author

21) F. Donati, G. Fratesi, M. Passoni, C.S. Casari, A. Mairov, C.E. Bottani, M.I. Trioni, and A. Li Bassi

“Strain effect on local electronic properties of Fe nanoislands grown on Au(111)”

Phys. Rev. B 83, 153404 (2011)

ISSN: 1098-0121, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.83.153404>

Role of GF: First theoretical author

20) F. Carone Fabiani, G. Fratesi, and G.P. Brivio

“Adsorption of H₂S, HS, S, and H on a stepped Fe(310) surface”

Eur. Phys. J. B 78, 455 (2010)

ISSN: 1434-6028, URL and DOI: <http://dx.doi.org/10.1140/epjb/e2010-10616-8>

19) G. Fratesi

“First-principles investigation of the early stages of Pd adsorption on Au(111)”

J. Phys.-Condens. Matter 23, 015001 (2011)

ISSN: 0953-8984, URL and DOI: <http://dx.doi.org/10.1088/0953-8984/23/1/015001>

Role of GF: Single author

18) C. Huang, G. Fratesi, D.A. MacLaren, W. Luo, G.P. Brivio, and W. Allison

“Charge redistribution in the formation of one-dimensional lithium wires on Cu(001)”

Phys. Rev. B 82, 081413(R) (2010)

ISSN: 1098-0121, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.82.081413>

Role of GF: First theoretical author

17) G. Fratesi, A. Pace, and G.P. Brivio

“Short-range lateral interactions and depolarization of Na atoms on Cu surfaces”

J. Phys.-Condens. Matter 22, 304005 (2010)

ISSN: 0953-8984, URL and DOI: <http://dx.doi.org/10.1088/0953-8984/22/30/304005>

Role of GF: First author

16) A. Picone, G. Fratesi, A. Brambilla, P. Sessi, F. Donati, S. Achilli, L. Maini, M.I. Trioni, C.S. Casari, M. Passoni, A. Li Bassi, M. Finazzi, L. Duò, and F. Ciccacci

“Atomic corrugation in scanning tunneling microscopy images of the Fe(001)-p(1×1)O surface”

Phys. Rev. B 81, 115450 (2010)

ISSN: 1098-0121, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.81.115450>

Role of GF: First theoretical author

15) H. Hedgeland, P.R. Kole, H.R. Davies, A.P. Jardine, G. Alexandrowicz, W. Allison, J. Ellis, G. Fratesi, and G.P. Brivio

“Surface dynamics and friction of K/Cu(001) characterized by helium-3 spin-echo and density functional theory”

Phys. Rev. B 80, 125426 (2009)

ISSN: 1098-0121, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.80.125426>

Role of GF: First theoretical author

14) P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G.L. Chiarotti, M.

Cococcioni, I. Dabo, A. Dal Corso, S. de Gironcoli, S. Fabris, G. Fratesi, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Sclauzero, A.P. Seitsonen, A. Smogunov, P. Umari, and R.M. Wentzcovitch

“QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials”

J. Phys.-Condens. Matter 21, 395502 (2009)

ISSN: 0953-8984, URL and DOI: <http://dx.doi.org/10.1088/0953-8984/21/39/395502>

13) G. Fratesi

“Potential energy surface of alkali atoms adsorbed on Cu(001)”

Phys. Rev. B 80, 045422 (2009)

ISSN: 1098-0121, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.80.045422>

Role of GF: Single author

12) M.I. Trioni, G. Fratesi, S. Achilli, and G.P. Brivio

“Dynamics of electron distributions probed by helium scattering”

J. Phys.-Condens. Matter 21, 264003 (2009)

ISSN: 0953-8984, URL and DOI: <http://dx.doi.org/10.1088/0953-8984/21/26/264003>

11) M.I. Trioni, A. Zanetti, G. Fratesi, and G.P. Brivio

“Spin polarized Auger electrons in Core-Valence-Valence decays of 3d impurities in metals”

Phys. Rev. B 79, 165115 (2009)

ISSN: 1098-0121, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.79.165115>

10) G. Fratesi, M.I. Trioni, G.P. Brivio, S. Ugenti, E. Perfetto, and M. Cini

“Ab initio calculation of core-valence-valence Auger spectra in closed shell systems”

Phys. Rev. B 78, 205111 (2008)

ISSN: 1098-0121, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.78.205111>

Role of GF: First author

9) G. Fratesi, G. Alexandrowicz, M.I. Trioni, G.P. Brivio, and W. Allison
“Crucial electronic contributions to measures of surface diffusion by He atom scattering”
Phys. Rev. B 77, 235444 (2008)
ISSN: 1098-0121, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.77.235444>
Role of GF: First author

8) T. Classen, M. Lingenfelder, Y. Wang, R. Chopra, C. Virojanadara, U. Starke, G. Costantini, G. Fratesi, S. Fabris, S. de Gironcoli, S. Baroni, S. Haq, R. Raval, and K. Kern
“Hydrogen and Coordination Bonding Supramolecular Structures of Trimesic Acid on Cu(110)”
J. Phys. Chem. A 111, 12589 (2007)
ISSN: 1089-5639, URL and DOI: <http://dx.doi.org/http://dx.doi.org/10.1021/jp076037o>
Role of GF: First theoretical author

7) G. Fratesi, P. Gava, and S. de Gironcoli
“Direct methane-to-methanol conversion: insight from first-principles calculations”
J. Phys. Chem. C 111, 17015 (2007)
ISSN: 1932-7447, URL and DOI: <http://dx.doi.org/10.1021/jp074134b>
Role of GF: First author

6) G.P. Brivio, G. Butti, S. Caravati, G. Fratesi, and M.I. Trioni
“Theoretical approaches in adsorption: alkali adatom investigations”
J. Phys.-Condens. Matter 19, 305005 (2007)
ISSN: 0953-8984, URL and DOI: <http://dx.doi.org/10.1088/0953-8984/19/30/305005>

5) A. Kokalj, N. Bonini, S. de Gironcoli, C. Sbraccia, G. Fratesi, and S. Baroni
“Methane dehydrogenation on Rh@Cu(111): A first-principles study of a model catalyst”
J. Am. Chem. Soc. 128, 12448 (2006)
ISSN: 0002-7863, URL and DOI: <http://dx.doi.org/10.1021/ja060114w>

4) G. Fratesi and S. de Gironcoli
“Analysis of methane-to-methanol conversion on clean and defective Rh surfaces”
J. Chem. Phys. 125, 044701 (2006)
ISSN: 0021-9606, URL and DOI: <http://dx.doi.org/10.1063/1.2219448>
Role of GF: First author

3) T. Classen, G. Fratesi, G. Costantini, S. Fabris, F. Stadler, C. Kim, S. de Gironcoli, S. Baroni, and K. Kern
“Templated growth of metal-organic coordination chains at surfaces”
Angew. Chem. Int. Edit. 44, 6142 (2005)
ISSN: 1433-7851, URL and DOI: <http://dx.doi.org/10.1002/anie.200502007>
Role of GF: First theoretical author

2) G. Fratesi, G.P. Brivio, and L.G. Molinari
“Many-body method for infinite nonperiodic systems”
Phys. Rev. B 69, 245113 (2004)
ISSN: 1098-0121, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.69.245113>
Role of GF: First author

