

## Fabio Ricci

## curriculum vitae et studiorum

University of Liège  
Physique Théorique de Matériaux  
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## Personal informations

Born in Teramo (Italy) the August 28th 1980.  
Residing in Liège, Boulevard D'Avroy, 75 - 4000 Liège (Belgium).  
Living in Liège (Belgium).

## Education

March 18th 2010 - PhD in Physics obtained at the University of L'Aquila (Italy) in condensed matter physics. Dissertation title: "Theoretical and experimental study of magnetic materials for spintronic applications".

April 26th 2006 - Master degree in Physics at L'Aquila University (Italy), course of study in condensed matter, with grade 106/110. Master thesis: "Firts principles calculations of magneto-optical properties of magnetic films for spintronic interests" ("Calcolo a principi primi delle proprietà magneto-ottiche di film in materiali magnetici di interesse in spintronica").

April 2nd 2003 - Bachelor in Physics at L'Aquila University (Italy). Bachelor thesis: "Magneto-optical films spectra and hysteresis cycles study for possible spintronic applications" ("Studio degli spettri magneto-ottici e dei cicli d'isteresi di film, con possibili applicazioni nel campo della spintronica").

High school-leaving certificate on the July 5th 1999.

## Experiences

*2019/10/01 - Present day*

Post-Doctoral assistant at the University of Liège (Belgium) for the theoretical optimisation and development of *ab-initio* utilities in the Abinit code.

*2019/01/25*

Advisory Board Member in the IOP Publishing "Journal of Physics: Condensed Matter".

*2016/10/01 - 2019/09/30*

Post-Doctoral assistant at the University of Liège (Belgium) for the theoretical optimisation and development of *ab-initio* utilities in the FEDER FMF: Energy "LoCoTED" project between the European Union and the Wallon Region with title: "Harvesting heat waste from industrial machines with low cost thermoelectric modules".

*2015/03/26 - Present day*

Teaching activity at the University of Liège in the Master course of "Magnetism" directed by Dr. Eric Bousquet: fundamentals of magneto-optics effects (classical and quantum mechanic explanations; experiments vs theory); exchange constants calculation on simple magnetic systems from first principles.

*2014/10/24*

Winner of SEED Young 2014 project at the SPIN-CNR Institute (Italy). The project concerns the “Synthesis, experimental and theoretical investigation of Ca-112 a new family of iron based superconductors”, and it is in collaboration with the University of Genoa (Italy) and the AIST Institute of Tsukuba (Japan).

*2014/10/22 - 2014/10/23*

Attendance to the CISM (Centre de calcul intensif et stockage de masse) training sessions at the Catholic University of Louvain (Louvain-La-Neuve, Belgium), on the following topics:

- 1) Compilers and compiling, optimized libraries, profiling and debugging.
- 2) Parallel programming with MPI.
- 3) Parallel programming with OpenMP.

*2014/10/13 - 2014/10/17*

Attendance to the CECAM-HQ-EPFL tutorial school on “Basic techniques and tools for development and maintenance of atomic-scale software”, Lausanne (Switzerland).

*2014/09/01 - 2016/09/30*

Post-Doc Fellowship at the University of Liège (BE) and FRS-FNRS (Fonds de la Recherche Scientifique), with project: “Perturbative treatment of response functions in magnetic field”, with Dr. Eric Bousquet as supervisor.

*2013/10/15 - 2014/02/18*

Teaching support activity to the “Elettromagnetismo” (Electromagnetism) course of study, directed by Prof. A. D’Altorio.

*2013/08/19 - 2014/08/18*

Post-doc at SPIN-CNR at L’Aquila University with project: “Theoretical and computational study of electronic, magnetic and superconducting properties of Iron-based materials and their interfaces”, with Dr. Gianni Profeta as supervisor, funded under the European Commission FP7 EU “Super Iron” Project.

*2013/03/22*

Approved ISCRA C HP10CY7J7J project at High Performance Computing Cineca: “Interfaces and hetero-structures in Fe-based superconductors”.

*2012/04/02 - 2013/04/02*

Post-doc fellowship L’Aquila University with project: “First principles modeling of Fe-based superconductors”, with supervisor Dr. Gianni Profeta, funded under the European Commission FP7 EU “Super Iron”.

