ALLEGATO B

UNIVERSITÀ DEGLI STUDI DI MILANO
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Guido Fratesi
CURRICULUM VITAE

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

COGNOME	**FRATESI**
NOME	**GUIDO**
DATA DI NASCITA	28 SETTEMBRE 1978

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1 Recent research focus and activities

This section summarizes the activities during the 3-year fixed-term researcher (RTDA) at Università degli Studi di Milano (UNIMI), from 20/12/2013 to 19/12/2016.

It is UNIMI policy that researchers concluding such appointment present a Portfolio of research and teaching activities, which is sent for evaluation to two external assessors. A numerical score is then attributed by a Department committee, on a 1-100 scale. GF's Portfolio resulted in a score 91/100, the highest among those evaluated by the Physics Department in 2016.

The research activity of GF focuses on the theoretical study of electronic, structural and spectroscopic properties of condensed matter systems, in tight connection with experiments. In particular, his interests span the **ab-initio investigation of real materials**, including surfaces of solids, molecular adsorbates, and nanostructures. Beside applications GF worked on the **development of theoretical methods and computational tools** for an improved description of the system's electronic structure at the nanometer lengthscale, with no empirical parameters.

The **main topics** developed in the 3-year period are:

I. Hybrid interfaces between adsorbed organic molecules and metals/semiconductors.

II. Two-dimensional materials, graphene and emerging atom-thick systems.

III. Thin magnetic films on magnetic surfaces.

As **main achievements** in the same period one mentions:

- The development of a Green's function approach, adopting concepts from the fields of quantum-transport simulations and theoretical core-level spectroscopy, to determine the **charge injection from a molecule to a substrate** in the presence of core-level excitations (as occurring in the experiments) [Ref31-JPCC-2014]. The method has been applied to real systems in collaboration with world-leading experimental groups showing the opening of back (substrate-to-molecule) charge transfer induced by the excitation [Ref48-PCCP-2016]. (Topic-I)
- The theoretical characterization and interpretation of experimental data for the **adsorption properties** of various technologically relevant molecules [Ref37-2015-JPCL; Ref39-2015-JPCC; Ref43-2015-ACSNano]. (Topic-I)
- Highlighting the disruption of the spin-polarization of **covalently-functionalized graphene** by electronic core-level excitations [Ref45-2016-SciRep]. (Topic-II)
- Demonstrating the delocalization onto the substrate, and subsequent metallic character of the optically excited states, for **2D silicon grown on a metal** [Ref50-2016-ACSNano; Ref41-2015-PRB]. (Topic-II)
- Showing the impact of the **softening of a metastable magnetic film** on the atomic diffusion as a structural transition is approached [Ref34-2015-PRL]. (Topic-III)

The **development of theoretical and methodological tools** has been instrumental to achieve the results above. Most of those developments are now part of software packages freely available to the community and of world-wide use, especially Quantum-ESPRESSO (of which he is contributor [Ref14-2009-JPCM; >5000 citations]).

Since 2014 GF published 20 articles (50 since 2003) in international, peer reviewed high-quality journals with Impact Factor (18/20 are classified in the First Quartile by the Journal Citation Reports) and 1 conference article, and he delivered 16 talks/seminars (of which 4 invited to international conferences).

In the same period GF has been PI of a project for high-performance computing (3 more projects earlier), responsible of grants obtained from external bodies for a conference organization, and successfully applied for research grants from his host University. GF presented, as PI of the local research unit, two research projects, under EU-H2020 and MIUR-Italian ministry calls both having a strong experimental counterpart.

GF supervised/co-supervised 5 undergraduate and 3 Ph.D. students. GF has been teaching Surface Physics and Mathematical Methods for Physics, for the Master and Bachelor's degree in Physics, respectively.

He has been organizer (and the lead local organizer) of WDPS17 (http://wdps17.fisica.unimi.it), a workshop belonging to an international series established since 1983 as a regular meeting point of experimental/theoretical surface physicists.

GF contributed to the organizational activity of the Physics Department by operating as webmaster of the Department website and member of the outreach committee.

