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SIMONA ACHILLI - CURRICULUM VITAE

PERSONAL DATA

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1. CURRENT POSITION

Fixed-term University Researcher (Ricercatore a tempo determinato RTD-A)

Università degli Studi di Milano, Dipartimento di Fisica "Aldo Pontremoli".

Italian scientific sectors:

SSD: FIS/03 (Fisica della materia)

SC: 02/B2 (Fisica teorica della materia)

2. NATIONAL SCIENTIFIC ABILITATION

Abilitazione scientifica nazionale a professore di seconda fascia (Associate Professor).

SSD: FIS/03 (Fisica della materia)

SC: 02/B2 (Fisica teorica della materia)

3. RESEARCH POSITIONS HELD

Feb. 2020 – Present **Fixed-term University Researcher (Ricercatore a tempo determinato RTD-A)**
Università degli Studi di Milano, Dipartimento di Fisica "Aldo Pontremoli".

Feb. 2019 – Jan. 2020 **Senior Post Doctoral Fellowship**
Catalan Institute of Nanoscience and Nanotechnology.
Research projects:
"Topological valley currents in graphene/hBN".
"Tuning the magnetoresistance of carbon nanotubes by functionalization with magnetic molecules".

Feb. 2017 – Jan. 2019 **Post Doctoral Fellowship ("Assegno di ricerca di tipo B")**
Università degli Studi di Milano, Dipartimento di Fisica.
Research project:
"Deep atomic States of Germanium dopants in Silicon".

Mar. 2015 – Jan. 2017 **Post Doctoral Fellowship ("Assegno di ricerca di tipo A")**
Università Cattolica del Sacro Cuore, Dipartimento di Fisica, Brescia.
Research Project: "Joined theoretical and experimental investigation of physical properties of graphene interfaces".

Jan. 2012 – Feb. 2015 **Post Doctoral Fellowship ("Assegno di ricerca di tipo A")**
Università degli Studi di Milano, Dipartimento di Chimica.
Research Project: "Theoretical study of the electronic transport in defective graphene and carbon nanostructures".

Oct. - Nov. 2011 **Visiting Researcher (2 months)**
Donostia International Physics Center, San Sebastian.
Opportunity of enlarging the network of international collaborations under the supervision of Prof. E. Chulkov.

Apr. 2010 – Apr. 2011 **Post Doctoral Fellowship ("Assegno di ricerca di tipo B")**
Università di Milano Bicocca, Dipartimento di Scienze dei Materiali.
Research project: "Theoretical study of the spin polarized tunnel microscopy".

Feb. - Jun. 2008

Visiting Researcher (4 months)

Donostia International Physics Center, San Sebastian.

Research activity focused on the implementation of a DFT embedding code for the description of an isolated adatom on an extended substrate.

Three Maternity leaves:

From Sep. 2009 to Jan. 2010 (5 months)

From Feb. 2012 to Jul. 2012 (5 months)

From Jun. 2014 to Feb. 2015 (8 months)

4. EDUCATION

May 3rd 2010

PhD in Materials Science – Università di Milano Bicocca.

Achieved in 3 years and 5 months (including 5 month of maternity leave)

Dissertation: "Spectral properties of adsorbates on metal surfaces via the embedding method". Supervisor: Dr. M. I. Trioni.

and

European Doctorate in Physics and Chemistry of Advanced Materials

Attending courses (300 hours) of the Master in Nanoscience of the University of Basque Countries, San Sebastian.

Jul. 17th 2006

Master Degree in Physics (Laurea Magistrale) - Università di Milano Bicocca.

Grade: 110/110 cum laude. Achieved in 1 year and 8 months

Thesis title: "Studio teorico delle proprietà elettroniche e magnetiche di film sottili di Fe/Cu(001)". Supervisor: Prof. G. P. Brivio.

Oct. 4th 2004

Bachelor Degree in Physics (Laurea Triennale) - Università di Milano Bicocca.

Grade: 110/110 cum laude. Achieved in 3 years

Thesis title: "Studio teorico computazionale di spettri Auger di adatom su superfici metalliche". Supervisor: Prof. G. P. Brivio.

5. PARTICIPATION TO RESEARCH GROUPS

During my research activity I joined 5 research groups, collaborating to research, management of research projects, supervision of students, scientific publications.

- **2006-2010:** "Theory of adsorption and of solid surface group".

Università di Milano Bicocca, Dipartimento di Scienze dei Materiali.

13 scientific papers published (1-13 in the "Publication List").

- **2012-2015:** "Chemical Dynamics Theory Group"

<http://users.unimi.it/cdtg/index.php?page=members&personale=martinazzo>

Università degli Studi di Milano, Dipartimento di Chimica.

3 scientific papers published (Ref. 14, 18, 25 in the "Publication list").

- **2015-2017** “Interdisciplinary Laboratories for Advanced Materials Physics”

<https://centridiricerca.unicatt.it/ilamp-home>

Università Cattolica del Sacro Cuore, Dip. Di Fisica, Brescia.

Director: Prof. Gabriele Ferrini.

5 scientific papers published + 1 reply (Refs. 16, 17, 21, 22, 26, 28, in the “Publication list”).

- **2017-2019** and **2020-present**: “Solid State Physics Theory Group”

<http://www.fisica.unimi.it/ecm/home/ricerca/gruppi-di-ricerca/struttura-della-materia/spettroscopia-teorica>

Università degli Studi di Milano, Dip. di Fisica.

≥ 15 scientific papers published.

- **2019 – 2020**: “Theory and Simulation Group”

<https://icn2.cat/en/theory-and-simulation-group>

Catalan Institute of Nanoscience and Nanotechnology, Barcelona.

Director: Pablo Ordejón.

1 scientific paper published (Ref. 47 in the “Publication list”).

Other affiliations:

- **Jan 2014 – Mar 2018** **Associated Member of “Istituto di Scienze e Tecnologie Molecolari”**

Consiglio Nazionale delle Ricerche (ISTM-CNR), Milano. <https://www.istm.cnr.it/>

Director: Rinaldo Psaro.

3 scientific papers published (Ref. 15, 20, 28 in the “Publication list”).

- **Mar 2020 – Present** **Associated member of INFN-Gruppo 4** (Sezione di Milano)

Research collaborations:

- Dr. L. da Costa Pereira - Institute for Nuclear and Radiation Physics, Leuven, Belgium.
- Prof. P. Ordejón, Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain.
- Prof. Z. Zanolli - Utrecht University, The Netherlands.
- Prof. A. Brambilla and co-workers, Scanning Tunneling Microscopy Laboratory, Politecnico di Milano.
- Prof. C. Casari, Nano-LAB, Politecnico di Milano
- Dr. A. Molle - CNR-IMM Unit, Agrate Brianza.
- Prof. S. Pagliara, Università Cattolica del Sacro Cuore, Brescia.
- Prof. E. Chulkov, Donostia International Physics Center, San Sebastian, Spain.