1) G. Fratesi, G.P. Brivio, P. Rinke, and R.W. Godby
“Image resonance in the many-body density of states at a metal surface”
Phys. Rev. B 68, 195404 (2003)
ISSN: 1098-0121, URL and DOI: <http://dx.doi.org/10.1103/PhysRevB.68.195404>
Role of GF: First author

Book chapters

3) G.P. Brivio and G. Fratesi
“Energetic Ground State Calculations, Electronic Band Structure at Surfaces”
Chapter in book: “Springer Handbook of Surface Science”, Mario Rocca, Luca Vattuone, Talat Rahman Editors, Springer (2020).
ISSN: 978-3-030-46906-1, URL and DOI: http://dx.doi.org/10.1007/978-3-030-46906-1_16

2) G. Fratesi, A. Ravikumar, and G.P. Brivio

“Graphene Properties by Functionalization with Organic Molecules”

Chapter in book: “World Scientific Reference of Hybrid Materials. Volume 2: Devices from Hybrid and Organic Materials”, Vida Turkovic, Morten Madsen, Horst-Günter Rubahn Editors, World Scientific 2019.

ISBN: 978-981-3270-48-0, URL and DOI: http://dx.doi.org/10.1142/9789813270541_0002

Role of GF: First author

1) G. Fratesi, E. Molteni, and G. Onida

“Spectroscopy of Adsorbates and the Role of Interfacial Interactions”

Chapter in book “Toward a Science Campus in Milan : A Snapshot of Current Research at the Physics Department Aldo Pontremoli”, P.F. Bortignon, G. Lodato, E. Meroni, M.G.A. Paris, L. Perini, and A. Vicini Editors, Springer 2018.

ISBN: 978-3-030-01628-9, URL and DOI: http://dx.doi.org/10.1007/978-3-030-01629-6_9

Role of GF: First author

Conference papers

4) G. Fratesi, S. Achilli, F. Orlando, M. Marino, E. Molteni, and G. Onida

“Tuning Electronic and Magnetic Properties of Ultrathin and Bulk Magnetic Oxides by Adsorption of Organic Molecules”

Il Nuovo Cimento C (accepted 2023)

ISSN: 1826-9885

Role of GF: Last author

3) E. Cinquanta, G. Fratesi, S. dal Conte, C. Grazianetti, F. Scotognella, S. Stagira, C. Vozzi, G. Onida, and A. Molle
“Ultrafast carrier dynamics of epitaxial silicene”

Proc. of SPIE Vol. 10102, 101020J (2017)

ISSN: 1996-756X, URL and DOI: <http://dx.doi.org/10.1117/12.2252009>

Role of GF: First theoretical author

2) A. Calloni, G. Berti, A. Brambilla, G. Bussetti, M. Finazzi, L. Duò, F. Ciccacci, and G. Fratesi

“Magnetism in thin Cr films grown on Fe(001)-p(1×1)O: a spin-resolved investigation of single and multi-layers”

Proc. SPIE 9551, Spintronics VIII, 95511K (2015)

ISSN: 1996-756X, URL and DOI: <http://dx.doi.org/10.1117/12.2188435>

Role of GF: Sole theoretical author

1) S. Ugenti, M. Cini, E. Perfetto, F. Da Pieve, C. Natoli, R. Gotter, F. Offi, A. Ruocco, G. Stefani, F. Tommasini, G. Fratesi, M.I. Trioni, and G.P. Brivio

“Spin selectivity by Auger-photoelectron coincidence spectroscopy”

J. Phys.: Conf. Ser. 100, 072020 (2008)

ISSN: 1742-6596, URL and DOI: <http://dx.doi.org/10.1088/1742-6596/100/7/072020>

Ph.D. Thesis

Ph.D. in Theoretical Condensed Matter at the International School for Advanced Studies (SISSA), Trieste, Italy (equivalent to the title of “Dottore di Ricerca in Fisica”, Ph.D. in Physics, according to the D.M. 24.04.87).

Title: “Low temperature methane-to-methanol conversion on transition metal surfaces”.

Supervisor: Prof. Stefano de Gironcoli.

The thesis has been approved cum laude on 24/10/2005.

Download link. <http://hdl.handle.net/20.500.11767/4087> .

3.3 Conferences and seminars

Organization of international conferences

- **CMD30 – FisMat2023** (<https://eventi.cnism.it/cmd30-fismat>, Milan, Italy, 4-8 September 2023).
 - Co-organizer of the mini-colloquium “Novel 2D magnetic materials and heterostructures” [José J. Baldoví (ICMOL, Universitat de València), Alberto Brambilla (Politecnico di Milano), GF, Ilaria Bergenti (CNR ISMN).
- **25th ETSF Workshop on Electronic Excitations** (<http://ws25.pcpm.ucl.ac.be/>, Leuven, Belgium, 13-17 June 2022). The workshop focused on fundamental challenges for theoretical spectroscopy posed by cutting-edge present and future technologies, thereby promoting a fruitful exchange between academia and industry. It counted more than 100 participants from Europe and outside the EU. The participation by young researchers and Ph.D students was supported with waived fees and grants for travel expenses.
 - Member of the organizing committee [Claudia Rödl (Friedrich-Schiller-Universität Jena, Germany), Gabriele D'Avino (CNRS, France), Michiel van Setten (IMEC, Leuven, Belgium), GF, Elena Cannuccia (Università degli Studi di Roma "Tor Vergata"), Pedro Melo (Universiteit Utrecht - Utrecht (Netherlands))].
 - Member of the program committee.
- **24th ETSF Workshop on Electronic Excitations** (<http://ws24.pcpm.ucl.ac.be/>, Jena, Germany, 16-20 September 2019). The workshop focused on light-matter interaction and optical spectroscopy from infrared to X-rays and counted more than 100 participants from Europe and outside the EU. The participation by young researchers and Ph.D students was supported with waived fees and grants for travel expenses.
 - Member of the organizing committee [Claudia Rödl (Friedrich-Schiller-Universität Jena, Germany), Gabriele D'Avino (CNRS, France), Michiel van Setten (IMEC, Belgium), GF, Elena Cannuccia (Università degli Studi di Roma "Tor Vergata"), Carina Faber (Universite Catholique de Louvain, Louvain-la-Neuve, Belgium)].
 - Member of the program committee.
- **Atoms and Molecules On Solid Surfaces** (<https://sites.google.com/view/amoss>, Milan, 23 November 2018). A one-day conference as a tribute to Gian Paolo Brivio for his 70th birthday, organized within the PhD Course in Materials Science and Nanotechnology at the University of Milano-Bicocca and counting ~50 attendants from Italy, abroad, and overseas.
 - Member of the organizing committee [GF, Giorgio Benedek (University of Milano-Bicocca), Marco Bernasconi (University of Milano-Bicocca)].
 - Member of the program committee and of the local committee.
 - Responsible of the workshop website.
- **23rd ETSF Workshop on Electronic Excitations** (<http://ws23.pcpm.ucl.ac.be/>, Milan, 10-14 September 2018). The workshop focused on interdisciplinary views on quantum many-body theory

and counted more than 80 participants, mostly from abroad. The participation by young researchers and Ph.D students was supported with waived fees and grants for travel expenses.