2 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: https://cm.sissa.it/thesis/2005/fratesi
- 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)

3 Research positions held

Fixed-term University researcher (RTD-A) (3 years):

(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).

4 Scientific output

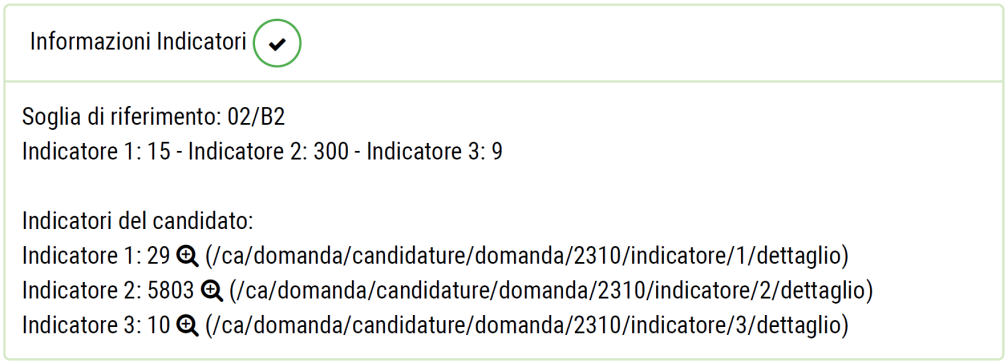
4.1 Overview of the scientific production

- **H index: 11** (Source: Web of Science, Dec. 29th 2016)
- **N. of citations: 5930** (Source: Web of Science, Dec. 29th 2016)
- **50 research articles** published on international peer-reviewed journals with Impact Factor.
    - Classification according to the Journal Citation Reports:
      39/50 first quartile (Q1)
      9/50 second quartile (Q2)
      2/50 third quartile (Q3)
- **2 conference papers**
- **1 international conference organized**
- **5 invited talks** at international conferences and workshops
- **22 oral presentations** at international conferences and workshops
- **17 invited seminars** at research institutes / Universities

"Abilitazione Scientifica Nazionale" (ASN): GF has applied on 30/11/2016 to the National Scientific Qualification for associate professors in the sector 02/B2 (ASN, DM 602 29/07/2016). The application is currently under evaluation.
All three thresholds established by the MIUR of Italy for this sector are fulfilled:

- ✔ N. of articles in the five years: **29**(*) (> threshold: **15**)
- ✔ N. of citations in the ten years: **5803**(*) (> threshold: **300**)
- ✔ H-index for publications in the five years: **10**(*) (> threshold: **9**)

(*) Source: MIUR https://asn16.cineca.it/ca/domanda/2310/show (password protected), 23/12/2016:



4.2 Publications

Publications on peer-reviewed journals with Impact Factor

The 12 publications selected for this application are highlighted in bold.

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 Just Accepted (29th Dec. 2016)
URL and DOI: http://dx.doi.org/10.1021/acsnano.6b07593
IF (2015): 13.334; Quartile: Q1 (6/144 Chemistry, Physical), ISSN: 1936-0851
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)
URL and DOI: http://dx.doi.org/10.1103/PhysRevB.94.195155
IF (2015): 3.718; Quartile: Q1 (16/67 Physics, Condensed Matter), ISSN: 1098-0121
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)
URL and DOI: http://dx.doi.org/10.1039/C6CP04099C
IF (2015): 4.449; Quartile: Q1 (6/35 Physics, Atomic, Molecular & Chemical), ISSN: 1463-9084
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)
URL and DOI: http://dx.doi.org/10.1016/j.elspec.2016.06.002
IF (2015): 1.561; Quartile: Q3 (25/43 Spectroscopy), ISSN: 0368-2048

46) D. Giofré, D. Ceresoli, G. Fratesi, and M.I. Trioni
"Electronic transport in B-N substituted bilayer graphene nanojunctions"
Phys. Rev. B 93, 205420 (2016)
URL and DOI: http://dx.doi.org/10.1103/PhysRevB.93.205420
IF (2015): 3.718; Quartile: Q1 (16/67 Physics, Condensed Matter), ISSN: 1098-0121