6. RESEARCH FOCUS AND MAIN ACHIEVEMENTS

My research activity is devoted to the theoretical study of electronic, magnetic and transport properties of low dimensional systems, interfaces and functionalized materials, mainly studied with ab initio Density Functional Theory methods.

Most of my research has been performed in tight collaborations with experimental groups.

Since my Master Degree I carried on different Research Lines (RL) as summarized below:

RL.1 Extended Substrate Approach

In my initial research, during Bachelor, Master and PhD, I exploited the method proposed by J. Inglesfield for the ab initio study of semi-infinite surfaces and interfaces. By introducing appropriate boundary conditions the method allows one to overcome the limit of the fictitious periodicity required by standard slab calculations and permits to describe both continuous bands and discrete states, giving access for example to the elastic lifetime of surface states (energy broadening due to the hybridization with the extended substrate states).

In this context, during my PhD, I have implemented and coded the necessary routines for the study of an isolated adatom on extended metal substrates. The major improvement achieved was a more realistic modeling of the substrate with respect to the already available jellium model. The theory and the code were successfully applied for the interpretation of spectroscopic measurements in a joined theoretical-experimental study of desorption processes induced by electronic excitations (Ref. 5 in the publication list).

RL.2 Electronic transport in low dimensional heterostructures

My work exploits the Non Equilibrium Green's function theory to study the ballistic electronic transport through 2D materials and heterostructures, also in presence of an external bias. This topic is strictly related to RL.1, from which my research was started, being the extended substrate approach a required guess to describe propagating electronic states.

My studies in this field concerned the electronic transport in carbon chains and patterned graphene. As main result I showed that the decoration of graphene with hydrogen dimers lines allows the confinement of electronic current, as in nanoribbons (Ref. 14 in the publication list). I also focused on the transport properties of doped graphene, studying the spin-filtering effect induced by the adsorption of magnetic atoms (Refs. 15 and 20 in the publication list). Moreover I developed a semiclassical description of the graphene conductivity in diffusive regime in order to address the role of neutral scatterers in limiting the transport properties of the carbon sheet. This research line is currently active.

RL.3 Theoretical Spectroscopy

This is the wide research field devoted to predicting spectroscopic properties of different materials via ab initio methods. My activity started in 2004, in the context of the European Theoretical Spectroscopy Facility (ETSF) network and benefits of the strong ongoing collaboration with two experimental groups of Politecnico di Milano, the ILAMP laboratories of Università Cattolica del Sacro Cuore, the group of A. Molle (CNR).

Among the spectroscopic properties I predicted through ab initio electronic structure calculations one can mention those explaining the inverse-, linear- and time-resolved photoemission experiments, as well as the simulation of STM and STS images to compare with experimental ones.

Among the studied systems are:

- hybrid sp/sp² carbon systems on metals
- graphene on metal surfaces
- functionalized carbon nanotubes
- organic molecules on magnetic and non magnetic substrates
- graphene doped with substitutional magnetic atoms

This research line is currently active.

RL.4 Point defects in semiconductors for high temperature q-bits

This is the most recent RL that I developed during the last three years in collaboration with experimental groups of CNR-IFN and Waseda University (Tokyo). I started this activity by characterizing the excited-state

electronic properties and transport of Ge-vacancy complexes in silicon through a multi-scale approach that combines ab initio + tight binding methods. These point defects, that can be obtained by Ge implantation followed by thermal annealing, appear particularly promising for exploitation as q-bits working at high temperature or Hubbard simulators (Refs. 29 and 43 in the publication list).

Based on these recent achievements I also recently started a project in collaboration with two researchers of Pure and Applied Quantum Mechanic Group of the Physics Department of the University of Milan to study the transport of quantum information through an array of such defects (e.g. random quantum walk).

Perspectives:

In the future I plan to extend both RL.3 and RL.4 towards the inclusion of optical properties.

In particular, concerning RL.4 I will include the effect of phonons with the purpose to extend the formalism to the description of single-photon emitters. This will boost my collaboration with the “Quantum Technology” theoretical group of the Physics Department, tightening the growing links among the Condensed Matter Theory group and colleagues working on quantum computing, quantum metrology, and quantum machine learning.

7. NUMERICAL AND COMPUTATIONAL SKILLS

I am an [experienced user of several ab-initio simulation packages](#), such as SIESTA/TRANSIESTA, QUANTUM ESPRESSO, CRYSTAL, FLEUR.

Software development

- I am a developer of the embedding code (FA code) for the description of isolated adatoms on metal surfaces by a modulated potential model (Ref. 12 in the Publication List).
- I implemented the routines for the calculation of the Zeeman energy due to an external applied magnetic field in the SIESTA code.

8. RESEARCH OUTPUT

8.1 OVERVIEW OF THE SCIENTIFIC PRODUCTION

H-index: 12 (Scopus)

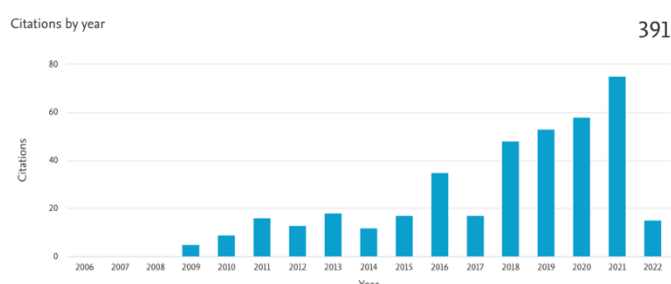
Number of Citations

Scopus: **391**

Scholar: **490**

Author of:

- **47 research articles** in peer reviewed journals (29/47 first quartile Q1)
of which 15 as first author, 5 as unique theoretical author
- **2 reviews**
- **2 conference proceedings** (both as first author)
- **14 invited presentations + 20 oral contributions**



8.2 PUBLICATIONS

Articles on peer-reviewed journals with impact factor

(the 12 publications selected for this application are highlighted in bold)