- Member of the organizing committee [Giovanni Onida (UNIMI), GF, Zeila Zanolli (Aachen University, Germany), Gabriele D'Avino (CNRS, France), Michiel van Setten (Universite Catholique de Louvain, Louvain-la-Neuve, Belgium), Claudia Rödl (Friedrich-Schiller-Universität Jena, Germany)].
- Member of the program committee and of the local committee.
- Grant holder for the financial support provided by the Physics Department of UNIMI.
- **17th Workshop on Dynamical Phenomena at Surfaces** (<http://wdps17.fisica.unimi.it>, Milan, 19-21 September 2016). The workshop counted more than 50 surface physicists and chemists, with a similar number from the theoretical and experimental community. The international participation was predominant, including 8 invited speakers from EU and overseas. Participation by young researchers and Ph.D. students was fostered through the support of travel and accommodation expenses.
 - Member of the organizing committee [GF, William Allison (University of Cambridge, UK), Giulio Casati (Università dell'Insubria, Italy), Talat Shahnaz Rahman (University of Central Florida, FL, USA), and Gian Paolo Brivio (Università di Milano-Bicocca, Italy)].
 - Member of the program committee. Main proponent and contact person of the invited speakers. Evaluator of the submitted abstracts.
 - Grant holder for the financial support provided by the Psi-K fundation, by SAES Getters S.p.A., and by the Physics Department of UNIMI.
 - Lead local organizer.
 - Responsible of the workshop website.

Invited talks at international conferences and workshops

7) 6th International Meeting on Silicene, SOLEIL Saint-Aubin, Paris, France (<http://www.silicene.org/IMS-5/>)
“Using a buffer layer to tune electron injection dynamics at the organic-graphene/metal interface” (14/12/2017)

6) International Conference on Novel nanomaterial: Engineering and properties, CEA-SOLEIL Saint-Aubin, Paris, France (<http://iramis.cea.fr/meetings/ICON2-2017/index.php>)
“Femto-Magnetism and Electron Transport at Core-Excited Organic Molecule/Graphene Interfaces” (18/10/2017)

5) CMD26 - Condensed Matter in Groningen, Groningen, The Netherlands (<http://cmd26.eu/>)
“Femtomagnetism in graphene induced by core level excitation of organic adsorbates” (04/09/2016)

4) 5th International Meeting on Silicene, Orlando, FL, US (<http://www.silicene.org/IMS-5/>)
“Optical response and ultrafast carrier dynamics of the silicene-silver interface” (15/12/2015)

3) 3rd Euro-Mediterranean Conference on Materials and Renewable Energies, Marrakech, Morocco (<http://www3.emcmre.com/>) “Theoretical core-level spectroscopy from adsorbed organic molecules” (03/11/2015)

2) Italian National Conference on Condensed Matter Physics, Palermo, Italy (<http://eventi.cnism.it/fismat2015>)
“Theoretical core-level spectroscopy from adsorbed organic molecules” (02/10/2015)

1) Summer school on “Emerging renewable energy conversion and storage”, Como, Italy (<http://www.pcam-doctorate.eu/events-news/index.php?new=22>)
“Charge injection processes from adsorbed organic molecules” (11/09/2013)

Other oral presentations at conferences and workshops

- 38) Graphene2023, Manchester, UK
"Crystal Phase Engineering of Silicene by Sn-modified Ag(111)" (28/06/2023)
- 37) 4th Workshop - 2023 "Condensed Matter Highlights", Milano, Italy
"Two-Dimensional Silicene–Stanene Heterostructures by Epitaxy" (14/02/2023)
- 36) 108 Congresso Nazionale SIF 2020, Milano, Italy
"Tuning Electronic and Magnetic Properties of Ultrathin and Bulk Magnetic Oxides by Adsorption of Organic Molecules " (13/09/2022)
- 35) ECOS 35, Luxembourg, Luxembourg
"Tuning Electronic and Magnetic Properties of Ultrathin and Bulk Magnetic Oxides by Adsorption of Organic Molecules " (31/08/2022)
- 34) 106 Congresso Nazionale SIF 2020, Milano (online event), Italy
"Elusive central-atom dependence in the adsorption of M-tetra-phenyl porphyrin molecules on Fe(001)-p(1x1)O" (14/09/2020)
- 33) 15th European Conference on Molecular Electronics (ECME), Linköping, Sweden
"Spectroscopic fingerprints of sp¹ hybridized C in surface-grown molecular assemblies" (30/08/2019)
- 32) Theory Meets Experiment in Low-Dimensional Structures with Correlated Electrons, Prague, Czech Republic
"Electronic and spectral properties of clean and C₆₀-covered atom-thick Chromium oxide at the Fe(001) surface" (04/07/2019)
- 31) 3rd Workshop Condensed Matter Highlights, Milano, Italy
"Tuning ultrafast electron injection dynamics at organic-graphene interfaces" (15/02/2019)
- 30) Atoms and Molecules On Solid Surfaces, Milano, Italy
"Quantum and Classical Image Charges at Metal Surfaces" (23/11/2018)
- 29) Materials.it 2018, Bologna, Italy
"Fingerprints of sp¹-carbon hybridization in the core-level spectra of surface-grown materials" (23/10/2018)
- 28) Molecular Simulation and Engineering 2018, Milano, Italy
"Lattice mismatch and spectroscopy of buckybowl on Ag(111)" (26/09/2018)
- 27) 2018 E-MRS Spring Meeting, Strasbourg, France
"Lattice mismatch drives spatial modulation of corannulene tilt on Ag(111)" (18/06/2018)
- 26) Italian National Conference on Condensed Matter Physics, Trieste, Italy
"Evidence of corannulene tilting on Ag(111)" (05/10/2017)
- 25) ETSF2017 workshop, Frascati, Italy
"Will simple free-standing graphene put an end to simple calculations of molecule-substrate electron dynamics?" (06/09/2017)
- 24) Congress of the Department of Physics, Milano, Italy
"Spectroscopy of adsorbates and the role of interfacial interactions" (29/06/2017)
- 23) USD10 - Ultrafast Surface Dynamics, Inzell, Germany
"Substrate induced ultrafast electron injection dynamics at organic-graphene interfaces" (15/06/2017)
- 22) Materials.it 2016, Catania, Italy
"Femtosecond electron transfer at core-excited adsorbed molecules" (15/12/2016)
- 21) CMD26 - Condensed Matter in Groningen, Groningen, The Netherlands
"Optical response and ultrafast carrier dynamics of silicene on silver" (05/09/2016)
- 20) 3rd Workshop on Surfaces, Interfaces and Functionalization Processes in Organic Compounds and Applications,

Naples, Italy

“Electron transfer with core-level excitations at hybrid interfaces” (28/06/2016)

19) Italian National Conference on Condensed Matter Physics, Palermo, Italy

“Optical response of epitaxial silicene on silver probed by transition reflectance spectroscopy” (29/09/2015)

18) 2nd Workshop Condensed Matter Highlights, Milano, Italy

“Optical response and ultrafast carrier dynamics of the silicene-silver interface” (24/09/2015)