*2011/03/06 - 2011/06/06*

Teaching job (2 hours/week) in the “Microfisica Quantistica” (Quantum Mechanics) course (Prof. Carlo Pierleoni) for the first level degree on physics at L’Aquila University.

*2011/03/01 - 2012/03/01*

Post-doc fellowship at L’Aquila University with project: “Characterization and experimental modelling of magnetic multilayered structures”, with supervisor Dr. Franco D’Orazio.

*2011/01/10 - 2011/02/19*

Temporary teaching job at public high school Istituto Tecnico e Professionale ”U. Follador” (Belluno) in physics and laboratories.

*2010/12/13 - 2010/12/23*

Temporary teaching job at public high school Istituto Magistrale "G. Renier", Agordo (Belluno) in mathematics.

*11/19/2010 - 12/02/2010*

Collaboration with the Milan University, invited by Prof. G. Onida. Seminar title: "Magneto-optical effects: a theoretical and experimental point of view in layered and inhomogeneous media" the 25 November 2010.

*2010/07/06 - 2010/07/09*

Participation at the course "Technical and scientific calculation within Fortran95" at CASPUR in via dei Tizii, 2/c Rome (RM).

*2010/03/04 - 2010/09/04*

Master student scholarship at L'Aquila University with title project: "Theoretical and experimental study of multilayers for spintronic applications" with Dr. Franco D'Orazio as supervisor.

*2009/09/05 - 2009/11/29*

Research period at Northwestern University, 2145 Sheridan Road - Evanston, IL 60208-3112 USA under the supervision of A. J. Freeman, Morrison Professor of Physics and Dr. Jung-Hwan Song, Department of Physics and Astronomy.

*2008/5/7 - 2010/12/31*

Guide in the physics and astrophysics museum "Galileium" in Teramo (IT).

*2006/11/01 - 2010/03/18*

PhD at L'Aquila University under the supervision of Dr. F. D'Orazio and Prof. F. Lucari.

*2006/10/02 - 2006/11/01*

Stage at the Regional Agency for the Ambient Safety (A.R.T.A.), as physicist, under the supervision of Dr. C. Cimatori. Activities: study of pollution from non-ionizing electromagnetic radiation and acoustic phenomena.

*2005/11/08 - 2011/01/09*

Teaching of physics and mathematics at private high school and university students at CEPU (European Center of university studies).

*2005/01/15 - 2005/06/15*

Temporary assistant professor position to the course related to the "Laboratorio di Introduzione alla Fisica" (Physics introductory laboratory) at L'Aquila University. Activities: didactic innovation methods, laboratory experiences planning, web-site ideation of the Physics Department.

*2004/09/15 - 2005/06/30*

Teaching activity of physics and mathematics for high school and university students at "G. Cameli" (Teramo, IT) private institute; Organization and setting of practical physics experiences with students.

*2003/05/05 - 2004/07/31*

Collaboration at "Graphite Technologies S.p.A" private factory: realization of components in carbon for submarine pumping systems. Activities: chemical laboratory assistant and responsible of the quality of the processes.

*2002/10/10 - 2003/6/30*

Teaching activity of physics and mathematics for high school and university students at "G. Cameli" (Teramo, IT) institute.

## List of Awards

*October 2017:* Elsevier *Certificate of outstanding contribution in reviewing* manuscripts in the “Computational Material Science” journal.

*August 2017:* “Elsevier Reviewer Recognition” for reviewing manuscripts in the Elsevier “Computational Material Science” journal.

*October 2016:* Elsevier *Certificate of outstanding contribution in reviewing* manuscripts in the “Materials Chemistry and Physics” journal.

*September 2016:* Best Poster Award at the European Conference on Thermoelectrics 2016.

*July 2016:* “Elsevier Reviewer Recognition” for reviewing manuscripts in the Elsevier “Computational Material Science” journal.