47. S. Achilli, C. Besson, X. He, P. Ordejón, C. Meyer, Z. Zanolli, "Magnetic properties of coordination clusters with {Mn₄} and {Co₄} antiferromagnetic cores", *Phys. Chem. Chem. Phys.* **24** (6), 3780-3787 (2022); DOI: [10.1039/d1cp03904k](https://doi.org/10.1039/d1cp03904k) ISSN: 1463-9084. IF (2020): 3. 676.
46. S. Mor, V. Gosetti, A. Molina-Sánchez, D. Sangalli, S. Achilli, V. F. Agekyan, P. Franceschini, C. Giannetti, L. Sangaletti, S. Pagliara, "Photoinduced modulation of the excitonic resonance via coupling with coherent phonons in a layered semiconductor", *Phys. Rev. Res.* **3**(4), 043175 (2021); DOI: [10.1103/PhysRevResearch.3.043175](https://doi.org/10.1103/PhysRevResearch.3.043175) ISSN: 2643-1564 (Online).
45. S. Achilli, A. Milani, G. Fratesi, F. Tumino, N. Manini, G. Onida, C. S. Casari, "Graphdiynes interacting with metal surfaces: First-principles electronic and vibrational properties", *2D Mater.* **8** (4), 044014 (2021); DOI: [10.1088/2053-1583/ac26ad](https://doi.org/10.1088/2053-1583/ac26ad) ISSN: 20531583 – E-ISSN:2053-1583. IF (2020): 8.7.
44. D. S. Dhungana, C. Grazianetti, C. Martella, S. Achilli, G. Fratesi, A. Molle, "Two-Dimensional Silicene–Stanene Heterostructures by Epitaxy", *Adv. Funct. Mater.* **31** (30), 2102797 (2021); DOI: [10.1002/adfm.202102797](https://doi.org/10.1002/adfm.202102797) ISSN: 1616-301X (print). 1616-3028 (online). IF (2020): 18.808.
43. S. Achilli, N. H. Le, G. Fratesi, N. Manini, G. Onida, M. Turchetti, G. Ferrari, T. Shinada, T. Tanii, E. Prati, "Position-Controlled Functionalization of Vacancies in Silicon by Single-Ion Implanted Germanium Atoms", *Adv. Funct. Mater.* **31** (21), 2011175 (2021); DOI: [10.1002/adfm.202011175](https://doi.org/10.1002/adfm.202011175) ISSN: 1616-301X (print). 1616-3028 (online). IF (2020): 18.808.
42. F. Orlando, G. Fratesi, G. Onida, 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** (13), 7948-7954 (2021); DOI: [10.1039/D0CP05848C](https://doi.org/10.1039/D0CP05848C) ISSN: 1463-9084. IF (2020): 3.676.
41. P.-C. Lin, R. Villareal, S. Achilli, H. Bana, M. N. Nair, A. Tejada, K. Verguts, S. De Gendt, M. Auge, H. Hofsäss, S. De Feyter, G. Di Santo, L. Petaccia, S. Brems, G. Fratesi, L. M. C. Pereira, "Doping Graphene with Substitutional Mn", *ACS Nano* **15** (3), 5449-5458 (2021); DOI: [10.1021/acsnano.1c00139](https://doi.org/10.1021/acsnano.1c00139) ISSN: 1936-0851(print); 1936-086X (online). IF (2020): 15.881.

40. G. Ambrosio, S. Achilli, S. Pagliara, “Resonance intensity of the $n=1$ image potential state of graphene on SiC via two-photon photoemission”, *Surf. Sci.* 703, 121722 (2021);
DOI: [10.1016/j.susc.2020.121722](https://doi.org/10.1016/j.susc.2020.121722)
ISSN: 0039-6028. IF (2020): 1.942.
39. A. Rabia, F. Tumino, A. Milani, V. Russo, A. Li Bassi, N. Bassi, A. Luccotti, S. Achilli, G. Fratesi, N. Manini, G. Onida, Q. Sun, W. Xu, C. S. Casari “Structural, Electronic, and Vibrational Properties of a Two dimensional Graphdyine-like carbon nano-network synthesized on Au(111): Implications for the engineering of $sp-sp^2$ carbon nanostructures”, *ACS Appl. Nano Mater.* 3, 12, 12178–12187 (2020);
DOI: [10.1021/acsanm.0c02665](https://doi.org/10.1021/acsanm.0c02665)
ISSN: 2574-0970 (online). IF (2020): 5.097.
38. G. Fratesi, S. Achilli, A. Ugolotti, A. Lodesani, A. Picone, A. Brambilla, L. Floreano, A. Calloni, G. Bussetti, “Nontrivial central-atom dependence in the adsorption of M-TPP molecules ($M=Co, Ni, Zn$) on $Fe(001)-p(1\times1)O$ ”, *Appl. Surf. Sci.* 530, 147085 (2020);
DOI: [10.1016/j.apsusc.2020.147085](https://doi.org/10.1016/j.apsusc.2020.147085)
ISSN: 0169-4332. IF (2020): 6.707.
37. S. Freddi, S. Achilli, R. Soave, S. Pagliara, G. Drera, A. De Poli, F. De Nicola, M. De Crescenzi, P. Castrucci, L. Sangaletti, “Dramatic efficiency boost of single-walled carbon nanotube-silicon hybrid solar cells through exposure to ppm nitrogen dioxide in air: An ab-initio assessment of the measured device performances”, *Journal of Colloid and Interface Science* 566, 60-68 (2020);
DOI: [10.1016/j.jcis.2020.01.038](https://doi.org/10.1016/j.jcis.2020.01.038)
ISSN: 0021-9797. IF (2020) 8.128.
36. R. Constantini, L. Colazzo, L. Batini, M. Stredansky, M. S. G. Mohammed, S. Achilli, L. Floreano, G. Fratesi, D. G. de Oteyza, A. Cossaro, “Keto–enol tautomerization drives the self-assembly of leucoquinizarin on Au (111)”, *Chem. Commun.* 56, 2833-2836 (2020);
DOI: [10.1039/C9CC09915H](https://doi.org/10.1039/C9CC09915H)
Online ISSN: 1364-548X. IF (2020): 6.222.
35. 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, L. Floreano, “Cobalt atoms drive the anchoring of Co-TPP molecules to the oxygen-passivated $Fe(001)$ surface”, *Applied Surface Science* 505, 144213 (2020); DOI: [10.1016/j.apsusc.2019.144213](https://doi.org/10.1016/j.apsusc.2019.144213)
ISSN: 0169-4332. IF (2020): 6.707.
34. A. Rabia, F. Tumino, A. Milani, V. Russo, A. Li Bassi, S. Achilli, G. Fratesi, G. Onida, N. Manini, Q. Sun, W. Xu, C. S. Casari, “Scanning tunneling microscopy and Raman spectroscopy of polymeric $sp-sp^2$ carbon atomic wires synthesized on the Au(111) surface”, *Nanoscale* 11, 18191 (2019);
DOI: [10.1039/c9nr06552k](https://doi.org/10.1039/c9nr06552k)
ISSN 2040-3372. IF (2020): 7.79.