17) 14th European Conference on Organised Films, Genova, Italy

“Anchoring and Bending of Pentacene on Aluminum (001)” (30/06/2015)

16) 16th Workshop on Dynamical Phenomena at Surfaces, Madrid, Spain

“Resonant Lifetime of Core-Excited Organic Adsorbates from First Principles” (29/10/2014)

15) 2nd Surfaces, Interfaces and Functionalization processes in Organic Compounds and Applications, Trieste, Italy

“Resonant Lifetime of Core-Excited Organic Adsorbates from First Principles” (26/06/2014)

14) 18th NANOQUANTA-ETSF Workshop on Electronic Excitations, Luxembourg, Luxembourg

“Fast electron transfer at molecule-substrate interfaces” (01/10/2013)

13) Italian National Conference on Condensed Matter Physics, Milano, Italy

“Azimuthal dichroism in near-edge X-ray absorption fine structure spectra of planar molecules” (10/09/2013)

12) Magnetic order in nanostructures and spectroscopy, Roma, Italy

“Theory and first principle calculation of CVV Auger spectra of magnetic systems” (13/09/2012)

11) APS March Meeting 2012, Boston MA, US, Boston, MA, US

“Depolarization and bonding in quasi-one-dimensional Na structures on Cu(001)” (29/02/2012)

10) APS March Meeting 2012, Boston MA, US, Boston, MA, US

“Probing the surface magnetic properties via Auger-photoelectron coincidence spectroscopy” (27/02/2012)

9) 14th Workshop on Dynamical Phenomena at Surfaces, Tegernsee, Germany

“Observation of charge redistribution during bond formation in one-dimensional alkali-metal wires” (19/07/2010)

8) APS March Meeting 2010, Portland, OR, US

“Observation of charge redistribution during bond formation in one-dimensional alkali-metal wires” (18/03/2010)

7) APS March Meeting 2008, New Orleans, LA, US

“Crucial electronic contributions to measures of surface diffusion by He atom scattering” (13/03/2008)

6) 12th NANOQUANTA-ETSF Workshop on Electronic Excitations, Aussois, France

“CVV Auger spectra by first principles” (18/09/2007)

5) Psi-K conference, Schwabisch Gmund, Germany

“Low temperature methanol synthesis on transition metal surfaces” (17/09/2005)

4) Theory @ ELETTRA, Trieste, Italy

“Low temperature methanol synthesis on transition metal surfaces” (06/07/2005)

3) 16th International Vacuum Congress, Venezia, Italy

“Molecular self-assembly of trimesic acid on Cu(110) surfaces” (30/06/2004)

2) INFMeeting, Genova, Italy

“Molecular self-assembly of trimesic acid on Cu(110) surfaces” (08/06/2004)

1) II Giornata di studio interazione molecola-superficie, Milano, Italy

“Many-body properties of semi-infinite jellium” (Jan. 2002)

Invited seminars at research institutes / Universities

- 20) Donostia International Physics Center, San Sebastian, Spain
“Atom-thick oxides at the Fe(001) surface: from the playground for theory and experiments to applications”
(04/04/2019)
- 19) Premiazione Olimpiadi di Fisica, Milano, Italy
“Tocchiamo con mano la Fisica Teorica” (05/06/2017)
- 18) Open Day di Ateneo, Milano, Italy
“Tocchiamo con mano la Fisica Teorica” (20/05/2017)
- 17) Seminar within the Ph.D. School in Materials Science at Università degli Studi di Milano-Bicocca, Milano, Italy
“Silicene: two-dimensional silicon” (19/01/2016)
- 16) CNR-NANO S3, Modena, Italy
“Theoretical core-level spectroscopy from adsorbed organic molecules” (25/11/2015)
- 15) Laboratoire des Solides Irradiés, École Polytechnique, Palaiseau, France
“Questions about core to valence excitations from adsorbed molecules” (09/12/2014)
- 14) Graz University of Technology, Graz, Austria
“Orientation and coupling of adsorbed organic molecules by first-principle theoretical spectroscopy methods”
(05/02/2014)
- 13) Donostia International Physics Center, San Sebastian, Spain
“Orientation and coupling of adsorbed aromatic molecules by theoretical spectroscopy” (16/07/2013)
- 12) Università degli Studi di Milano, Milano, Italy
“Molecule-substrate interaction by first-principle theoretical spectroscopy methods” (18/06/2013)
- 11) Donostia International Physics Center, San Sebastian, Spain
“Strain effect on electronic and structural properties of metal nanoislands grown on reconstructed Au(111)”
(22/11/2011)
- 10) Laboratorio Nazionale TASC, Trieste, Italy
“Strain effect on electronic and structural properties of metal nanoislands grown on reconstructed Au(111)”
(28/06/2011)
- 9) Department of Physics, University of Cambridge, Cambridge, UK
“Strain effect on electronic and structural properties of metal nanoislands grown on reconstructed Au(111)”
(13/04/2011)
- 8) Università degli Studi di Genova, Genova, Italy
“Crucial electronic contributions to measures of surface diffusion by He atom scattering” (15/12/2008)
- 7) International School for Advanced Studies, Trieste, Italy
“Crucial electronic contributions to measures of surface diffusion by He atom scattering” (28/04/2008)
- 6) Università degli Studi di Roma Tor Vergata, Roma, Italy
“Crucial electronic contributions to measures of surface diffusion by He atom scattering” (21/02/2008)
- 5) Seminar within the Ph.D. School in Materials Science at Università degli Studi di Milano-Bicocca, Milano, Italy
“Low temperature methane to methanol conversion on transition metal surfaces - an ab initio study”
(02/04/2007)
- 4) Department of Physics, University of Cambridge, Cambridge, UK
“Low temperature methanol synthesis on transition metal surfaces” (02/10/2006)

3) IRRMA, Lausanne, Switzerland

“Molecular self-assembly of trimesic acid on Cu(110) surfaces” (07/03/2005)

2) Seminar within the Ph.D. School in Materials Science at Università degli Studi di Milano-Bicocca, Milano, Italy

“Molecular self-assembly of trimesic acid on Cu(110) surfaces” (29/03/2004)

1) Institute of Solid State Research, Juelich, Germany

“Many-body approach to infinite non-periodic systems: application to the surface of semi-infinite jellium” (Sept. 2003)