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)
URL and DOI: http://dx.doi.org/10.1038/srep24603
IF (2015): 5.228; Quartile: Q1 (7/63 Multidisciplinary Sciences), ISSN: 2045-2322
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)
URL and DOI: http://dx.doi.org/10.1021/acs.jpcc.5b11885
IF (2015): 4.509; Quartile: Q1 (30/144 Chemistry, Physical), ISSN: 1932-7447

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)
URL and DOI: http://dx.doi.org/10.1021/acsnano.5b07145
IF (2015): 13.334; Quartile: Q1 (6/144 Chemistry, Physical), ISSN: 1936-0851

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)
URL and DOI: http://dx.doi.org/10.3762/bjnano.6.230
IF (2015): 2.778; Quartile: Q1 (30/145 Physics, Applied), ISSN: 2190-4286
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)
URL and DOI: http://dx.doi.org/10.1103/PhysRevB.92.165427
IF (2015): 3.718; Quartile: Q1 (16/67 Physics, Condensed Matter), ISSN: 1098-0121
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)
URL and DOI: http://dx.doi.org/10.1103/PhysRevB.92.115434
IF (2015): 3.718; Quartile: Q1 (16/67 Physics, Condensed Matter), ISSN: 1098-0121
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)
URL and DOI: http://dx.doi.org/10.1021/jp512337y
IF (2015): 4.509; Quartile: Q1 (30/144 Chemistry, Physical), ISSN: 1932-7447

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)
URL and DOI: http://dx.doi.org/10.1088/0953-8984/27/8/085003
IF (2015): 2.209; Quartile: Q2 (28/67 Physics, Condensed Matter), ISSN: 0953-8984

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)
URL and DOI: http://dx.doi.org/10.1021/jz502523u
IF (2015): 8.539; Quartile: Q1 (1/35 Physics, Atomic, Molecular & Chemical), ISSN: 1948-7185
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)
URL and DOI: http://dx.doi.org/10.1039/C4CP04476B
IF (2015): 4.449; Quartile: Q1 (6/35 Physics, Atomic, Molecular & Chemical), ISSN: 1463-9084

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)
URL and DOI: http://dx.doi.org/10.1103/PhysRevB.90.201401
IF (2015): 3.718; Quartile: Q1 (16/67 Physics, Condensed Matter), ISSN: 1098-0121
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)
URL and DOI: http://dx.doi.org/10.1103/PhysRevLett.113.046102
IF (2015): 7.645; Quartile: Q1 (6/80, Physics, Multidisciplinary), ISSN: 1079-7114
Role of GF: Sole theoretical author

33) F. Sirotti, N. Beaulieu, A. Bendounan, M. G. Silly, C. Chauvet, G. Malinowski, G. Fratesi, V. Véniard, and G. Onida
“Multiphoton k-resolved photoemission from gold surface states with 800-nm femtosecond laser pulses”
Phys. Rev. B 90, 035401 (2014)
URL and DOI: http://dx.doi.org/10.1103/PhysRevB.90.035401
IF (2015): 3.718; Quartile: Q1 (16/67 Physics, Condensed Matter), ISSN: 1098-0121
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)
URL and DOI: http://dx.doi.org/10.1039/C4CP01625D
IF (2015): 4.449; Quartile: Q1 (6/35 Physics, Atomic, Molecular & Chemical), ISSN: 1463-9084
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)
URL and DOI: http://dx.doi.org/10.1021/jp500520k
IF (2015): 4.509; Quartile: Q1 (30/144 Chemistry, Physical), ISSN: 1932-7447
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)
URL and DOI: http://dx.doi.org/10.1103/PhysRevB.87.235431
IF (2015): 3.718; Quartile: Q1 (16/67 Physics, Condensed Matter), ISSN: 1098-0121
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)
URL and DOI: http://dx.doi.org/10.1021/jp312569q
IF (2015): 4.509; Quartile: Q1 (30/144 Chemistry, Physical), ISSN: 1932-7447
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)
URL and DOI: http://dx.doi.org/10.1103/PhysRevB.87.075415
IF (2015): 3.718; Quartile: Q1 (16/67 Physics, Condensed Matter), ISSN: 1098-0121

