



Elena Cannuccia

Maître de Conférences - Aix-Marseille Université

Personal

Name **Elena Cannuccia**
Date of birth **22nd January 1981**
Place of birth **Fano (Italy)**
Marital Status **Married, a daughter born in August 2013 and a son born in June 2016**
Affiliation **Aix-Marseille Université, PIIM UMR 7345 13397 Marseille, (France)**
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Education

2007–2010 **PhD in Condensed Matter Physics,**
"Tor Vergata" University, Rome (Italy),
Thesis title: "Giant Polaronic Effects in Polymers: breakdown of the electronic picture"
Supervisors: R. Del Sole and A. Marini.
2004–2007 **M. S. Degree in Condensed Matter Physics,**
"Tor Vergata" University, Rome (Italy),
Thesis title: "Ab initio study of optical properties of a biological molecule: the flavin"
Supervisors: R. Del Sole and O. Pulci.
2000–2004 **B. S. Degree in Physics,**
"Tor Vergata" University, Rome (Italy),
Thesis title: "Study of roughness for what concerns the Poissonian processes: 1D and 2D cases"
Supervisors: M. Fanfoni and M. Tomellini.

Postdoctoral Experience

Feb 2013 - Jul 2014 **PostDoc Fellowship, Institut Laue Langevin (ILL), Grenoble (France).**

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Jun 2011 - **PostDoc Fellowship**, *Universidad del Pais Vasco*, San Sebastian (Spain).
Jan 2013
Nov 2010 - **PostDoc Contract**, "*Tor Vergata*" University, Rome (Italy) .
May 2011

Experience

Vocational

Mar 2020 - **Maître de Conférences**, Laboratoire de Physique des Interactions Ioniques et
present Moléculaires, Aix-Marseille Université (France).
Mar 2017-Feb **Researcher in Condensed Matter Physics (Rita Levi Montalcini research**
2020 **fellowship)**, Secondment in Department of Physics, University of Rome "Tor
Vergata" (Italy).
Sep 2014-Feb **Maître de Conférences**, Laboratoire de Physique des Interactions Ioniques et
2017 Moléculaires, Aix-Marseille Université (France).

Awards and Honors

2021-2025 **Partial release from teaching obligations (96 hours per academic year) from**
Aix-Marseille Université and financed by Agence Nationale de la Recherche,
(France).
2017-2020 **Rita Levi Montalcini fellowship research program from "Ministero**
dell'Istruzione Università e Ricerca" (MIUR), (Italy).
2014-2016 **Partial release from teaching obligations (64 hours per academic year) from**
Aix-Marseille Université.
2014 **Prime d'installation chercheurs, Ville de Marseille**, (France).

Languages

Italian **Native**
French **Advanced**
English **Advanced**
Spanish **Intermediate**

Teaching Experience

Lecturer at Aix-Marseille Université, for the classes:

- **Modern Density-Functional Theory Applied to Solids and Nanostructures: Structural, Electronic, and Optical properties** (CM:5 hours), Doctoral School 352 (ED352). Academic years 2023-2024.
- **Low Dimensional Systems** (CM/TD:9 hours), Master of Nanoscience and Nanotechnology (M2). Academic year 2024-2025.
- **Mécanique Quantique/Quantum Mechanics** (TD:30 hours), Master of Fundamental Physics (M1). Since academic year 2020-2021 to 2024-2025.
- **Optique Géométrique/Geometrical Optics** (CM+TD:22 hours), Portail Marie-Curie (L1). Since academic year 2020-2021 to 2024-2025.