3.4 Software development

Contributions to publicly available software

- Quantum-ESPRESSO (www.quantum-espresso.org) is among the most widely used software packages for ab initio electronic structure simulation. GF is co-author of its presenting papers [Ref14-2009-JPCM, Ref55-2017-JPCM] and is contributing to the package and to the developer's and user's forums. Main contributions by GF are:
 - The initial implementation of the Projector Augmented Wave method (collaboration with Dr. R. Mazzarello and Prof. S. de Gironcoli, SISSA, 2005).
 - Lead developer of the code `molecularpdos.x` for the projection of the electronic structure of a complex system such as molecules adsorbed on a surface onto the orbitals of a molecule. Adopted in, e.g., [Ref39-2015-JPCC] and included in the stable release of Quantum-ESPRESSO since v.5.1.2 (released 08/03/2015) with updates for wavevector-resolved quantities included in v.5.4.0 (released 25/04/2016).
 - Lead developer of the code `molecularnexafs.x` for the analysis of core-level (photoemission and X-ray absorption) spectra of a molecule including inequivalent atoms of the same species. Adopted in, e.g., [Ref32-2014-PCCP] and included in the stable release of Quantum-ESPRESSO since v.6.0 (released 05/10/2016).
 - Extension of the code `sumpdos.x` to the analysis of wavevector-resolved quantities. Adopted in, e.g., [Ref49-2016-PRB] and included in the stable release of Quantum-ESPRESSO since v.5.4.0 (released 25/04/2016).
- YAMBO (www.yambo-code.org) is a code for Many-Body calculations in solid-state physics. GF has contributed an extension to evaluate the spacial origin of the optical absorption spectra, as done in [Ref41-2015-PRB].
- SIESTA (www.icmab.es/siesta) adopts a localized basis set approach to the electronic structure problem. GF has extended the transmission code TBTrans to evaluate the resonant lifetime of molecular orbitals of adsorbed molecules, as done in [Ref48-2016-PCCP] and [Ref31-2014-JPCC].

Development of other research software

- Contributor to a code for the evaluation of angular-resolved Core-Valence-Valence Auger spectra in systems with cylindrical symmetry, leading to results published in [Ref25-2012-PRL] and [Ref23-2011-JPCA].

- Sole developer of a code for the evaluation of the jellium surface Green's function including many body effects and avoiding the thin-slab approximation, leading to results published in [Ref02-2004-PRB] and [Ref01-2003-PRB].

4 Coordination of research activities

- **Scientist in charge** of the User project No. 443 accepted in 2023 by the Nanoscience Foundries and Fine Analysis - Europe|PILOT (NEP, www.nffa.eu) and being carried out since June 2023. The collaboration includes experimental researchers from an institution abroad and from the CNR-IOM node of the project. GF leads the theoretical study.
- **Scientist in charge** of the User project No. 647 accepted in 2018 by the Nanoscience Foundries and Fine Analysis (NFFA, www.nffa.eu) and carried out during 2019. The collaboration included experimental researchers from an institution abroad. GF lead the study and is the corresponding and senior author of a resulting manuscript [Ref79-2022-PCCP].
- **Scientist in charge** of the User project No. 544 “Simulation of the core-level excitation spectra of possible superconducting organic molecules” accepted in 2014 by the European Theoretical Spectroscopy Facility (ETSF, www.etsf.eu) and carried out during 2014-2015. The collaboration included 7 researchers from 6 institutions (2 outside Italy). GF lead the study and is the corresponding and senior author of a resulting manuscript [Ref61-2018-JPCC].
- **Principal investigator** in the following 9 projects for high-performance computing (HPC):
 - HP10BC1AM9 “ORGA FINT Theoretical development of hybrid ORGanic/AF INTerfaces”, 20/10/2022 – 20/10/2023, ISCRA initiative. Group GF, Dr. Simona Achilli, and Dr. Elena Molteni
 - HP10C8E33M “PORPHOXI Porphyrins interaction with thin and bulk oxides”, 09/09/2022 – 09/06/2023, ISCRA initiative. Group GF, Dr. Simona Achilli, and Dr. Elena Molteni
 - HP10CEC0H6 “HOMSI Hybrid Organic-Magnetic Substrate Interfaces”, 17/06/2021 – 17/03/2022, ISCRA initiative. Group: GF and Dr. Simona Achilli
 - HP10CB0ZW2 “APOCAPOF Adsorption Properties Of C60 And Porphyrins On Fe(001)-derived surfaces”, 10/10/2019 – 10/07/2020, ISCRA initiative. Group: GF, Dr. Elena Molteni, and Dr. Simona Achilli
 - HP10C2SVDP “MOLATO Molecular adsorption on Atom-Thick Oxides”, 05/07/2018 – 05/04/2019, ISCRA initiative. Group: GF, Dr. Elena Molteni, Dr. Simona Achilli, Mr. Federico Orlando, and Dr. Anu Baby.
 - HP10CESYLM “ADOXIS Atomic diffusion on oxidized iron surfaces”, 12/11/2014 – 12/08/2015, ISCRA initiative. Group: GF, Mrs. Anu Baby, Prof. Gian Paolo Brivio, and Mr. He Lin.
 - HP10C0TP0R “SENSO molecular SENSitizers at SOLid surfaces”, 22/03/2013 – 22/12/2013, ISCRA initiative. Group: GF and Prof. Gian Paolo Brivio.
 - HP10C3YWUA “PACO Perylene adsorption on Copper(110)”, 19/12/2011 – 19/02/2013, ISCRA initiative. Group: GF and Prof. Gian Paolo Brivio.

- HP10C7B0DN “MetAlk Metallization of alkali atom films on metal surfaces”, 11/03/2011 – 11/12/2011, ISCRA initiative. Group: GF and Prof. Gian Paolo Brivio.

5 Other scientific and organizational responsibilities

- **Local Coordinator** of the European Doctorate in Physics and Chemistry of Advanced Materials (PCAM) (<http://www.pcam-doctorate.eu>), established with 15 partners across Europe, since October 2018.
- **Participant** to the activities of the following European scientific facilities:
 - Nanoscience Foundries and Fine Analysis (NFFA, www.nffa.eu)
This international collaboration collected EU grants for a 26MEUR EU grant (grant agreements: no. 654360 from 01/09/2015 to 28/02/2021; no. 101007417 from 01/03/2021 to 28/02/2026) and includes UNIMI and more than 20 partner institutions across Europe; GF has participated to the research activities and he has been scientist in charge of two user projects (see Section Error: Reference source not found).
 - European Theoretical Spectroscopy Facility (ETSF, www.etsf.eu)
This international collaboration includes 68 research teams and about 200 researchers across Europe and the US; GF is an ETSF Research Team Leader and has been scientist in charge of a user project (see Section Error: Reference source not found).
- **Webmaster** of the Physics Department website (www.fisica.unimi.it) since November 2018. From November 2015, already in charge of the “News”, “Focus On”, and “Scientific Comments” sections.
- **Committee member** of the outreach committee of the Physics Department (representative for the Physics of Matter group since July 2016).
- **Co-responsible** of a former scientific collaboration agreement between the Physics Department of UNIMI and the Materials Science department of the University of Milano-Bicocca (approved by the Physics Department council on 17/09/2014, lasting for 3 years).
- **Member** of the Ph.D. Council (2014-2015, 2015-2016, and 2017-2018 until 2022-2023), Department Council, and Teaching Council, at the Physics Department of UNIMI (since 2013).