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)
URL and DOI: http://dx.doi.org/10.1103/PhysRevB.87.085403
IF (2015): 3.718; Quartile: Q1 (16/67 Physics, Condensed Matter), ISSN: 1098-0121
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)
URL and DOI: http://dx.doi.org/10.1021/jp309566s
IF (2015): 4.509; Quartile: Q1 (30/144 Chemistry, Physical), ISSN: 1932-7447

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)
URL and DOI: http://dx.doi.org/10.1103/PhysRevLett.109.126401
IF (2015): 7.645; Quartile: Q1 (6/80, Physics, Multidisciplinary), ISSN: 1079-7114
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)
URL and DOI: http://dx.doi.org/10.1103/PhysRevB.84.155424
IF (2015): 3.718; Quartile: Q1 (16/67 Physics, Condensed Matter), ISSN: 1098-0121
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)
URL and DOI: http://dx.doi.org/10.1021/jp2005875
IF (2015): 2.883; Quartile: Q2 (11/35 Physics, Atomic, Molecular & Chemical), ISSN: 1089-5639

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)
URL and DOI: http://dx.doi.org/10.1021/am200267u
IF (2015): 7.145; Quartile: Q1 (25/271 Materials Science, Multidisciplinary), ISSN: 1944-8244
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)
URL and DOI: http://dx.doi.org/10.1103/PhysRevB.83.153404
IF (2015): 3.718; Quartile: Q1 (16/67 Physics, Condensed Matter), ISSN: 1098-0121
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)
URL and DOI: http://dx.doi.org/10.1140/epjb/e2010-10616-8
IF (2015): 1.223; Quartile: Q3 (47/67 Physics, Condensed Matter), ISSN: 1434-6028

19) G. Fratesi
“First-principles investigation of the early stages of Pd adsorption on Au(111)”
J. Phys.-Condens. Matter 23, 015001 (2011)
URL and DOI: http://dx.doi.org/10.1088/0953-8984/23/1/015001
IF (2015): 2.209; Quartile: Q2 (28/67 Physics, Condensed Matter), ISSN: 0953-8984
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)
URL and DOI: http://dx.doi.org/10.1103/PhysRevB.82.081413
IF (2015): 3.718; Quartile: Q1 (16/67 Physics, Condensed Matter), ISSN: 1098-0121
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)
URL and DOI: http://dx.doi.org/10.1088/0953-8984/22/30/304005
IF (2015): 2.209; Quartile: Q2 (28/67 Physics, Condensed Matter), ISSN: 0953-8984
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)
URL and DOI: http://dx.doi.org/10.1103/PhysRevB.81.115450
IF (2015): 3.718; Quartile: Q1 (16/67 Physics, Condensed Matter), ISSN: 1098-0121
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)
URL and DOI: http://dx.doi.org/10.1103/PhysRevB.80.125426
IF (2015): 3.718; Quartile: Q1 (16/67 Physics, Condensed Matter), ISSN: 1098-0121
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)
URL and DOI: http://dx.doi.org/10.1088/0953-8984/21/39/395502
IF (2015): 2.209; Quartile: Q2 (28/67 Physics, Condensed Matter), ISSN: 0953-8984

13) G. Fratesi
“Potential energy surface of alkali atoms adsorbed on Cu(001)”
Phys. Rev. B 80, 045422 (2009)
URL and DOI: http://dx.doi.org/10.1103/PhysRevB.80.045422
IF (2015): 3.718; Quartile: Q1 (16/67 Physics, Condensed Matter), ISSN: 1098-0121
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)
URL and DOI: http://dx.doi.org/10.1088/0953-8984/21/26/264003
IF (2015): 2.209; Quartile: Q2 (28/67 Physics, Condensed Matter), ISSN: 0953-8984

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)
URL and DOI: http://dx.doi.org/10.1103/PhysRevB.79.165115
IF (2015): 3.718; Quartile: Q1 (16/67 Physics, Condensed Matter), ISSN: 1098-0121