## List of Scientific Publications

16. X. Gonze *et al.*, “ABINIT: Overview and focus on selected capabilities”, in preparation for submission.
15. S. Lemal, F. Ricci, D. I. Bilc, M. J. Verstraete and Ph. Ghosez, “Magnetic instabilities in doped  $\text{Fe}_2\text{YZ}$  full-Heusler thermoelectric compounds”, *Phys. Rev. B* **100**, 161201(R) (2019).
14. X. Gonze *et al.*, “The ABINIT project: impact, environment and recent developments”, submitted to the Computer Physics Communications.
13. F. Belviso *et al.*, “Viewpoint: Atomic-scale design protocols towards energy, electronic, catalysis and sensing applications”, *Inorganic Chemistry* **58**, 14939 (2019).
12. F. Ricci, S. Prokhorenko, M. Torrent, M. J. Verstraete, E. Bousquet, *Phys. Rev. B* **99**, 184404 (2019) *Editors’ Suggestion*.
11. I. Pallecchi, M. Pani, F. Ricci, S. Lemal, D. I. Bilc, P. Ghosez, C. Bernini, N. Ardoino, G. Lamura and D. Marré, *Phys. Rev. Mat.* **2**, 075403 (2018).
10. F. Ricci and E. Bousquet, *Phys. Rev. Lett.* **116**, 227601 (2016).
9. C. Tresca, F. Ricci and G. Profeta, *2D Mater.* **2**, 015001 (2014).
8. V. Grinenko *et al.*, *Phys. Rev. B* **90**, 094511 (2014).
7. F. Ricci, G. Profeta, *Phys. Rev. B* **87**, 184105 (2013).
6. F. Ricci, F. D’Orazio, F. Lucari, A. Continenza, *J. Supercond. Nov. Magn.* **26**, 1005 (2013).
5. D. R. Cavicchia, F. D’Orazio, L. Rossi, F. Ricci and F. Lucari, *EPJ Web of Conferences* **40**, 13002 (2013).
4. F. Cagliaris, F. Ricci, G. Lamura, A. Martinelli, A. Palenzona, I. Pallecchi, A. Sala, G. Profeta and M. Putti, *Sci. Technol. Adv. Mater.* **13**, 054402 (2012).
3. F. Ricci, F. D’Orazio, A. Continenza, F. Lucari, and A. J. Freeman, *Phys. Rev. B* **83**, 224421 (2011).
2. F. Ricci, F. D’Orazio, A. Continenza, F. Lucari, M. Passacantando, G. Impellizzeri, F. Priolo and A. J. Freeman, *J. Phys.: Conf. Ser.* **200**, 072079 (2010).

1. F. Ricci, F. D’Orazio, A. Continenza, F. Lucari, and A. J. Freeman, Phys. Rev. B **78**, 134411 (2008).
0. F. Ricci, S. Picozzi, A. Continenza, F. D’Orazio, F. Lucari, K. Westerholt, M. Kim, and A. J. Freeman, Phys. Rev. B **76**, 014425 (2007).

## List of Conferences and Workshops

*2019/07/11 - 2019/07/12*

Attendance to the “Advanced Energy Materials and Research” with an *invited* presentation entitled “Magnetic instability in heavily n-doped Fe-based full-Heusler compounds: origin and impact on thermoelectric properties”, held in Zurich (CH).

*2019/05/20 - 2019/05/22*

Attendance to the “Abinit Developers Workshop 2019”, held in Louvain-la-Neuve (Belgium), with a contributed poster presentation entitled “Doping effects and magnetic instabilities in full-Heusler  $\text{Fe}_2\text{YZ}_{1-x}\text{A}_x$  thermoelectric compounds”.

*2019/03/04 - 2019/03/08*

Attendance to the “APS March Meeting 2019”, held in Boston (MA, USA), with two contributed oral communications entitled: 1) “The second-principles MULTIBINIT software project” and 2) “Doping effects and magnetic instabilities in full-Heusler  $\text{Fe}_2\text{YZ}_{1-x}\text{A}_x$  thermoelectric compounds”

*2018/09/17 - 2018/09/20*

Attendance to the “EMRS Fall Meeting”, held in Warsaw (Poland), with a contributed oral communication entitled “The second-principles MULTIBINIT software project”.

*2018/07/01 - 2018/07/05*

Attendance to the “37th Annual International Conference on Thermoelectrics and 16th Annual European Conference on Thermoelectrics”, held in Caen (France), with a contributed poster entitled “Magnetic instability in heavily *n*-doped Fe-based full-Heusler compounds for thermoelectric applications”.

*2018/05/29*

Attendance to the “2nd Principles Workshop”, held in Liège (Belgium), with a contributed presentation entitled “A first preliminary second-principles effective potential in the full-Heusler  $\text{Fe}_2\text{VAI}$  for thermoelectrics”.