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- **Mécanique Quantique/Quantum Mechanics** (TD:15 hours), Licence Physique Chimie (L3). Since academic year 2019-2020 to 2024-2025.
- **Advanced Numerical Simulations** (CM+TP:16 hours), Master of Nanoscience and Nanotechnology (M2). Academic years 2019-2020, 2020-2021, 2021-2022 and 2023-2024.
- **Physics Practical Sessions (Electricity)** (TP:12 hours), Portail Marie-Curie (L1). Academic years 2020-2021, 2021-2022.
- **Optique, Mécanique et ondes: introduction/Introduction to Physics** (CM+TD+TP:38 hours), Année de Remise à Niveau Scientifique (AMNS). Academic year 2020-2021.
- **Physics** (TD:42 hours), Année de Remise à Niveau Scientifique (AMNS). Academic years 2019-2020, 2020-2021.
- **Electricité/Electricity** (TD:16 hours) Portail Snell-Descartes (L1). Academic years 2020-2021.
- **Physics Practical Sessions (Optics)** (TP:18 hours), Année de Remise à Niveau Scientifique (AMNS). Academic years 2019-2020, 2020-2021.
- **Physique pour la Biologie/Physics for Biology** (TD:22 hours). Academic years: 2014-2015, 2015-2016, 2016-2017
- **Physics Practical Sessions (Electronics and Optics)**. Academic years: 2014-2015 (TP:60 hours), 2015-2016 (TP:45hours).
- **Optique Géométrique/Geometrical Optics**. Parcours des écoles d'ingénieurs Polytech. Academic years: 2015-2016 (CM:48 hours), 2016-2017 (CM:24 hours).
- Basic **Mathematics** course (40 hours of Analysis) addressed to students willing to get the High School Certificate. The DAEU training course is supervised by the University of Aix-Marseille.

Lecturer at Department of Physics at University of Rome "Tor Vergata" for the classes:

- **Quantum and Statistical Mechanics** (CM:48 hours), Material Science (L2). Academic years 2017-2018, 2018-2019.

Supervising activities

- Supervision of **PhD students**: Martino Silvetti, financed by ANR-JCJC project NOTISPERF, co-supervised with Cedric Pardanaud (Oct 2021 - Sep 2024). Thesis title: "Thermodynamics and optical properties of point defects in wurtzite Boron Nitride", Thesis defended on 7th October 2024.

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- Supervision of **Master Students**:
 (1) Paul Giraud from Université des Sciences et Technologies Lille 1, co-supervised with Prof. A. Rubio (Apr-Sep 2012). Title of the Thesis: *Study of the Electronic Structure of hexagonal Boron Nitride on metals substrates*.
 (2) Mathilde Pouyot from Aix-Marseille University (Apr-Jun 2022 (stage M1), and Feb-May 2023 (stage M2)). Title of the internships: "A Configuration Coordinate Diagram study of defects in semiconductors : the case of C substitutional atom in hexagonal Boron Nitride monolayer" and "Étude de niveaux d'énergie électroniques et de l'énergie de formation d'un défaut ponctuel, le dimère de carbone, dans le nitrure de bore en phase wurtzite".
- **Internship Students**: Simone Grillo, an ERASMU+ student from Tor Vergata University: (Project:"Tunable second harmonic generation in 2D materials: comparison of different strategies").
- **Science Watch AA 2021-2022** teaching unit hosted by Master of Fundamental Physics, Aix-Marseille Université. Supervision of students: Mathilde Pouyot (Project:"Defects in semiconductors: Combining experiment and theory")

Grants

As PI:

- **Psi-K European Network** for the organization of the 27th ETSF Workshop on Electronic Excitations (2024). Organizing Committee: Maryam Azizi, Guido Fratesi, Vitaly Gorelov, Roberta Poloni, Rajarshi SINHA ROY; budget 6 k€
- **FIR-AMU** for the organization of the 27th ETSF Workshop on Electronic Excitations (2024); budget 1.2 k€
- **AMUTECH** for the organization of the 27th ETSF Workshop on Electronic Excitations (2024); budget 1 k€
- **Ville de Marseille** for the organization of the 27th ETSF Workshop on Electronic Excitations (2024); budget 1 k€
- **ANR 2020** "Jeunes Chercheuses et Jeunes Chercheurs" (French National Research Agency Young Investigator Grant); Title:"NOThing IS PERFect: Defects in hexagonal Boron Nitride (NOTISPERF)". Funding starting March 15th 2021; budget 174k€. Collaborators:Claudio Attaccalite, Alberto Zobelli, Adam Gali. ANR-20-CE47-0009-01 - NOTISPERF.
- Italian National "Rita Levi Montalcini" young researcher fellowship program. Funding started on 1st March 2017 for a period of 3 years; budget 175,873.66 €.
- Funding from University of Rome Tor Vergata for the participation to the 24th ETSF Workshop on Electronic Excitations (2019); budget 1.5 k€.

