



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

Teaching Experience

Lecturer at Aix-Marseille Université, for the classes:

- **Mécanique Quantique/Quantum Mechanics** (TD:30 hours), Master of Fundamental Physics (M1). Academic years 2020-2021, 2021-2022.
- **Optique Géométrique/Geometrical Optics** (CM+TD:22 hours), Portail Marie-Curie (L1). Academic years 2020-2021, 2021-2022.
- **Physics Practical Sessions (Electricity)** (TP:12 hours), Portail Marie-Curie (L1). Academic years 2020-2021, 2021-2022.
- **Mécanique Quantique/Quantum Méchanics** (TD:15 hours), Licence Physique Chimie (L3). Academic years 2019-2020, 2020-2021, 2021-2022.

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- **Advanced Numerical Simulations** (CM+TP:16 hours), Master of Nanoscience and Nanotechnology (M2). Academic years 2019-2020, 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.

Other experiences

- Maths Teacher, "Villa Sora" high school, Frascati, Italy (2007-2009).
- Private Maths Lessons (2007-2010).

Supervising activities

- **Science Watch** teaching unit hosted by Master of Fundamental Physics, Aix-Marseille Université. Supervision of students: Mathilde Pouyot (Project:"Defects in semiconductors: Combining experiment and theory")
 - Supervision of **PhD students**: Martino Silveti, financed by ANR-JCJC project NOTISPERF, co-supervised with Cedric Pardanaud (Oct 2021 - Sep 2024).
 - Supervision of **Master Student**: 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.*

Grants

As PI:

- ANR "Jeunes Chercheuses et Jeunes Chercheurs" 2020 (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:

- 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

- "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)

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- PRACE: "Opto-electronic properties of 2D Transition Metal Dichalcogenides with DFT and post-DFT simulations (OPTEL2D)", Coordinator: Maurizia Palumbo. (2018-2019)

Organizational Experience

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

Publications

Published in peer reviewed journals:

1. **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 (submitted 2019) arXiv preprint arXiv:1906.12231
2. **Thermal evolution of silicon carbide electronic bands**
E Cannuccia, A Gali Phys. Rev. Materials **4**, 014601 (2020)
3. **Lattice vibrations and electronic properties of GaSe nanosheets from first principles**
M. Bejani et al. (submitted 2019) arXiv preprint arXiv:1906.06933
4. **Second-harmonic generation in single-layer monochalcogenides: A response from first-principles real-time simulations**
C. Attaccalite, M. Palumbo, **E. Cannuccia** and M. Grüning
Physical Review Materials **3** (7), 074003 (2019)
5. **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)
6. **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)
7. **Excitonic effects in third harmonic generation: the case of carbon nanotubes and nanoribbons**
C. Attaccalite, **E. Cannuccia**, M. Grüning

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Phys. Rev. B **95**, 125403 (2017)

8. **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. Lepeit
J. Phys. Chem. C, **121** (2017)
9. **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)
10. **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)
11. **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)
12. **Orbital-ordering-driven multiferroicity and magnetoelectric coupling in GeV4S8**
K. Singh, C. Simon, E. Cannuccia, M.-B. Lepeit, B. Corraze, E. Janod, and L. Cario
Phys. Rev. Lett. **113** , 137602 (2014)
13. **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)
14. **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. Coté, X. Gonze
Computational Materials Science **83**, 341–348 (2014)
15. **Artificially stacked atomic layers: towards new van der Waals solids**
G. Gao, W. Gao, E. Cannuccia, et al.
Nano Letters **12**, 3518-3525 (2012)
16. **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)
17. **Effect of the quantum zero-point atomic motion on the optical and electronic properties of diamond and trans-polyacetylene**
E. Cannuccia, A. Marini,

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Phys. Rev. Lett. **107**, 255501 (2011)

18. **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)
19. **Ab-initio optical spectra of complex systems**
E. Cannuccia, O. Pulci, M. Palumbo, V. Garbuio and R. Del Sole
Phys. Stat. Sol. **5**, 2543-2550 (2008)

Conference proceedings and other publications:

20. **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. **E. Cannuccia** *Phonon-assisted luminescence in hexagonal Boron Nitride*, "9th Annual Meeting of Mediterranean Institute of Fundamental Physics", Marino, February 27 - March 2, 2019.
2. **E. Cannuccia** *Exploring phase diagram of super cooled water*, "Eighth Annual Meeting of Mediterranean Institute of Fundamental Physics", Marino, February 28 - March 3, 2018.
3. **E. Cannuccia** *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.
4. **E. Cannuccia** *Neutral electronic excitations: a Many-Body approach to the optical absorption spectra*, "9^o Young Researchers' Meeting - ETSF", Brussels, May 21-25, 2012.
5. **E. Cannuccia** *Giant polaronic effects in polymers: breakdown of the electronic picture*, "15^o Nanoquanta-ETSF Series of Workshops on Electronic Excitations: *New Frontiers in Theoretical Spectroscopy and Quantum Transport*", Berlin, Oct 11-15, 2010.

Invited Seminars

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

Invited Lectures

- **E. Cannuccia** *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).
- **E. Cannuccia** *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

- **E. Cannuccia** *Phonon-assisted luminescence in hexagonal Boron Nitride*, "Nanoscience and Nanotechnology", Frascati, Oct 15-18, 2019.
- **E. Cannuccia** *Phonon-assisted luminescence in hexagonal Boron Nitride*, "Lavoisier Discussion on Quantum Simulation", Barcelona, May 8-9, 2019.
- **E. Cannuccia** *Phonon-Induced Breakdown of Quasi Particle Approximation in Conjugated Polymers*, "10^o International Conference on Nanostructured Materials (NANO 2010)", Rome, Sep 13-17, 2010.
- **E. Cannuccia** *Exciton-Vibron Coupling in one-dimensional Conjugated Polymers*, "6^o 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*, "13^o 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*, "5^o Young Researchers' Meeting - Nanoquanta ETSF, Modena, May 20-23, 2008.
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".

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- 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

- Online Prace Training, Introduction to ScaLAPACK library @ Mdis/Ildris, 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

- 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.
- Member of thesis jury: Abdullah SHUKRI, "Ab initio electronic stopping power" 30 novembre 2015 INSTN, CEA.

Memberships

European Theoretical Spectroscopy Facility, as a Research Team Leader.