33. A. Brambilla, A. Picone, S. Achilli, G. Fratesi, A. Calloni, G. Bussetti, M. Finazzi, L. Duò, F. Ciccacci, "Effects of the introduction of a Chromium Oxide monolayer at the C60/Fe(001) interface", Journal of Applied Physics 1125, 142907 (2019); DOI: [10.1063/1.5075531](https://doi.org/10.1063/1.5075531)
EISSN: 1089-7550. IF (2020): 2.146.
32. 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, F. Ciccacci
"Correction to: Enhanced Magnetic Hybridization of a Spinterface through Insertion of a Two-Dimensional Magnetic Oxide Layer", Nano Lett. 19 (3), 2186 (2019). DOI: [10.1021/acs.nanolett.9b00190](https://doi.org/10.1021/acs.nanolett.9b00190)
ISSN: 1530-6984. IF (2020): 11.189.
31. S. Tognolini, S. Achilli, S. Ponzoni, L. Longetti, C. Mariani, M. I. Trioni and S. Pagliara "On- and off-resonance measurement of the IPS lifetime at the graphene/Ir(111) interface", Surf. Sci. 679, 11-16 (2019). DOI: [10.1016/j.susc.2018.08.010](https://doi.org/10.1016/j.susc.2018.08.010)
ISSN: 0039-6028. IF (2020): 1.942.
30. 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 sp-C Hybridization in the Near-Edge X-Ray Absorption Spectra of Surface-Grown Materials", Materials 11 (12), 2556 (2018); DOI: [10.3390/ma11122556](https://doi.org/10.3390/ma11122556)
EISSN 1996-1944. IF (2020): 3.623.
- 29. S. Achilli, N. Manini, G. Onida, T. Shinada, T. Tanii, E. Prati**
**"GeV_n complexes in silicon: a viable route towards single-electron transport at room temperature", Scientific Reports 8, 18054 (2018). DOI: [10.1038/s41598-018-36441-w](https://doi.org/10.1038/s41598-018-36441-w)
ISSN: 2045-2322 (online). IF (2020): 4.13.**
28. S. Achilli, S. Tognolini, E. Fava, S. Ponzoni, C. Cepek, L. L. Patera, C. Africh, E. del Castillo, M. I. Trioni, and S. Pagliara "Surface states characterization in the strongly interacting graphene/Ni(111) system", New Journal of Physics 20, 103039 (2018). DOI: [10.1088/1367-2630/aae7a0](https://doi.org/10.1088/1367-2630/aae7a0)
ISSN: 1367-2630. IF (2020): 3.729.
27. Marco Bragato, Simona Achilli, Fausto Cargnoni, Davide Ceresoli, Rocco Martinazzo, Raffaella Soave, Mario Italo Trioni, "Magnetic Moments and Electron Transport through Chromium-based Antiferromagnetic Nanojunctions", Materials 11 (10), 2030 (2018). DOI: [10.3390/ma11102030](https://doi.org/10.3390/ma11102030)
ISSN: 1996-1944. IF (2020): 3.623.
26. S. Achilli, E. Cavaliere, T. H. Nguyen, M. Cattelan, S. Agnoli "Growth and electronic structure of 2D hexagonal nanosheets on highly anisotropic rectangular substrate", Nanotechnology 29 (48), 485201 (2018). DOI: [10.1088/1361-6528/aadfd2](https://doi.org/10.1088/1361-6528/aadfd2)
ISSN: 1361-6528. IF (2020): 3.874.
25. M. Bonfanti, S. Achilli, R. Martinazzo "Sticking of Hydrogen atoms on graphene" TOPICAL REVIEW in J. Phys. Condens. Matter 30, 283002 (2018). DOI: [10.1088/1361-648X/aac89f](https://doi.org/10.1088/1361-648X/aac89f)
ISSN: 1361-648X (online). IF (2020): 2.333.

24. 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, F. Ciccacci
“Enhanced Magnetic Hybridization of a Spinterface through Insertion of a Two-Dimensional Magnetic Oxide Layer”, *Nano Lett.* **17**, 7440 (2017). DOI: [/10.1021/acs.nanolett.7b03314](https://doi.org/10.1021/acs.nanolett.7b03314)
ISSN: 1530-6984. IF (2020): 11.189.

23. A. Calloni, G. Fratesi, S. Achilli, G. Berti, G. Bussetti, A. Picone, A. Brambilla, P. Folegati, F. Ciccacci, L. Duò
“Combined spectroscopic and ab-initio investigation of monolayer range Cr oxides on Fe(001): the effect of an ordered vacancy superstructure” *Phys. Rev. B* **96** (8), 085427 (2017). DOI: [/10.1103/PhysRevB.96.085427](https://doi.org/10.1103/PhysRevB.96.085427)
ISSN: 1944-8244. IF (2020): 4.036.

22. S. Ponzoni S. Achilli, C. Pintossi, G. Drera, L. Sangaletti, P. Castrucci, M. De Crescenzi, S. Pagliara.
“Hybridized C–O–Si Interface States at the Origin of Efficiency Improvement in CNT/Si Solar Cells”
Applied Materials & Interfaces **9** (19), 16627-16634 (2017). DOI: [/10.1021/acsami.7b01766](https://doi.org/10.1021/acsami.7b01766)
ISSN: 1944-8244. IF (2020): 9.229.

21. S. Tognolini, S. Achilli, L. Longetti, E. Fava, C. Mariani, M. I. Trioni, S. Pagliara
Reply, *Phys. Rev. Lett.* **117** (23), 239702 (2015). DOI: [/10.1103/PhysRevLett.117.239702](https://doi.org/10.1103/PhysRevLett.117.239702)
ISSN: 1079-7114. IF (2020): 9.161.

20. E. del Castillo, S. Achilli, F. Cargnoni, D. Ceresoli, R. Soave, M. I. Trioni
“Spin filtering in graphene junction with Ti and Co adsorbates”
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ISSN: 1521-4095. IF (2020): 30.849.

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ISSN: 1463-9084. IF (2020): 3.676.

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“Rashba Spin-Orbit Coupling in Image Potential States”,
Phys. Rev. Lett. **115**, 046801 (2015). DOI: [/10.1103/PhysRevLett.115.046801](https://doi.org/10.1103/PhysRevLett.115.046801)
ISSN: 1079-7114. IF (2020): 9.161.

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Phys. Rev. B **91**, 195440 (2015). DOI: [/10.1103/PhysRevB.91.195440](https://doi.org/10.1103/PhysRevB.91.195440) ISSN: 1944-8244. IF (2020): 4.036.

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 "Spin asymmetric band gap opening in graphene by Fe adsorption"
 Surf. Sci. 634, 62 (2015). DOI: [/10.1016/j.susc.2014.11.012](https://doi.org/10.1016/j.susc.2014.11.012)
 ISSN: 0039-6028. IF (2020): 1.214.

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"Hydrogen-dimer lines and electron waveguides in graphene",
Phys. Chem. Chem. Phys. 16 (33), 17610-17616 (2014). DOI: [/10.1039/C4CP01025F](https://doi.org/10.1039/C4CP01025F)
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 "Key ingredients of the alkali atom – metal surface interaction: Chemical bonding versus spectral properties", Prog. Surf. Sci. 88 (2), 160-170 (2013). DOI: [/10.1016/j.progsurf.2013.03.002](https://doi.org/10.1016/j.progsurf.2013.03.002)
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 J. Phys Chem. A, 115 (30), 8498-8503 (2011). DOI: [/10.1021/jp2005875](https://doi.org/10.1021/jp2005875)
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10. P. Gargiani, M. G. Izzo, F. Bussolotti, M. G. Betti, S. Achilli and M. I. Trioni
 "Bi ordered phases on Cu(100): periodic arrays of dislocations influence the electronic properties"
 J. Chem. Phys., 132, 174706 (2010). DOI: [/10.1063/1.3424741](https://doi.org/10.1063/1.3424741)
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 "Detailed features of the surface electronic states of K/Cu(111) by density functional theory"
 Phys. Rev. B 81, 165444 (2010). DOI: [10.1103/PhysRevB.81.165444](https://doi.org/10.1103/PhysRevB.81.165444)
 ISSN: 1098-0121. IF (2020): 4.036.