As Collaborator:

- **Marie-Curie Doctoral Network 2023**; Title:"Time-resolved simulations of ultra-fast phenomena in quantum materials (TIMES): Tailoring materials from first principles". (<https://times.uv.es>)

- **ANR 2022** (French National Research Agency Young Investigator Grant); Title: "CORreLated photoemission spectra from the three-Body GRreen's function (COLIBRI)". Funding starting October 1st 2022; budget 300k€. Collaborators: Pina Romaniello, Claudio Attaccalite, ANR-22-CE30-0027-02 - COLIBRI.
- PhD grant from University of Aix-Marseille on "Electronic structure calculations for energy-producing systems: Hydrogen-metal interaction in fusion science and hybrid organic-inorganic heterostructures for solar cells applications", Coordinators: E. Cannuccia and Y. Ferro
- Funding from Psi-K European Network for the organization of the 24th ETSF Workshop on Electronic Excitations (2019) and 25th ETSF Workshop on Electronic Excitations (2022). Organizing Committee: Gabriele D'Avino, Elena Cannuccia, Carina Faber, Guido Fratesi, Pedro Melo, Claudia Roedl and Michiel van Setten; budget 12 k€

Computer time (As PI):

Aix-Marseille Mésocentre

- "An intensive ab initio DFT study of point defect electronic and optical properties of wurtzite Boron Nitride, 1 000 000 CPU hours
- "Dependence on pressure of electronic and vibrational properties of wurtzite Boron Nitride", 110000 CPU hours

French CEA GENCI

- "Ab initio Study of Electronic, Vibrational and Optical Properties of wurtzite BN under pressure", 400000 CPU hours on IRENE-ROME machine.

Italian CINECA, ISCRA-C projects:

- "Nothing is perfect: defects in hexagonal boron nitride". Collaborators: O. Pulci (2019) (360000 CPU hours).
- "Structural, dynamical and optical properties of confined water inside carbon nanotubes". Collaborators: O. Pulci (2019) (200000 CPU hours).
- "High temperature extrapolation of SiC polytypes operating limits in space missions. Collaborators: O. Pulci (2018) (320000 CPU hours).
- "Super Cooled Water: Self Consistent GW corrections and hybrid functionals". Collaborators: O. Pulci, M. Marsili, V. Armuzza (2018) (200000 CPU hours).

Computer time (As collaborator):

- "PRACE Distributed European Computing Initiative (DECI-7) project DIAVIB". Coordinator: Marton Voros. (2011)
- PRACE: "Opto-electronic properties of 2D Transition Metal Dichalcogenides with DFT and post-DFT simulations (OPTEL2D)", Coordinator: Maurizia Palummo. (2018-2019)

Conference and Workshop Organisation

1. Yambo School "Excited states in complex materials by MBPT methods" (Modena, May 2025)
2. Minicolloque "Excitations électroniques et optiques dans les solides et les structures de basse dimensionnalité" at Journée de la Matière Condensée 2024 (Marseille, France, Oct, 28-31, 2024)

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3. **Local Organizer** of the 27th ETSF Workshop on Electronic Excitations (Marseille, France, Jun 3-7, 2024)
4. Member of the organizing committee of the 25th Workshop on Electronic Excitations (Leuven, Belgium, Jun 13-17, 2022)
5. Member of the organizing committee of the 24th Workshop on Electronic Excitations (Jena, Germany, Sep 16-20, 2019)
6. 1^o meeting of the French Research Scientific Group GDR-REST (Roscoff, France, May 23-27, 2016)
7. International Workshop on Models and Data for Plasma-Material Interaction (Aix-Marseille Université, France, May 23-25, 2015)
8. 1^o *Roman Young Researchers' Meeting* (University of Rome "Tor Vergata", July 21, 2009)

Publications

Published in peer reviewed journals:

1. **Tunable second harmonic generation in 2D materials: comparison of different strategies**
S Grillo, E Cannuccia, M Palummo, O Pulci, C Attacalite, arXiv:2410.07661 (2024)
2. **Pressure Dependence of Electronic, Vibrational and Optical Properties of wurtzite-Boron Nitride**
M Silveti, C Attacalite, E Cannuccia, Physical Review Materials 7, 055201 (2023)
3. **Electronic structure, vibrational properties, and optical spectra of two- and three-dimensional hexagonal InSe: Layer-dependent ab initio calculations**
M Bejani, O Pulci, N Karimi, E Cannuccia, F Bechstedt Physical Review Materials 6 (11), 115201, (2022)
4. **Influence of anisotropy, tilt and pairing of Weyl nodes: The Weyl semimetals TaAs, TaP, NbAs and NbP**
D Grassano, O Pulci, **E Cannuccia**, F Bechstedt The European Physical Journal B 93 (8), 1-12, (2020)
5. **Thermal evolution of silicon carbide electronic bands**
E Cannuccia, A Gali Phys. Rev. Materials 4, 014601 (2020)
6. **Lattice vibrations and electronic properties of GaSe nanosheets from first principles**
M. Bejani et al., Physical Review Materials 3 (12), 124003 (2019)
7. **Second-harmonic generation in single-layer monochalcogenides: A response from first-principles real-time simulations**
C. Attacalite, M. Palummo, **E. Cannuccia** and M. Gruning
Physical Review Materials 3 (7), 074003 (2019)

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8. **Many-body perturbation theory calculations using the yambo code**
D. Sangalli, A. Ferretti, H. Miranda, C. Attaccalite, I. Marri, **E. Cannuccia**, et al.
J. Phys.: Condens. Matter **31** 325902 (2019)
9. **Theory of phonon-assisted luminescence in solids: Application to hexagonal boron nitride**
E. Cannuccia, B. Monserrat, C. Attaccalite
Phys. Rev. B **99**, 081109(R) (2019)
10. **Excitonic effects in third harmonic generation: the case of carbon nanotubes and nanoribbons**
C. Attaccalite, **E. Cannuccia**, M. Grüning
Phys. Rev. B **95**, 125403 (2017)
11. **Combined First Principle Calculations and Experimental Study of the Phonon Modes in the Multiferroic Compound GeV4S8**
E. Cannuccia, V. Ta Phuoc, B. Briere, L. Cario, E. Janod, B. Corraze, M. Lepetit
J. Phys. Chem. C, **121** (2017)
12. **Electron-vibration coupling induced renormalization in the photoemission spectrum of diamondoids**
A. Gali, T. Demján, M. Voros, G. Thiering, **E. Cannuccia**, A. Marini
Nature communications **7** (2016)
13. **Strong second harmonic generation in SiC, ZnO, GaN two-dimensional hexagonal crystals from first-principles many-body calculations**
C. Attaccalite, A. Nguer, **E. Cannuccia**, M. Grüning Physical Chemistry Chemical Physics **17**, 9533-9540 (2015)
14. **Exploring approximations to the GW self-energy ionic gradients**
C. Faber, P. Boulanger, C. Attaccalite, **E. Cannuccia**, I. Duchemin, T. Deutsch, X. Blase
Physical Review B **91**, 155109 (2015)
15. **Orbital-ordering-driven multiferroicity and magnetoelectric coupling in GeV4S8**
K. Singh, C. Simon, **E. Cannuccia**, M.-B. Lepetit, B. Corraze, E. Janod, and L. Cario
Phys. Rev. Lett. **113** , 137602 (2014)
16. **Electron-electron and electron-phonon correlation effects on the finite temperature electronic and optical properties of zb-GaN**
H. Kawai, K. Yamashita, **E. Cannuccia**, A. Marini
Phys. Rev. B. **89**, 085202 (2014)
17. **Verification of first-principles codes: Comparison of total energies, phonon frequencies, electron-phonon coupling and zero-point motion correction to the gap between ABINIT and QE/Yambo**
S. Poncé, G. Antonius, P. Boulanger, **E. Cannuccia**, A. Marini, M. Côté, X. Gonze
Computational Materials Science **83**, 341–348 (2014)
18. **Artificially stacked atomic layers: towards new van der Waals solids**