6 Research grants

- **Principal investigator of the UNIMI unit** in the MIUR of Italy PRIN project “FUnctionalized surfaces by True molecUlar bottom-up gROwth” (FUTURO), approved in 2023. Total budget: 254’994 EUR. Budget of the UNIMI research unit: 83’655 EUR
- **Principal investigator of the UNIMI unit** in the EU FET-OPEN project “Selectively activated INFOrmation technology by hybrid Organic Interfaces” (SINFONIA), 01/04/2021 – 30/04/2025. Total EU contribution 3’327’678.61EUR. Contribution to the UNIMI research unit: 321’671.25EUR. <https://cordis.europa.eu/project/id/964396>.
- Individual grant from MIUR of Italy, “Fondo per il finanziamento delle attività base di ricerca – FFABR” 2017, granted 3’000EUR.
- Grants for access to 9 high-performance computing (HPC) projects, already mentioned in Section Error: Reference source not found Error: Reference source not found, through the Italian SuperComputing Resource Allocation – ISCRA, with contributions in kind:(*)
 - **Principal investigator** of the project “HP10BC1AM9”, 20/10/2022 – 20/10/2023, 527’610 CPUh allocated on MARCONI100 and 73’500 CPUh on GALILEO100
 - **Principal investigator** of the project “HP10C8E33M”, 09/09/2022 – 09/06/2023, 64’000 CPUh allocated on MARCONI100.
 - **Principal investigator** of the project “HP10CEC0H6”, 17/06/2021 – 17/03/2022, 64’000 CPUh allocated on MARCONI100.
 - **Principal investigator** of the project HP10CB0ZW2 “APOCAPOF”, 10/10/2019 – 10/07/2020, 400’000 CPUh allocated on MARCONI-A2 (estimated value:~3’200EUR +VAT).
 - **Principal investigator** of the project HP10C2SVDP “MOLATO”, 05/07/2018 – 05/04/2019, 60’000 CPUh allocated on MARCONI-A1 and 176’432 CPUh on MARCONI-A2 (estimated value:~2300EUR +VAT).
 - **Principal investigator** of the project HP10CESYLM “ADOXIS”, 12/11/2014 – 12/08/2015, 700’000 CPUh allocated on FERMI (estimated value:~9’000EUR +VAT).
 - **Principal investigator** of the project HP10C0TP0R “SENSO”, 22/03/2013 – 22/12/2013, 1’000’000 CPUh allocated on FERMI (estimated value:~13’000EUR +VAT).
 - **Principal investigator** of the project HP10C3YWUA “PACO”, 19/12/2011 – 19/02/2013, 100’000 CPUh allocated on FERMI (estimated value:~1’300EUR +VAT).
 - **Principal investigator** of the project HP10C7B0DN “MetAlk”, 11/03/2011 – 11/12/2011, 15’000 CPUh allocated on SP6.

(*) One of the main requirements for the theoretical/numerical research in condensed matter Physics is the access to High Performance Computing facilities. This is often gained through competitive calls where a given amount of CPU time is granted, rather than money to buy the same CPU time. To facilitate comparison to projects granting money, one can refer to the 2015 agreement between CINECA and UNIMI which consisted of 109’000EUR+VAT for 1.7M “standard hours” (1 standard

hour = 5 CPUh on the FERMI supercomputer and 8 CPUh on MARCONI-A2), corresponding to a cost/hour of about 0.064EUR/h(standard)+VAT from which the given estimate is deduced.

- Research grants from UNIMI:
 - **Principal investigator** of the project “Ab initio investigation of tailored molecular layers on solid surfaces”.
UNIMI call “Piano di Sostegno alla Ricerca - Linea 2, Azione A” (2019).
Funded for 2'900EUR.
 - **Principal investigator** of the project “Electronic and structural properties of surface-supported organic molecules”.
UNIMI call “Piano di Sostegno alla Ricerca - Linea 2, Azione A” (2018).
Funded for 3'500EUR.
 - **Principal investigator** of the project “Tuning the adsorbate-substrate interaction and electronic coupling”.
UNIMI call “Piano di Sostegno alla Ricerca - Linea 2, Azione A” (2017).
Funded for 4'275EUR.
 - **Principal investigator** of the project “Valence and core-level theoretical spectroscopy of adsorbed organic molecules”.
UNIMI call “Piano di Sostegno alla Ricerca (2015-2017) - Linea 2, Azione A” (2016).
Funded for 4'500EUR.
 - **Principal investigator** of the project “Theoretical spectroscopy of molecules at hybrid organic/inorganic interfaces”.
UNIMI call “Piano di Sostegno alla Ricerca (2015-2017) - Linea 2, Azione A” (2015).
Funded for 3'270EUR.
 - **Principal investigator** of the project “Theory and simulation of electron transfer from adsorbed molecules”.
UNIMI call “Piano Sviluppo UNIMI - Linea B (2014-2015)” (2014).
Funded for 2'610EUR.
- Grants for the organization of the conference “17th Workshop on Dynamical Phenomena at surfaces”, 19-21 September 2016 (wdps17.fisica.unimi.it)
 - Psi-K Charity (UK), “Call for Psi-K workshop proposals for 2016”
Role: Project coordinator and presenter
Funded application for 3'000EUR.
 - SAES Getters S.p.A.
Role: grant holder and responsible
Sponsorship for 3'000EUR.

Positively evaluated projects since 2013

- MIUR, call PRIN 2017, proposal “Surface-supported Molecular Architectures Responsive To External Stimuli: Theory Allied To Experiment (SMART ESTATE)”, PI: Maurizio Casarin, University of Padua.

Role of G.F.: lead of the UNIMI research unit.
Score 91/100, ranked 17th among projects in the PE4 sector.

- EU, call H2020-NMP-2015, proposal “COMPOSITE” (No. 685562)
Role: Leader of the UNIMI unit
Other partners: Milano-Bicocca (IT), Fraunhofer Institut Silicatforschung (DE), Centrum Organické Chemia S.R.O. (CZ), LCS life cycle simulation GMBH (DE), Acreo Swedish ICT AB (SE), University of Birmingham (UK), COATEMA gmbh (DE), POLYERA (US), GRAPHENEA (ES).
First-stage evaluation: 7/10, missing by 1 point the threshold (8/10) for the access to the second stage of evaluation.
- MIUR, call FIRB 2013, proposal “Molecular sensitizers at solid surfaces: theory and simulation of electron transfer processes”.
Role: Principal investigator.
Score (19/04/2013): 8.33/10, where 8/10 was set to be between 95th and 90th percentile.

7 Scientific collaborations

Participation to funded projects

- EU, H2020-FETOPEN-2018-2020 “Selectively activated INFORMATION technology by hybrid Organic Interfaces (SINFONIA)”, 01/04/2021-31/03/2025, European consortium with 10 partners.
Role: **local principal investigator** of the UNIMI research unit.
<https://cordis.europa.eu/project/id/964396>
- EU, H2020-INFRAIA-2018-2020 “Nanoscience Foundries and Fine Analysis – Europe|PILOT (NEP)”, 01/03/2021-28/02/2026, European consortium with 26 partners. Role: participant to the UNIMI research unit. <https://cordis.europa.eu/project/id/101007417>
- EU, H2020-INFRAIA-2014-2015 “Nanoscience Foundries and Fine Analysis (NFFA-EUROPE)”, 01/09/2015-28/02/2021, European consortium with 21 partners. Role: participant to the UNIMI research unit. <https://cordis.europa.eu/project/id/654360>
- MIUR, call PRIN 2010-2011, project No. 20104XET32_003: “Dispositivi Solari a Coloranti di Nuova Generazione: Sensibilizzatori e Conduttori Nano-Ingegnerizzati (DSSCX)” 01/02/2013-01/02/2016 (National coordinator: Prof. Carlo Alberto Bignozzi, Ferrara).
Role: participant (writing and research activity).
- MIUR, call PRIN 2008, project No. 2008AKZSXY_004: “Teoria e calcolo da principi primi di spettri Auger di sistemi magnetici” 22/03/2010–22/09/2012 (National coordinator: Prof. Michele Cini, Roma Tor Vergata).
Role: participant (writing and research activity).
- Fondazione CARILO, call “Ricerca scientifica e tecnologica sui materiali avanzati – 2008”, project “IMaging MAGnetic Interfaces and NAnostructures for applications in spintronics (IMMAGINA)” (National coordinator: Prof. Marco Finazzi, Politecnico di Milano).
Role: participant (writing and research activity).