*2017/12/11 - 2017/12/12*

Attendance to the “1st Workshop on thermoelectric transport in nanowires”, held in Eindhoven (Netherlands), with a contributed poster entitled “Magnetic instability in heavily n-doped Fe-based full-Heusler compounds for thermoelectric applications”.

*2017/07/31 - 2017/08/03*

Attendance to the “36th Annual International Conference on Thermoelectrics”, in Pasadena California (USA), with a contributed poster entitled “About the electronic properties of  $\text{Fe}_2\text{VAI}$  and related thermoelectric compounds”.

*2017/07/03 - 2017/07/06*

Attendance to the “Thermoelectric Materials: From Theoretical Design to Industrial Application” Workshop, in Cork (Ireland), with a contributed talk entitled “About the electronic properties of  $\text{Fe}_2\text{VAI}$  and related thermoelectric compounds”.

*2017/05/09 - 2017/05/12*

Attendance to the “8th Abinit Developers Workshop”, in Frejus (France), with an *invited* presentation entitled “Non-collinear magnetism in the Abinit Density Functional Perturbation Theory”.

2017/01/12 - 2017/01/14

Attendance to the “18th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods”, in Trieste (Italy), with a contributed poster presentation with title “Non-collinear magnetism in the Abinit Density Functional Perturbation Theory”.

2016/09/20 - 2016/09/23

Attendance to the “14th European Conference on Thermoelectrics” (ECT2016) with a contributed poster with title “First-principles study of heavily doped full-Heusler  $\text{Fe}_2YZ$  for high thermoelectric power factor”. **Awarded** with poster prize by the ECT committee.

2016/04/22

Attendance to the “8th CECI Scientific Meeting”: scientific meeting of the group for massive calculations of the FNRS ”Calcul Intensif” unit.

2016/01/31 -2016/02/03

Attendance to the Workshop “Fundamental Physics of Ferroelectrics and Related Materials 2016”, Washington DC (USA), with an oral presentation with title: “Unveiling the room temperature magnetoelectricity of troilite  $\text{FeS}$ ”.

2015/11/29 - 2015/12/4

Attendance to the “MRS Fall Meeting” Conference in Boston (MA, USA), with an oral presentation with title: “First-principles investigations of multiferroicity in  $\text{FeS}$ ”.

2015/10/12 - 2015/10/14

Attendance to the “Challenges in Multiferroics and Magnetoelectrics” Workshop in Jülich (Germany), with a poster presentation with title: “First-principles investigations of multiferroicity in  $\text{FeS}$ ”.

2015/09/06 - 2015/09/10

Attendance to the “Psi-k 2015” Conference in San Sebastian (Spain), with a poster presentation with title: “First-principles investigations of multiferroicity in  $\text{FeS}$ ”.

2015/06/29 - 2015/07/03

Attendance to the “European Meeting on Ferroelectricity EMF 2015” in Porto (Portugal), with a poster presentation with title: “First-principles investigations of multiferroicity in  $\text{FeS}$ ”.

2015/05/11 - 2015/05/15

Attendance to the “E-MRS Spring Meeting 2015” in Lille (France), with a poster presentation with title: “First-principles investigations of multiferroicity in  $\text{FeS}$ ”.

2015/04/28 - 2015/04/30

Attendance to the “7<sup>th</sup> Abinit Developers Workshop” held at the University of Liège, with *invited* presentation: “Density functional perturbation theory within non-collinear magnetism”.

2014/10/17 - 2014/10/18

Attendance to the “First SCALE-UP workshop: a joint initiative supported by ABINIT, HiT4FiT and TheMoTherm”, University of Liège (Belgium).

2014/09/09 - 2014/09/13

Attendance to the “Workshop on Superconductors and Functional Oxides” SuperFox 2014 (University of Rome La Sapienza) with a poster presentation: “Pressure dependent critical temperature on  $\text{KFe}_2\text{As}_2$ ”.

2013/09/09 - 2013/09/13

Attendance to the “Italian National Conference on Condensed Matter Physics” FisMat 2013 with oral contribution: “Electronic structure of Iron-Chalcogenide thin films”.

*2013/05/06 - 2013/05/08*

Attendance to the Mid-Term Meeting of the FP7 EU Super Iron Project as Guest Scientist in Dresden (Germany).