8. 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(1x1)O Surface"
 Phys. Rev. B 81, 115450 (2010). DOI: [10.1103/PhysRevB.81.115450](https://doi.org/10.1103/PhysRevB.81.115450)
 ISSN: 1098-0121. IF (2017): 4.036.

7. M. I. Trioni, G. Fratesi, S. Achilli and G. P. Brivio
 "Dynamics of electron distributions probed by helium scattering"
 J. Phys. Condens Matter 21 (29), 264003 (2009). DOI: [/10.1088/0953-8984/21/26/264003](https://doi.org/10.1088/0953-8984/21/26/264003)
 ISSN: 0953-8984. IF (2020): 2.333.

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“Electronic structure and lifetime broadening of a quantum-well state on p(2x2) K/Cu(111)”

Phys. Rev. B 80 (19), 195419 (2009). DOI: [/10.1103/PhysRevB.80.195419](https://doi.org/10.1103/PhysRevB.80.195419)

ISSN: 1098-0121. IF (2020): 4.036.

5. S. Achilli, M. I. Trioni, E. V. Chulkov, P. M. Echenique, V. Sametoglu, N. Pontius, A. Winkelmann, A. Kubo, J. Zhao, and H. Petek

“Spectral properties of Cs and Ba on Cu(111) at very low coverage: Two-photon photoemission spectroscopy and electronic structure theory”.

Phys. Rev. B 80 (24), 245419 (2009). DOI: [/10.1103/PhysRevB.80.245419](https://doi.org/10.1103/PhysRevB.80.245419)

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4. F. Donati, P. Sessi, S. Achilli, A. Li Bassi, M. Passoni, C. S. Casari, C. E. Bottani, A. Brambilla, A. Picone, M. Finazzi, L. Duò, M. I. Trioni, and F. Ciccacci

“Scanning tunneling spectroscopy of the Fe(001)-p(1x1)O surface”.

Phys. Rev. B 79 (19), 195430 (2009). DOI: [/10.1103/PhysRevB.79.195430](https://doi.org/10.1103/PhysRevB.79.195430) ISSN: 1098-0121. IF (2020): 4.036.

3. S. Achilli, S. Caravati, M. I. Trioni

“Ultrathin Fe film on Cu(001): Exchange splitting of image states from first principles”

Surf. Sci. 601 (18), 4048 (2007). DOI: [/10.1016/j.susc.2007.04.175](https://doi.org/10.1016/j.susc.2007.04.175) ISSN: 0039-6028. IF (2020): 1.942.

2. S. Achilli, S. Caravati, M. I. Trioni “Ab initio electronic and magnetic properties of 1 ML Fe/Cu(001)”

J. Phys. Condens. Matter 19 (30), 305021 (2007). DOI: [/10.1088/0953-8984/19/30/30502.1](https://doi.org/10.1088/0953-8984/19/30/30502.1)

ISSN: 0953-8984. IF (2020): 2333.

1. S. Achilli, G. P. Brivio, M. I. Trioni

“New feature in the Auger peak of adsorbed oxygen”

Surf. Sci. 600 (18), 3610 (2006). DOI: [/10.1016/j.susc.2006.01.065](https://doi.org/10.1016/j.susc.2006.01.065). ISSN: 0039-6028. IF (2020): 1.942.

Conference Proceedings

1. S. Achilli, N. H. Le, G. Fratesi, N. Manini, G. Onida, M. Turchetti, G. Ferrari, T. Shinada, T. Tanii, E. Prati
“Quantum transport through a disordered array of Ge-vacancy defects in silicon for applications in quantum technologies”, Proceeding of the 2021 Silicon Nanoelectronics Workshop, SNW 2021.

2. S. Achilli, N. Manini, G. Onida, E. Prati

“Theoretical spectroscopy characterization of deep electronic states of defects in silicon via Density Functional Theory with hybrid potentials” Chapter of “Toward a Science Campus in Milan” - p. 17-24,. Editors: P. F. Bortignon, G. Lodato, E. Meroni, M. Paris, L. Perini, A. Vicini, Springer Edition (2018).

DOI: [/10.1007/978-3-030-01629-6](https://doi.org/10.1007/978-3-030-01629-6).

PhD Thesis

Title: “Spectral properties of adsorbates on metal surfaces via the embedding method”.

Available online: <https://www.semanticscholar.org/paper/Spectral-properties-of-adsorbates-on-metal-surfaces-Achilli/fe1f39eb4b6d36dd57c3881a9c2644618301108a>

8.3 CONFERENCES AND SEMINARS

Invited talks at international Conferences and Workshops

- 1) **13-17 September 2021** 107° Congresso Nazionale SIF (<https://www.sif.it/attivita/congresso/107>). Invited talk in the session “Fisica della Materia”. Title: “Point defects in silicon for quantum technologies at room temperature”.
- 2) **31 Aug - 4 Sept 2020** GEFES Conference. Invited talk at the Minicolloquium “Molecularly Functionalized Low-Dimensional Systems” (<https://eventos.uam.es/files/event/28512/editorFiles/file/44533.pdf>). Title: “Carbon nanotubes functionalization for antiferromagnetic spintronic”, CMD2020.
- 3) **16 Sept 2020** RES (Red Espanola de Supercomputacion) User Conference (<https://www.res.es/en/events/14th-users-conference>). Invited talk.
“Carbon nanotubes functionalization for antiferromagnetic spintronic”
- 4) **1-4 Jul 2019** 14th International Conference of Advanced Nanomaterials Aveiro (Portugal).
Plenary invited talk to present NFFA.eu infrastructure.
- 5) **19-21 Feb 2019** “2nd NFFA-Europe Scientific Workshop”, Milano (<http://workshop2019.nffa.eu/>). Invited talk.
Title: “GeV complex in silicon: a viable route toward room temperature quantum information technology.”
- 6) **18 Dec 2018** “QTech Fall meeting” Workshop, Milano (<https://sites.unimi.it/aqm/qtech-fall-workshop-2018/>). Invited talk.
Title: “GeV complex in silicon: a viable route toward room temperature quantum information technology.”
- 7) **23 Nov 2018** “Atoms and Molecules On Solid Surfaces” Workshop, Università di Milano Bicocca, Milano.
Invited talk.
Title: “Enhanced Magnetic Hybridization of C60 on Fe(001) by a two dimensional Chromium Oxide layer.”
- 8) **2 - 4 May 2017** IV Italy-Japan Workshop on Silicon nanoelectronics for advanced applications, Colico (Como lake). Invited talk.
Title: “Deep electronic states of defects due to implanted atoms in Silicon: tools and results from a theoretical spectroscopy approach.”