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)
URL and DOI: http://dx.doi.org/10.1103/PhysRevB.78.205111
IF (2015): 3.718; Quartile: Q1 (16/67 Physics, Condensed Matter), ISSN: 1098-0121
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)
URL and DOI: http://dx.doi.org/10.1103/PhysRevB.77.235444
IF (2015): 3.718; Quartile: Q1 (16/67 Physics, Condensed Matter), ISSN: 1098-0121
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)
URL and DOI: http://dx.doi.org/http://dx.doi.org/10.1021/jp076037o
IF (2015): 2.883; Quartile: Q2 (11/35 Physics, Atomic, Molecular & Chemical), ISSN: 1089-5639
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)
URL and DOI: http://dx.doi.org/10.1021/jp074134b
IF (2015): 4.509; Quartile: Q1 (30/144 Chemistry, Physical), ISSN: 1932-7447
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)
URL and DOI: http://dx.doi.org/10.1088/0953-8984/19/30/305005
IF (2015): 2.209; Quartile: Q2 (28/67 Physics, Condensed Matter), ISSN: 0953-8984

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)
URL and DOI: http://dx.doi.org/10.1021/ja060114w
IF (2015): 13.038; Quartile: Q1 (10/163 Chemistry, Multidisciplinary), ISSN: 0002-7863

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)
URL and DOI: http://dx.doi.org/10.1063/1.2219448
IF (2015): 2.894; Quartile: Q2 (9/35 Physics, Atomic, Molecular & Chemical), ISSN: 0021-

9606
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)
URL and DOI: http://dx.doi.org/10.1002/anie.200502007
IF (2015): 11.709; Quartile: Q1 (11/163 Chemistry, Multidisciplinary), ISSN: 1433-7851
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)
URL and DOI: http://dx.doi.org/10.1103/PhysRevB.69.245113
IF (2015): 3.718; Quartile: Q1 (16/67 Physics, Condensed Matter), ISSN: 1098-0121
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)
URL and DOI: http://dx.doi.org/10.1103/PhysRevB.68.195404
IF (2015): 3.718; Quartile: Q1 (16/67 Physics, Condensed Matter), ISSN: 1098-0121
Role of GF: First author

Conference papers

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

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: https://cm.sissa.it/thesis/2005/fratesi

4.3 Conferences and seminars

Organization of international conferences

- **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.
    - Sole responsible and developer of the workshop website.

Invited talks at international conferences and workshops

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

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

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)

4.4 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 paper [Ref14-2009-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]. This feature will be included in the future releases of YAMBO.
- 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].

5 Coordination of research activities

- **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 in preparation (one more to follow).
- **Principal investigator** in the following 4 projects for high-performance computing (HPC):
  - 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.
- **Leading scientist** in scientific collaborations not necessarily related to funded projects, as demonstrated by being last author (i.e., the “senior” scientist) in the related papers:
  - “Femtomagnetism in graphene induced by core level excitation of organic adsorbates”, Scientific Reports 6, 24603 (2016): result of a collaboration with Milano-Bicocca involving 5 scientists.
  - “Core-level spectra and molecular deformation in adsorption: V-shaped pentacene on Al(001)”, Beilstein J. Nanotechnol. 6, 2242 (2015): result of a collaboration with Milano-Bicocca and CNR-IOM, Trieste, involving 5 scientists.
  - “Modeling elastic charge transfer times including the effect of structural fluctuations at hybrid organic-semiconductor interfaces”, manuscript in preparation (presented at conferences in 2016): result of a collaboration with CSIC (San Sebastian, ES), Milano-Bicocca, and the Princeton University (Princeton, NJ), involving 6 scientists.

6 Other scientific and organizational responsibilities

- **Local Coordinator** of the European Doctorate in Physics and Chemistry of Advanced Materials (PCAM) (http://www.pcam-doctorate.eu/networks-partners/card.php?partner=University+of+Milan), established with 15 partners across Europe.
- **Participant** to the activities of the following European scientific facilities:

- 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 takes part through the Solid State Physics Theory Group of UNIMI and has been scientist in charge of a user project (see Section 5).
- Nanoscience Foundries and Fine Analysis (NFFA, www.nffa.eu)
  This international collaboration holds a 11MEUR EU grant (grant agreement no. 654360 from 01/09/2015 to 31/08/2019) and includes UNIMI and 19 partner institutions across Europe.