8 Teaching activities

8.1 Institutional courses at Universities

As Associate Professor in UNIMI (since 2020)

- Professor for the course “Fisica Generale 1” (General Physics 1, Degree in Mathematics at UNIMI) for 4 years: 2019-2020 (49h/year), 2020-2021 and 2021-2022 (51h/year), 2022-2023 (48h/year).
- Professor for the course “Struttura Elettronica” (Electronic Structure, Master in Physics at UNIMI) for 1 year: 2022-2023 (42h/year).
- Professor for the course “Fisica dei Solidi 2” (Solid State Physics 2, Master in Physics at UNIMI) for 2 years: 2020-2021 and 2021-2022 (42h/year).
- Professor for the course “Hpc@unimi: indaco for molecules and solids” (PhD in Physics and PhD in Chemistry at UNIMI) for 2 years: 2021-2022 and 2022-2023 (5h/year).
- Assistant professor for the course “Metodi Matematici della Fisica” (Mathematical Methods for Physics, Degree in Physics at UNIMI) for 4 years: 2019-2020 (20h/year), then 2020-2021, 2021-2022, and 2022-2023 (24h/year of full-class tutorials). Course responsible: Prof. Luca Guido Molinari.

During the RTDB contract in UNIMI (2017-2020)

The teaching assignment as fixed-term researcher (RTDB) at UNIMI was set to 60h/year.

- Assistant professor for the course “Fisica Generale 1” (General Physics 1, Degree in Mathematics at UNIMI) for 3 years: 2016-2017(*) (34h), then 2017-2018 and 2018-2019 (44h/year of full-class tutorials). Course responsible: Prof. Alessandra Guglielmetti.
- Assistant professor for the course “Metodi Matematici della Fisica” (Mathematical Methods for Physics, Degree in Physics at UNIMI) for 3 years: 2016-2017(*), 2017-2018, and 2018-2019 (20h/year of full-class tutorials). Course responsible: Prof. Luca Guido Molinari.

(*) Since the courses of 2016-2017 started before GF was enrolled as RTDB, these classes were initially attributed to GF as an external collaborator before the *a posteriori* assignment by the Physics Department. Independently of that, these classes were fully taken by GF alike the other years.

During the RTDA contract in UNIMI (2013-2016)

The teaching assignment as fixed-term researcher (RTDA) at UNIMI was set to 30h/year.

- Teacher for the course “Fisica delle Superfici 1” (Surface Physics, Master in Physics at UNIMI) for 4 years: 2013-2014, 2014-2015, 2015-2016, and 2016-2017 (10h in class/year). Course shared with Prof. Giovanni Onida.
- Assistant professor for the course “Metodi Matematici della Fisica” (Mathematical Methods for Physics, Degree in Physics at UNIMI) for 3 years: 2013-2014, 2014-2015, and 2015-2016 (20h/year of full-class tutorials). Course responsible: Prof. Luca Guido Molinari.

Previous teaching at Universities

- Tutor and examiner for the course of “Teoria della Materia Condensata” (Theory of Condensed Matter), for the Physics degree at Università degli Studi di Milano-Bicocca, for 3 years: 2011-2012, 2012-2013, 2013-2014 (ca 12h in class/year).
- Official tutor and examiner (“professore a contratto”) for the course of “Teoria della Materia Condensata” (Theory of Condensed Matter), for the Physics degree at Università degli Studi di Milano-Bicocca, for 2 years: 2009-2010 (12h in class) and 2010-2011 (24h in class).
- Official tutor and examiner (“professore a contratto”) for the course of “Fisica Atomica e Molecolare” (Atomic and Molecular Physics), for the Physics degree at Università degli Studi di Milano-Bicocca, 1 year: 2008-2009 (12h in class).
- Official tutor and examiner (“professore a contratto”) for the course of “Struttura della Materia” (Structure of Matter), for the Physics degree at Università degli Studi di Milano-Bicocca, 1 year: 2007-2008 (12h in class).
- Seminars for the course of “Teoria Quantistica dei Sistemi a Molti Corpi” (Quantum Theory of Many-Body Systems), for the Physics degree at Università degli Studi di Milano-Bicocca: 2005-2007.

8.2 Supervision of students

GF has been supervisor/co-supervisor of 5 graduate students (1 as main supervisor), 6 master students (1 as main supervisor), 7 bachelor students (3 as main supervisor), and 1 ERASMUS student.

Graduate students

- **Main supervisor** of Marco Marino
Title: Ph.D. in Physics
Institution: University of Milano
Thesis (provisional): “Theoretical development of hybrid organic/antiferromagnetic interfaces”
From 01/10/2021 to 30/09/2024 (expected).
- **Co-supervisor** of Aldo Ugolotti
Title: Ph.D. in Materials Science and Nanotechnology
Institution: University of Milano-Bicocca (within the PCAM joint doctorate)
Thesis: “Investigating metal-organic/inorganic interfaces with different dimensionalities from first-principles”
Defense: 20/02/2020
- **Co-supervisor** of Dr. Abhilash Ravikumar
Title: Ph.D. in Materials Science
Institution: University of Milano-Bicocca (within the PCAM joint doctorate)
Thesis: “Electronic, spin-dependent, conductive properties of modified graphene”
Defense: 10/07/2017
- **Co-supervisor** of Dr. He Lin
Title: Ph.D. in Materials Science
Institution: University of Milano-Bicocca

Thesis: “Ab initio Study of Organic Molecules Adsorbed on Technologically Relevant Surfaces”

Defense: 28/07/2016

- **Co-supervisor** of Dr. Anu Baby
Title: Ph.D. in Materials Science
Institution: University of Milano-Bicocca (within the PCAM joint doctorate)
Thesis: “Hybrid Interfaces: Adsorption of Aromatic Molecules on Metals”
Defense: 09/02/2016

Master students (“Laurea Magistrale”)