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- G. Gao, W. Gao, **E. Cannuccia**, et al.
Nano Letters **12**, 3518-3525 (2012)
19. **Zero point motion effect on the electronic properties of diamond, trans-polyacetylene and polyethylene**
E. Cannuccia and A. Marini
Europ. Phys. J. B. **85**, 320 (2012)
 20. **Effect of the quantum zero-point atomic motion on the optical and electronic properties of diamond and trans-polyacetylene**
E. Cannuccia, A. Marini,
Phys. Rev. Lett. **107**, 255501 (2011)
 21. **Optical properties of flavin mononucleotide: a QM/MM study of the protein environment effects**
E. Cannuccia, O. Pulci, R. del Sole and M. Cascella
Chemical Physics **389**, 35 (2011)
 22. **Ab-initio optical spectra of complex systems**
E. Cannuccia, O. Pulci, M. Palummo, V. Garbuio and R. Del Sole
Phys. Stat. Sol. **5**, 2543-2550 (2008)

Conference proceedings and other publications:

23. **First and Second Young Researchers Meetings in Rome**
E. Cannuccia, et al.
J. Phys.: Conf. Ser. **280**, 011001 (2011)
Proceedings of First and Second Young Researchers Meeting

Invited Talks

1. *Phonon-mediated optical properties*, <https://www.cecarn.org/workshop-details/1138>, Toulouse, November 2022.
2. *Phonon-assisted luminescence in hexagonal Boron Nitride*, "9th Annual Meeting of Mediterranean Institute of Fundamental Physics", Marino, February 27 - March 2, 2019.
3. *Exploring phase diagram of super cooled water*, "Eighth Annual Meeting of Mediterranean Institute of Fundamental Physics", Marino, February 28 - March 3, 2018.
4. *Finite temperature calculations of the electronic and optical properties of solids and nanostructures*, "11th ETSF Young Researchers' Meeting: evolution of ab-initio methods for condensed matter-connection with experiments and industry", Rome, May 12-16, 2014.
5. *Neutral electronic excitations: a Many-Body approach to the optical absorption spectra*, "9th Young Researchers' Meeting - ETSF", Brussels, May 21-25, 2012.
6. *Giant polaronic effects in polymers: breakdown of the electronic picture*, "15th Nanoquanta-ETSF Series of Workshops on Electronic Excitations: New Frontiers in Theoretical Spectroscopy and Quantum Transport", Berlin, Oct 11-15, 2010.

Invited Seminars

1. *Phonon-assisted luminescence in hexagonal Boron Nitride*, Belfast University, March 2019.
2. *Phonon-assisted luminescence in hexagonal Boron Nitride*, Cavendish Laboratories, Cambridge University, Jan 2019.

Invited Lectures

- *Phonon modes and electron-phonon coupling (DFPT)*, ICTP School "Ab-initio Many-Body Methods and Simulations with the Yambo Code", Trieste, Italy, April 4-8, 2022 (online).
- *Finite temperature calculations of the electronic and optical properties of solids and nano-structures*, CECAM-HQ-EPFL, Lausanne, Switzerland, April 8-12, 2013.

Contributed Talks

- *Thermodynamics and optical properties of point defects in wurtzite boron nitride*, "Journée de la matière condensée 2024", Marseille, Oct 28-31, 2024.
- *Phonon-assisted luminescence in hexagonal Boron Nitride*, "Nanoscience and Nanotechnology", Frascati, Oct 15-18, 2019.
- *Phonon-assisted luminescence in hexagonal Boron Nitride*, "Lavoisier Discussion on Quantum Simulation", Barcelona, May 8-9, 2019.
- *Phonon-Induced Breakdown of Quasi Particle Approximation in Conjugated Polymers*, "10th International Conference on Nanostructured Materials (NANO 2010)", Rome, Sep 13-17, 2010.
- *Exciton-Vibron Coupling in one-dimensional Conjugated Polymers*, "6th Young Researchers' Meeting - ETSF", Berlin, Jun 2-6, 2009.