Other oral contributions at conferences

- 1) **June 2021** 11th Conference: “New Generation in Strongly Correlated Electron Systems”, online.
Title: “Quantum transport of strongly correlated electrons through GeV complexes in silicon: a combined ab-initio and Hubbard model approach.”
- 2) **June 2021** “Silicon Nanoelectronics Workshop 2021”, online.
Title: “Quantum transport through Ge-vacancy defects in silicon for application in quantum technologies.”
- 3) **Jul 2019** Conference: “14th International Conference of Advanced Nanomaterials”, Aveiro.
Title: “GeV complex in silicon: a viable route toward room temperature quantum information technology.”

- 4) **Jun 2019** Conference: "Theory Meets Experiments", Prague.
Title: "GeV complex in silicon: a viable route toward room temperature quantum information technology."
- 5) **Feb 2019** Whorkshop: "3rd Workshop Condensed Matter Highlights", Milano.
Title: "Enhanced Magnetic Hybridization of C60 on Fe(001) by a two dimensional Chromium Oxide layer."
- 6) **Feb 2019** Conference: "Toward Reality in Nanoscale Materials X", Kittila.
Title: "GeV complex in silicon: a viable route toward room temperature quantum information technology."
- 7) **Oct 2018** Conference: "Materials.it", Milano.
Title: "GeV complex in silicon: a viable route toward room temperature single electron transport."
- 8) **Sep 2018** "2018 MolSimEng Workshop", Milano.
Title: "Enhanced Magnetic Hybridization of C60 on Fe(001) by a two dimensional Chromium Oxide layer."
- 9) **Sep 2018** "23rd ETSF Workshop on Electronic Excitations", Milano.
Title: "GeV_n complexes in silicon: a viable route toward room temperature single atom devices."
- 10) **Mar 2018** Conference: "American Physical Society March Meeting 2018", Los Angeles.
Title: "GeV_n complexes in silicon: a viable route toward room temperature single atom devices."
- 11) **Sep 2017** "ETSF Workshop 2017", INFN national Labs, Frascati.
Title: "Single electron quantum transport through deep atomic states."
- 12) **Jun 2016** DIPC-PAMS Theory Workshop: "Towards reality in modeling molecular electronics", Donostia International Physics Center, San Sebastian.
Title: "First principle semiclassical conductivity and quantum transport in graphene with resonant scatterers: the case of H and F adatoms and the carbon atom vacancies."
- 14) **Sep 2015** "FisMat 2015", Italian National Conference on Condensed Matter Physics, Palermo.
Title: "Unoccupied surface features induced by epitaxial graphene on metal surfaces."
- 15) **Sep 2010** 26th Congresso nazionale Società Italiana di Fisica, Modena.
Title: "Bi film on Cu: surface morphology and electronic properties."
- 16) **Aug 2010** 27th European Congress on Surface Science ECOS27, Groningen.
Title: "Interplay between electronic properties and surface morphology in Bi/Cu(100)".
- 17) **Jul 2008** 25th European Congress on Surface Science ECOS25, Liverpool.
Title: "In plane dispersion of the n=1 image state of Cu(111) via the embedding method and the phase shift model."
- 18) **Jul 2008** 44th Workshop: "Dynamical Phenomena in low-Dimensional Systems", International School of Solid State Physics, "Ettore Majorana" Foundation and centre for scientific culture, Erice.
Title: "In plane dispersion of the n=1 image state of Cu(111) via the embedding method and the phase shift model."

19) **May 2008** 5th ETSF Young Researcher's Meeting, Modena.

Title: "Elastic contribution to the lifetime of excited surface states of alkali overlayers on Cu(111)."

20) **Jul 2007** 42th Workshop: "Low dimensional Dynamical phenomena and simulation", International School of Solid State Physics, "Ettore Majorana" Foundation and centre for scientific culture, Erice.

Title: "Bi film on Cu: surface morphology and electronic properties."

21) **Jul 2006** 37th Workshop: "Low dimensional Dynamical phenomena and simulation", International School of Solid State Physics, "Ettore Majorana" Foundation and centre for scientific culture, Erice.

Title: "Ultrathin Fe film on Cu: Effects of the dimensionality reduction".

Invited seminars at research institutes and Universities

1) **15 February 2022** Nanolab Talk, Politecnico di Milano. Title: "Functionalization: an ab initio perspective".

2) **26 March 2021** ETSF Webinar. Title: "Quantum transport through Ge-vacancy defects in silicon for applications in quantum technologies".

3) **4 Oct 2017** Università di Torino, Dip. di Chimica. Host: Prof. R. Dovesi.

Title: "Single-electron quantum transport through deep atomic states of Ge dopants in silicon."

4) **6 Jun 2017** Università di Trieste, Dip. di Fisica. Host: Prof. F. Parmigiani.

Title: "Interface properties of graphene on metals and semiconductors: interplay between theory and experiments for an accurate characterization"

5) **Jun 2014** Università Cattolica del Sacro Cuore, Dip. di Fisica, Brescia. Host: Dr. S. Pagliara.

Title: "How DFT can support experimental analysis of low dimensional systems."

6) **Jun 2011** Università di Milano Bicocca, Dip. di Scienze dei Materiali. Seminar for the local PhD program.

Title: "Electronic properties of adatoms and overlayers on metals: extended substrate approach."

• **From 2005 to 2018** Several **posters presentations** at international conferences and schools

9. TEACHING ACTIVITIES

9.1 MEMBERSHIP OF TEACHING BOARDS

• Since May 2021: **board of the PhD** in Physics, Astrophysics and Applied Physics, Università degli Studi di Milano. (membro del Collegio Didattico del Dottorato, Cineca code: DOT1315144).

9.2 INSTITUTIONAL COURSES AT UNIVERSITIES

Post-graduate

1) **Lecturer** (Titolare di Modulo Didattico) of the course "Quantum Theory of Matter" for the PhD in "Physics, Astronomy and Applied Physics" Ciclo 37° - Università degli Studi di Milano (9 hours). Academic year 2021-2022.

2) **Lecturer** (Assistant Professor) of the course "Quantum Theory of Matter" for the PhD in "Physics, Astronomy and Applied Physics" Ciclo 36° - Università degli Studi di Milano (3 hours). Academic year 2020-2021.