- **Co-responsible** of a 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).
- **Webmaster** of the Physics Department website (www.fisica.unimi.it) since November 2015, 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).
- **Member** of the Ph.D. Council, Department Council, and Teaching Council, at the Physics Department of UNIMI, during the 3-year research position (2013-2016).

7 Research grants

- 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.
- Grants for access to 4 high-performance computing (HPC) projects, already mentioned in Section 5 above, through the Italian SuperComputing Resource Allocation – ISCRA, with contributions in kind:(*)
  - **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), corresponding to a cost/hour of about 0.013EUR/h+VAT from which the given estimate is deduced.

- Research grants from UNIMI:
  - **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.

Positively evaluated projects since 2013

- 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.

8 Scientific collaborations

National and international collaborations

Scientific collaborations (currently active but not necessarily related to running funded projects) with scientists at various international and national institutions include:

- CSIC (ES), Dr. Daniel Sanchez-Portal
- Princeton University (NJ), Prof. Annabella Selloni
- Columbia University (NY), Prof. Latha Venkataraman
- Graz University of Technology (AT), Prof. Egbert Zojer
- University of Ljubljana (SLO), Prof. Dean Cvetko
- Synchrotron SOLEIL (FR), Dr. Fausto Sirotti
- CNR-MDM (Agrate Brianza), Dr. Alessandro Molle
- CNR-IOM (Trieste), Prof. Alberto Morgante; Dr. Luca Floreano
- Sincrotrone ELETTRA (Trieste), Dr. Andrea Goldoni; Dr. Paolo Moras
- Università di Milano-Bicocca, Prof. Gian Paolo Brivio
- Politecnico di Milano, Prof. Marco Finazzi; Dr. Francesco Scotognella

Participation to funded projects

- 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 CARIPLO, 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).

9 Teaching activities

9.1 Institutional courses at Universities

Teaching duties during the RTDA contract in UNIMI

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 (ongoing) 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. Lectures held by Prof. Luca Guido Molinari. GF has been in charge of 20h in class/year full-class tutorials.

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.

9.2 Supervision of students

GF has been supervisor/co-supervisor of 3 graduate students, 4 master students (1 as main supervisor), and 4 bachelor students (1 as main supervisor):

Graduate students

- **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

- **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 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: expected July 2017

Master students (“Laurea Magistrale”)

- **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 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 Giofré
  Title: Bachelor in Physics
  Institution: Università degli Studi di Milano-Bicocca
  Thesis: “Proprietà elettroniche di molecole aromatiche cicliche”
  Defense: 2011

9.3 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 5 editions of the Quantum-ESPRESSO tutorial (package for simulation of electronic, structural and dynamical properties of materials):
  - 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).

10 Evaluation of research activities

- **Reviewer for peer-reviewed journals** with impact factor, for a total of 43 reviews including:
  - Physical Review Letters (16 articles) [IF 7.645] by the American Physical Society;
  - Physical Review B (4 articles) [IF 3.718] by the American Physical Society;
  - Scientific Reports (1 article) [IF 5.228] by the Nature Publishing Group;
  - ACSCatalysis (1 article) [IF 9.307] by the American Chemical Society;
  - Journal of Physical Chemistry Letters (1 article) [IF 8.539] by the American Chemical Society;
  - Journal of Physical Chemistry C (2 articles) [IF 4.509] by the American Chemical Society;
  - Journal of Chemical Theory and Computation (2 articles) [IF 5.301] by the American Chemical Society;
  - Physical Chemistry Chemical Physics (1 article) [IF 4.449] by the American Chemical Society.
- **Reviewer** of 1 conference paper (Journal of Physics: Conference Series).
- **Referee** for 2 projects for HPC access (ISCRA initiative).
- **External evaluator of a Ph.D. thesis** (Paolo Carrozzo, Ph.D. in Energy and Nuclear Science and Technology at Politecnico di Milano).

Data 29/12/2016 Luogo PAVIA