Posters

1. *Temperature dependence of electronic and optical properties of Silicon Carbide compounds*, "25th ETSF Workshop on Electronic Excitations (2022)", Leuven, Belgium, June 13-17, 2022.
2. *Phonon-assisted luminescence in hexagonal Boron Nitride*, "19th International Workshop on Computational Physics and Material Science: Total Energy and Force Methods", Trieste, January 9-11, 2019.
3. *Multiferroicity and para/ferroelectric transition in GeV4S8*, "Psi-k 2015", San Sebastian, September 6-10, 2015.
4. *Multiferroicity and para/ferroelectric transition in GeV4S8*, "GBB60, Computer Simulations for Condensed Phase Systems", Rome, May 4-6, 2015.
5. *Phonon spectrum of GeV4S8 compound: high versus low temperature phases*, "GDR-Matériaux et interactions en compétition", Gif-sur-Yvette (France), November 19-22, 2013.
6. *Ab-initio study of optical properties of flavin mononucleotide and related molecules: a QM/MM study*, "Ab Initio Modeling in BioSciences: Structure, Dynamics and Function", Uppsala University, Sweden, December 10-11, 2008.
7. *Ab-initio study of optical properties of flavin mononucleotide and related molecules: a QM/MM study*, "13th NANOQUANTA-ETSF Workshop on Electronic Excitations", Pugnochiuso (FG), Italy, September 22-27, 2008.
8. *Ab-initio study of optical properties of flavin mononucleotide and related molecules*, "SIBPA 2008", Rome, September 17-20, 2008.
9. *Ab-initio study of optical properties of flavin mononucleotide and related molecules*, "5th Young Researchers' Meeting - Nanoquanta ETSF, Modena, May 20-23, 2008.

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10. *Ab-initio study of optical properties of flavin mononucleotide and related molecules*, "Acta Biophysica Romana 2008", Rome, April 10-11, 2008.

Science Outreach

- 2018 **Academic Event: High School Open Day, guidelines for middle school students**,
Conference Title: "Innovazione e progresso: la scienza dei materiali rivoluziona le nostre vite".
- 2018 **Academic Event: Scienza Orienta, guidelines for high school students**,
Conference Title: "Innovazione e progresso: la scienza dei materiali rivoluziona le nostre vite".
- 2017 **Inauguration of the academic year at Dep. of Physics "Tor Vergata"**,
Conference Title: "Innovazione e progresso: la scienza dei materiali rivoluziona le nostre vite".

Training Courses

- Formation ANF 2024 - CNRS Physique "Femmes en science physique" Partager les expériences, Renforcer l'affirmation de soi, 15-16 Octobre, 2024
- Formation consacrée aux Violences Sexuelles et Sexistes (VSS) au travail NIVEAU 1 - "Les bases" : identifier, comprendre et réagir @Coop-Egal, October, 2023
- Oser s'exprimer en publique, Association AIL, Marseille, Avril/Mai 2023
- Construire un enseignement (CM, TD, TP) : ingénierie pédagogique de base (techniques, méthodes) @Aix-Marseille Université, February/March, 2023
- Online Prace Training, Introduction to ScaLAPACK library @ MdIS/Idris, March 15-16, 2022.
- 4th International Workshop and School - Time dependent Density-Functional Theory: Prospects and Applications (Benasque, Spain, January 2-15, 2010)
- 5^o CASPUR Summer School: Calcolo Avanzato (Grottaferrata (RM), September 1-12, 2008).
- Theoretical Spectroscopy Lectures: theory and codes (Lyon, December 10-14, 2007).

Administration

- Apr 2024 **Member of Council Organism of Laboratory PIIM.**
- Jun 2023 **Correspondante égalité du Laboratoire PIIM, Aix-Marseille Université.**
- Nov 2018 **Elected as a member of Physics Department Council Organism, University of Rome "Tor Vergata", Rome (Italy).**

Professional Services

- Peer-reviewer for major scientific journals, including Physical Review Letters, Physical Review B, European Physics Journal B.
- Peer-reviewer for DECI-Computing Resources Calls and for CECAM workshops.

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- Member of thesis jury: Abdullah SHUKRI, "Ab initio electronic stopping power" 30 novembre 2015 INSTN, CEA.
- Member of selection committee for a permanent position (Maitre de Conference) at Aix-Marseille University, Avr 2022.

Memberships

European Theoretical Spectroscopy Facility, as a Research Team Leader.

Activité de Bénévole

Responsable du Club Omnisport de la Recherche (COR) du CNRS pour le cours de natation enfants, depuis septembre 2023.