Undergraduate

- 1) **Lecturer** of the course (Titolare del corso) “Fisica” (36 hours frontal lessons) of the Master Degree in Biotechnology, Università degli Studi di Milano. Academic year 2021-2022.
- 2) **Lecturer** of the course (Titolare del corso) “Fisica” (36 hours frontal lessons) of the Master Degree in Biotechnology, Università degli Studi di Milano. Academic year 2020-2021.
- 3) Jun 2021 - present: **Examiner** (head of the commission - Presidente di Commissione) for 97 exams of the course “Fisica”, Master Degree in Biotechnology, Università degli Studi di Milano.
- 4) **Tutor and examiner** (Co-titolare del corso) for the course “Laboratorio di ottica elettronica e fisica moderna” of the Master Degree in Physics, Università degli Studi di Milano. Academic year 2019-2020 (Activity: Setup of virtual laboratories, tutoring of students, exams. Held during COVID lockdown.)
- 5) **Tutor and examiner** (by contract) for the course of “Fisica Generale” (15 hours in class + exams) of the Master Degree in Mathematics, Università degli Studi di Milano. Academic year 2018- 2019.
- 6) **Assistant Professor** (Esercitatore – by contract)for the course and laboratories of “Fisica A+B” (10 CFU, 40 hours in class + exams) of the Master Degree in Engineering Physics, Politecnico di Milano. Academic year 2018-2019.
- 7) **Tutor and examiner** (by contract) for the course of “Fisica Generale” (15 hours in class + exams) of the Master Degree in Mathematics, Università degli Studi di Milano. Academic year 2017- 2018.
- 8) **Assistant Professor** (Esercitatore – by contract) for the course and laboratories of “Fisica A+B” (10 CFU, 40 hours in class + exams) of the Master Degree in Engineering, Physics of Politecnico di Milano. Academic year 2017-2018.
- 9) **Lecturer** (Titolare di un Modulo Didattico) of the course “Statistical Mathematics” for the Master Degree in Physics, Università Cattolica del Sacro Cuore. Academic year 2015-2016.
- 10) **Assistant Professor** (Esercitatore - by contract) for the course of “Fisica A+B” (10 CFU, 40 hours in class + exams) of the Master Degree in Engineering Physics, Politecnico di Milano. Academic year 2013-2014.
- 11) **Tutor** (by contract) for the laboratory activity of “Fisica sperimentale I + B” (27 hours in laboratory) of the Master Degree in Engineering Physics, Politecnico di Milano. Academic year 2013-2014.
- 12) **Assistant Professor** (Esercitatore – by contract) for the course of “Fisica sperimentale I + B” (12 CFU, 48 hours in class + exams) of the Master Degree in Engineering Physics of Politecnico di Milano. Academic year 2010-2011.
- 13) **Tutor** (by contract) for the laboratory activity of “Fisica sperimentale I + B” (15 hours in laboratory) of the Master Degree in Engineering Physics, Politecnico di Milano. Academic year 2010-2011.
- 14) **Assistant Professor** (Esercitatore – by contract)for the course of “Fisica sperimentale I + B” (12 CFU, 48 hours in class + exams) of the Master Degree in Engineering Physics, Politecnico di Milano. Academic year 2008-2009.

9.3 SUPERVISION OF STUDENTS

Official supervisor of 2 Master Students:

- 2022 - Federico Orlando, Master Degree in Physics, Università degli Studi di Milano.
- 2022 - Federico Civaia (external supervisor), Master Degree in Nuclear Engineering, Politecnico di Milano.

Official supervisor of 4 Bachelor Students:

- 2020 – Francesco Melone, Bachelor Degree in Physics, Università degli Studi di Milano.
Thesis: “Electronic properties of vanadyl-tetraphenylporphyrin molecules from first principle calculations.”
- 2018 – Laura Batini, Bachelor Degree in Physics, Università degli Studi di Milano.
Thesis: “First-principle simulation of core-level spectra in molecules and dependence on tautomerism”.
- 2018 – Federico Orlando, Bachelor Degree in Physics, 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”
- 2011 – Simone Lampasona, Bachelor Degree in Physics, Università di Milano Bicocca.
Thesis: “Applicazione del metodo dello shift di fase per il calcolo degli stati legati di superfici metalliche”

Other mentoring activity

I personally followed the thesis work of other 2 PhD student, 3 Master student and 2 Bachelor students, without explicitly appearing as official supervisor:

- Since 2021 – Marco Marino, PhD in Physics, Astrophysics and Applied Physics, Università degli Studi di Milano. Thesis: “Theoretical development of hybrid organic/antiferromagnetic interfaces.”
- 2012-2013 – Paolo Bonardi, PhD in Chemistry, Università degli Studi di Milano.
Thesis: “First principles investigation of the electronic and transport properties of carbon atom wires.”
- 2017 – Marco Bragato, Master Degree in Chemistry, Università degli Studi di Milano.
Thesis: “Electron transport through antiferromagnetic nanojunctions.”
- 2014 – Simone Lampasona, Master Degree in Physics, Università di Milano Bicocca.
Thesis: “Influenza dei difetti di Ossigeno sul trasporto elettronico attraverso film ultrasottili di MgO inseriti tra elettrodi di Ag.”
- 2009 – Alessandra Zanetti, Master Degree in Physics, Università di Milano Bicocca.
Thesis: “Many-body effects in spin resolved Auger deexcitation from adatoms on metal surfaces.”
- 2015 – Luca Oggioni, Bachelor Degree in Physics, Università di Milano Bicocca.
Thesis: “Computational Study of electronic and transport properties of nanoscale-GeTe.”
- 2010 – Federico Guerra, Bachelor Degree in Physics, Università di Milano Bicocca.
Thesis: “Studio teorico computazionale di superfici metalliche: effetti di substrato esteso sulle proprietà elettroniche.”

Teaching activity abroad

- 28 June-2 July 2021: Tutor for the hands-on “Bands Unfolding” of the CECAM Siesta School 2021 (online).

10. NATIONAL AND INTERNATIONAL RESEARCH PROJECTS FUNDED BY COMPETITIVE GRANTS

10.1 COORDINATION:

- **co-PI** Project: “Quantum Information transport through special point defects in Silicon.”

UNIMI Call “Piano di Sostegno alla Ricerca” Linea 2, Azione A (2021). Funded with 11 Keuros.

- **co-PI** Project: “Fundamentals of quantum machine learning for physics.”

UNIMI Call “Piano di Sostegno alla Ricerca” Linea 2, Azione A (2022). Funded with 18 Keuros.

- **Principal Investigator** of **7 Iskra C** project of high-performance computing at CINECA:

1) “Adatoms on Modulated surface potential via the embedding method”, 20 khours on SP6.

2) “Electronic Transport Across Graphene based Nano-junctions”, 240 khours on FERMI.

3) “Scattering Cross Section of Neutral Defects on Graphene”, 2 MLN hours on FERMI.

4) “Ballistic conduction of phase change materials”, 100 K-hours on EURORA.

5) “Density functional characterization of morphology and electronic spectra of graphene on Pt surfaces”, 1MLN hours on FERMI.

6) “Deep energy levels of dopant atoms in Silicon for quantum transport”, 12500 Khours on MARCONI_A1 + 9375 on Marconi_A2.

7) “Interface between organic molecule and oxidized iron for spintronics”, 360 Khours on MARCONI_A2.