*2013/05/04 - 2013/05/06*

Attendance to the “Super Iron Student Workshop” in Bad Schandau (Germany) as Guest Scientist with oral presentation with title: “Theoretical investigation on iron chalcogenide superconductors”.

*2012/09/09 - 2012/09/14*

Participation to the Joint European Magnetic Symposia JEMS 2012 within the oral contribution: “Magneto-optics for uniaxial crystals: an application to strained  $\text{Fe}_{0.5}\text{Co}_{0.5}$ ”.

*2011/09/26 - 2011/09/30*

Participation to the Italian Physics Society (SIF) National Meeting, with oral presentation title: “Magneto-optical properties of uniaxial crystals”.

*2011/02/23 - 2011/02/25*

Participation to the Convegno Italiano di Magnetismo, Magnet 2011, with oral presentation within title: “Optical and magneto-optical properties of strained  $\text{Fe}_{0.5}\text{Co}_{0.5}$  alloy”.

*2009/07/26 - 2009/07/31*

Participation to the International Conference on Magnetism 2009 with a poster presentation.

*2009/06/03 - 2009/06/05*

Participation to IX Convegno Nazionale sui Materiali Nanofasici, Cagliari-Iglesias (IT), with oral contribution: “Magneto-optical spectra of spheroidal Mn-Ge nanoparticles”.

*2009/05/15 - 2009/05/30*

School on superconductors and functional oxides, Marina di Pisciotta, Salerno (Italy).

*1 July 2008*

Participation to the workshop on “Structural, Electronic and Magnetic Properties of Diluted Magnetic Semiconductors (DMSs)”, CRN, Rome (Italy).

*2008/10/11 - 2008/10/18*

INFN School on “Physics in Low Dimensions”, Lucca (Italy).

## Skills and Qualifications

- Excellent use of Unix, Linux and MacOS operating systems.
- Excellent knowledge of shell and Fortran programming languages.
- Good knowledge of parallel programming interfaces MPI and OpenMP.
- Good knowledge of WOLFRAM Mathematica for technical computing software.
- Advanced use of LabVIEW (C++ based graphic user interface) to build, program and setup measure devices.
- Advanced knowledge of High Performance Computing (HPC) facilities.
- Good knowledge of the following programming languages: Python, Perl, C, C++, Html, CSS.
- **Languages:** Fluent English and French; Italian: mother tongue.

## Research topics

I have strong experience in first-principle simulations of structural, electronic, magnetic, optical and magneto-optical (magneto-optical Faraday and Kerr effect) properties of crystals by means of Density Functional Theory. During my master thesis and part of my PhD, I studied the magnetic properties of full-Heusler alloys and diluted magnetic semiconductors via magneto-optical Kerr and Faraday effects measurements at the University of L'Aquila.

In the same period, in collaboration within the Dr. Franco D'Orazio, a theoretical model to calculate the Kerr effect on layered (with cubic symmetry) systems has been generalised and extended in order to systems with uniaxial symmetry. These results are, at present, in preparation for publication.

I have advanced knowledge of codes for ab-initio simulations ranging from all-electron (FLAPW) to pseudo-potential plan-wave based codes (VASP, ABINIT) and Hybrid Functionals (CRYSTAL).

I have a strong background in the following families of compounds:

- Heusler alloys for spintronic applications (I have worked on  $\text{Co}_2\text{MnGe}$  and  $\text{Co}_2\text{MnSn}$ ).
- magnetic diluted semiconductors like  $(\text{Ga},\text{Mn})\text{As}$ ,  $(\text{Ge},\text{Mn})\text{Ge}$ .
- soft magnetic materials (I worked on  $\text{Fe}_{1-x}\text{Co}_x$  alloys in the PRIN07 Project).
- Iron-based superconductors (working in the European Commission FP7 EU "Super Iron" Project).
- Magneto- and Ferro-electric materials (working on the troilite  $\text{FeS}$  in the FRS-FNRS project).
- Fe-based full-Heusler compounds for thermoelectric applications.

I have been working from the last three years in the ABINIT Developers community: I derived, developed and tested the density functional perturbation theory for non-collinear magnetism related to the phonon perturbations. At the moment, a publication related to this topic, is in preparation.

## Personal interests

- I am a volleyball trainer and player. I believe the sport is a good way to stay balanced.
- I am the president of the volleyball club "ASD Sart-Tilman" (asbl), reference number: LG0232.
- Music.
- Comics, books and games.