- **Co-supervisor** of Federico Orlando (matr. 867249)
Title: Master in Physics
Institution: Università degli Studi di Milano
Thesis: “Structural and electronic properties of a silicene/Ag₂Sn/Ag(111) heterostructure via an ab initio numerical approach”
Defense: 04/10/2022
- **Co-supervisor** of Pietro Fontana (matr. 938170)
Title: Master in Physics
Institution: Università degli Studi di Milano
Thesis: “Robust schemes for constructing maximally localized Wannier functions”
Defense: 09/07/2020
- **Main supervisor** of Matteo Ferri (matr. 843067)
Title: Master in Physics
Institution: Università degli Studi di Milano
Thesis: “Ab initio study of structural, electronic and optical properties of silicene nanoribbons”
Defense: 19/07/2016
- **Co-supervisor** of Marco Vanzini (matr. 790152)
Title: Master in Physics
Institution: Università degli Studi di Milano
Thesis: “Equazioni di Hedin e potenziale di Kohn-Sham nel formalismo dell'integrale funzionale”
Defense: 17/04/2014
- **Co-supervisor** of Aldo Ugolotti (matr. 774295)
Title: Master in Physics
Institution: University of Milano-Bicocca
Thesis: “Ab initio investigation of the adsorption of aromatic molecules on a platinum surface”
Defense: 29/06/2016
- **Co-supervisor** of Giuseppe Barbalinardo
Title: Master in Physics
Institution: Università degli Studi di Milano-Bicocca
Thesis: “Quantum theory of the inverse Faraday effect for ultrafast magneto-optics”
Defense: 2011

Bachelor students (“Laurea Triennale”)

- **Main supervisor** of Francesco Melone (matr. 886751)
Title: Bachelor in Physics
Institution: Università degli Studi di Milano
Thesis: “Electronic properties of vanadyl tetraphenylporphyrin molecules from first principle calculations”
Defense: 14/12/2020
- **Co-supervisor** of Federico Orlando (matr. 867249)
Title: Bachelor in Physics
Institution: Università degli Studi di Milano
Thesis: “Study of the magnetic properties and spin patterning of a 2D Cr4O5 layer by ab initio total energy calculations”
Defense: 26/02/2019
- **Main supervisor** of Laura Batini (matr. 867399)
Title: Bachelor in Physics
Institution: Università degli Studi di Milano
Thesis: “First-principle simulation of core-level spectra in molecules and dependence on tautomerism”
Defense: 18/12/2018
- **Main supervisor** of Nicolas Trojani (matr. 782591)
Title: Bachelor in Physics
Institution: Università degli Studi di Milano
Thesis: “Modellizzazione di effetti eccitonici nell'interazione tra raggi-X e materia”
Defense: 25/02/2016
- **Co-supervisor** of Pietro Torta (matr. 814287)
Title: Bachelor in Physics
Institution: Università degli Studi di Milano
Thesis: “Struttura elettronica di atomi a molti elettroni: implementazione del metodo di Hartree-Fock”
Defense: 21/04/2016
- **Co-supervisor** of Giacomo Mangiagalli
Title: Bachelor in Physics
Institution: Università degli Studi di Milano-Bicocca
Thesis: “Trasporto di carica e tempi di vita in sistemi ibridi di interesse fotovoltaico”
Defense: 2013
- **Co-supervisor** of Daniele Giofrè
Title: Bachelor in Physics
Institution: Università degli Studi di Milano-Bicocca
Thesis: “Proprietà elettroniche di molecole aromatiche cicliche”
Defense: 2011

ERASMUS students

- **Internship supervisor** of Zongyun Yang
Sending institution: Sorbonne, Paris (France)
Host institution: Università degli Studi di Milano
Internship title: “Electronic, Energetic and Spectral Properties in Mixed sp¹/sp² Carbon Nano-structures and Molecules by First Principle Methods”
Duration: 3 months (01/06/2019-31/08/2019)

8.3 Software tutorials

- Tutor and organizer of seminars in the Ph.D school of the University of Pavia: “Quantum-ESPRESSO mini-tutorial”, 1 year (2013-2014), 4h.
- Teacher at 6 editions of Quantum-ESPRESSO tutorials (package for simulation of electronic, structural and dynamical properties of materials):
 - Advanced Quantum ESPRESSO school: Hubbard and Koopmans functionals from linear response, University of Pavia, 28 August – 01 September 2023 (to be held);
 - African School on Electronic Structure Methods and Applications, AIMS (African Institute for Mathematical Sciences) Muizenberg, South Africa, 14-25 July 2008;
 - Summer School on Computational Materials Science: Ab Initio Molecular Dynamics Simulation Methods in Chemistry, University of Illinois at Urbana-Champaign, US, 2-4 August 2006;
 - Tutorial on the ab-initio simulation of the electronic, structural and dynamical properties of materials, SLACS and University di Cagliari, 26-30 September 2005;
 - ICTP – INFM-DEMOCRITOS – ISMO-IUT School on Electronic-structure calculations and their applications in materials science, Technical University of Isfahan, Iran, 25 April - 6 May 2005;
 - A hands-on introduction to the ESPRESSO package, Democritos and ICTP, Trieste, 17-21 January 2005
- Programmer of JAVA applets with Physics demonstrations for the training of high-school students, within the project “Fare Scienza con il Computer” by the CNR-INFM CRS Democritos (2009-2010).
- Tutor for the project “Training of University Students with the PWSCF code”: tutorials for the Physics degree at Università degli Studi di Trieste, 2 years (2004-2005 and 2005-2006).

9 Evaluation of research activities

- **Committee member for the selection of assistant professors (RTD):**
 - RTD-B at the University of Pavia, Italy (appointed on 11/04/2023)
 - RTD-A at the University of Milano-Bicocca, Italy (appointed on 31/01/2023)
 - RTD-A at the University of Trento, Italy (appointed on 21/12/2022)
- **Committee member for the selection of 6 post-doctoral positions** at the University of Milano.
- **Committee member for the admission to the Ph.D. in Physics** at the University of Milano, XXXVI cycle (2020), 119 candidates.
- **Referee** for 2 **grants**: calls by the Deutsche Forschungsgemeinschaft (Germany) and by the National Science Center (Poland).
- **Reviewer for peer-reviewed journals** with impact factor, for a total of over 150 reviews including:
 - Physical Review Letters (23 articles), Physical Review B (11 articles), Phys. Rev. Applied (3 articles) and Phys. Rev. Materials (3 articles) by the American Physical Society;
 - Journal of Physical Chemistry C (18 articles), ACS Advanced Materials and Interfaces (4), ACS Catalysis (1), ACS Omega (2), Journal of Physical Chemistry Letters (2), Journal of Chemical Theory and Computation (2), Physical Chemistry Chemical Physics (5), by the American Chemical Society;
 - Nature Communications (3 articles) and Scientific Reports (3 article) by the Nature Publishing Group;
 - Reports on Progress in Physics (2 article) by the Institute of Physics;
 - Nanoscale (1 article) by the Royal Society of Chemistry.
- **Referee** for 8 projects for HPC access (ISCRA initiative).
- **Member of Ph.D. evaluation committees:**
 - Ph.D. in Materials Science and Nanotechnology, University of Milano-Bicocca (March 2023).
 - Ph.D. in Physics, University of Cagliari, XXXII cycle (February 2020).
 - PhD in Physics of Nanostructures and Advanced Materials at Universidad del Pais Vasco, Donostia, Spain, DATA chair of the evaluation committee.
- **External evaluator of two Ph.D. theses** (Paolo Carrozzo, Ph.D. in Energy and Nuclear Science and Technology at Politecnico di Milano, 2014; Patrick Serafini, Ph.D. in Energy and Nuclear Science and Technology at Politecnico di Milano, 2022).

Data

22/07/2023

Luogo

PAVIA