- **Principal Investigator** of **1 LISA project** of high-performance computing at CINECA:

“Heterojunctions for antiferromagnetic spintronics”, 4MLN hours on MARCONI_A1

- **Principal Investigator** of **3 projects** of high-performance computing at the Red Espanola de Supercomputacion(RES):

1) “Fully ab initio relaxation of hBN/graphene stacking layers at very small twisting angle” 1MLN hours on Marenostrum.

2) “Ab initio spin transport properties of Co4/CNT” 200.000 hours on Marenostrum.

3) “Antiferromagnetic spinterfaces for new-concept Information technology devices.” 880 Khours on Nasertic.

The assigned amount of computing hours may be converted to euros on the basis of the typical cost adopted by INDACO facility of the University of Milan (<https://unitech.unimi.it/listino/indaco>)

- **Leading scientist of 4 NFFA-EUROPE projects:** responsible of the research activity and of the interaction with experimentalists.

1) Project ID 188: “Deep atomic states of germanium dopant in silicon”, assigned to Università degli Studi di Milano.

2) Project ID 517: Continuation project of “Deep atomic states of germanium dopant in silicon”, assigned to Università degli Studi di Milano.

3) Project ID 710: “Topological valley currents in graphene/hBN”, assigned to Catalan Institute of Nanoscience and Nanotechnology.

4) Project ID 753: “Tuning the magnetoresistance of carbon nanotubes by functionalization with magnetic molecules”, assigned to Catalan Institute of Nanoscience and Nanotechnology.

- **Leading scientist of 1 NEP projects:** responsible of the research activity and of the interaction with experimentalists.

1) Project ID 078: “Single-atom quantum magnets in two-dimensional h-BN” assigned to Università degli Studi di Milano.

10.2 PARTICIPATION:

1) 2021-2025 Project “Selectively activated INFORMATION technology by hybrid Organic Interfaces” (H2020-FETOPEN-01-2018-2019-2020, Grant Agreement n. 964396).

Role: proposal writing, scientific activity, training, reporting.

2) 2021-2026 Project “Nanoscience Foundries and Fine Analysis - Europe | PILOT” (H2020-INFRAIA-03-2020 Grant Agreement n. 101007417) .

Role: proposal writing, scientific activity, Infrastructure Node Official, reporting.

3) 2015-2021 Project “Nanoscience Foundries and Fine Analysis”

(H2020-INFRAIA-1-2014-2015 Grant Agreement n. 654360.

Role: proposal writing, scientific activity, reporting.

4) 2020-2022 Project “Advanced Theoretical methods for emerging 2D materials in Quantum Information Technology Studies. (TIME2QUEST)” - Progetto di Iniziativa specifica INFN. Funded with 12 Keuros.

Role: proposal writing, research activity.

5) Project: “Imaging Magnetic Interfaces and Nanostructures for applications in spintronics”

Call “Ricerca scientifica e tecnologica sui materiali avanzati – 2008”, Fondazione CARIPLO.

Role: scientific research and reporting.

10.3 SUBMITTED PROJECTS UNDER EVALUATION

- **Local-PI** (Coordinatore nodo di Milano) for the participation to the Doctoral Network (DN) TIMES: “Time-resolved simulations of ultrafast phenoMena in quantum matErialS” within the call HORIZON-MSCA-DN-2021

- **Local-PI** (Responsabile di Unità) of a project submitted to the call PRIN 2022 – under 40

11. OTHER GRANTS

- **CECAM grant** for organizing the Workshop “Transiesta + Tbtrans + SISL School”, 10.5 Keuros, **co-PI**

12. FELLOWSHIPS, HONORS AND AWARDS

- **Scholarship** at the “Theory Meets Experiments” conference in Prague, June 2018.

13. ORGANIZATION OF WORKSHOPS AND SCHOOLS

- **Member of the committee** for the organization of the “23th ETSF Workshop on Electronic Excitations”, Milano, 10-14 September 2018.

- **Member of the committee** for the organization of the “Transiesta + Tbtrans + SISL School”, San Sebastian, 23-30 March 2020.

14. PARTICIPATION TO EDITORIAL BOARDS

Since March 2018: Associated Editor of European Physical Journal B.

15. ACTIVITY OF REFEREE AND EVALUATOR:

- **Referee** of “ACS Applied Nanomaterials”, “Nanoscale”, “Journal of Physics D”, “Materials”, “European Physical Journal B”, “2D Materials”, “RSC Advances”, “Physica Status Solidi B”, “Physica E”, “Physical Review B”.
- **Scientific Evaluator** of IscraC and IscraB projects for high performance computing projects at CINECA.
- **Scientific Evaluator** of proposal for the Slovak Academic and Scientific Program (SASPRO 2) – Horizon2020 Marie Skłodowska Curie COFUND Action.
- **Member of the commission** for the public selection of 3 postdoc funded by research grants active at the Physics Department of the University of Milan. (Assegno di ricerca di tipo B)

16. OTHER INSTITUTIONAL ACTIVITIES

- European Theoretical Spectroscopy Facility (ETSF, www.etsf.eu).
Role: Elected member of the Steering Committee (6 members out of 65 Research Team Leaders).
- November 2020 - February 2022 Member of the “Consulta dei Ricercatori” UNIMI as designated alternate representative of the Researchers of the Physics Department.
- Infrastructure Node Official for the project “Nanoscience Foundries and Fine Analysis - Europe|PILOT” (H2020-INFRAIA-03-2020 Grant Agreement n. 101007417) .

17. LANGUAGE KNOWLEDGE

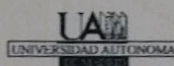
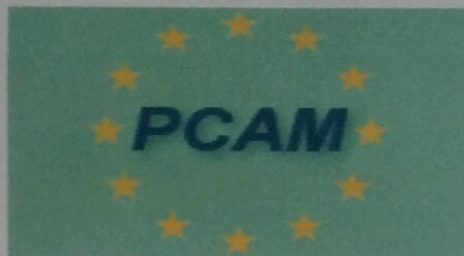
Italian: Native

English: B2 (Certified by evaluation after the attendance of a 6 months course organised by SLAM - University of Milan Language Centre. The course consisted of self-study on an online learning platform integrated by 20-hour one-to-one tutoring run remotely.

Spanish: Good

Milano, 30/3/2022

According to law 679/2016 of the Regulation of the European Parliament of 27th April 2016, I hereby express my consent to process and use my data provided in this CV



European Doctorate in Physics and Chemistry of Advanced Materials PCAM

It is hereby certified that a doctorate degree has been issued
by the University of Milano-Bicocca to

Simona Achilli

born in Vizzolo Predabissi (Milan) on 29 November 1982

The Rectors of the participating universities
and the PCAM coordinator have additionally called the degree as

**Doctor Europaeus
in Materials Science**

obtained within the collaborative network of doctorate programmes in
Physics and Chemistry of Advanced Materials,
in recognition of the fulfillment of the requirements for this degree
as agreed by the European Rectors' Confederation (27/11/1992)

Date, 3 May 2010

The PCAM Coordinator

The Rector's Nominee
University of Milano-Bicocca

The Rector's Nominee
University of the Basque Country