Curriculum vitae

First name: Michele
Last name: Casula
Place and date of birth: Trieste (Italy), 18/05/1977
Marital status: Married to Ilaria Cherubini, 14/04/2007
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Current position
CNRS DR2 permanent research fellow at the IMPMC, Paris, France; Head of the "Théorie Quantique des Matériaux" (TQM) team; Member of the CNRS Comité National Section 03.

Education and Qualifications

- since October 2020: CNRS DR2 at IMPMC, Paris, France
- September 2017 - October 2020: CNRS CR-CN permanent research fellow at IMPMC, Paris, France
- March 2015 - September 2017: CNRS CR1 permanent research fellow at IMPMC, Paris, France
- October 2010 - March 2015: CNRS CR2 permanent research fellow at IMPMC, Paris, France
- September 2008 - September 2010: Postdoctoral fellow at the Ecole Polytechnique in the "strongly correlated quantum materials" group of Professors Silke Biermann and Antoine Georges.
- October 2005 - August 2008: Postdoctoral fellow at the University of Illinois in Urbana-Champaign (UIUC), Illinois, USA in the group of Professors David M. Ceperley and Richard M. Martin.
- October 2005: *Doctor Philosophiæ* degree in Physics (approved magna cum laude) at SISSA.
  Thesis: *New QMC approaches for the simulation of electronic systems: a first application to aromatic molecules and transition metal compounds.*
  Supervisor: Prof. S. Sorella
- October 2002: *Magister Philosophiæ* degree in Physics (full marks, magna cum laude) at SISSA.
  Thesis: *The antisymmetrized geminal wave function in Quantum Monte Carlo calculations*
  Supervisor: Prof. S. Sorella
- November 2001: Degree in Physics (full marks, magna cum laude) at the University of Trieste
  Thesis: *Ottimizzazione della funzione d'onda per un gas di elettroni quasi unidimensionale e problemi di ergodicità* (*Wave function optimization for a quasi one dimensional electron gas and ergodicity problems*)
  Supervisor: Prof. G. Senatore
- Summer 1999: Summer student fellowship at CERN (Geneva, Switzerland) in collaboration with the ATLAS group (LHC project).
- From 1996/1997 to 2000/2001, Degree Course in Physics at the University of Trieste, Facoltà di Scienze MM.FF.NN., Specialization in Theoretical Physics.

Professional Habilitations

- French "Habilitation à diriger des recherches" (HDR) in Physics, released by the Université Pierre et Marie Curie. Thesis defence: 18/12/2017.
- Italian Scientific Habilitation as associate professor ("Seconda Fascia") in Theoretical Physics of Condensed Matter (02/B2), released by MIUR (Italian ministry for education, university and research). Validity: from 08/08/2018 to 08/08/2027.
- Italian Scientific Habilitation as full professor ("Prima Fascia") in Theoretical Physics of Condensed Matter (02/B2), released by MIUR (Italian ministry for education, university and research). Validity: from 08/08/2018 to 08/08/2027.

Awards

2013: "Prime d'excellence scientifique"

Research activity and interests

Methods:

- Density functional theory;
- Variational and diffusion Quantum Monte Carlo;
- Dynamical mean field theory;
- Molecular dynamics.

Applications:

- Strongly correlated systems;
- Electron-phonon coupling;
- Low-dimensional systems;
- Electronic structure from first principles.

Research funding

- 2012: INTELBIOMAT - Exchange Grant for funding a mid-term visit (12 weeks) of Simone Taioli, under the project "Theoretical and computational study of the electron-phonon coupling in potassium-doped fullerene crystals". It has been awarded by the European Science Foundation within the framework of Interdisciplinary Approaches to Functional Electronic and Biological Materials.
- 2016: Fellowship funded by the Sorbonne Excellence Cluster MATISSE (MATerials, InterfaceS, Surfaces, Environment) for a 18-month postdoctoral position in the group.
- 2019: Fellowship funded by the Sorbonne Excellence Cluster MATISSE (MATerials, InterfaceS, Surfaces, Environment) for a 18-month postdoctoral position in the group.
- 2020: ANR DesperQD (AAP in the "Projet de recherche collaboratif international" (PRCI) framework with NRF Singapore). The aim of the project is to develop the next generation of halide perovskite-based quantum dots for photonic applications. This will be done by both an experimental and a theoretical characterization of the optimal materials for quantum light emission. On the French side, M. Casula and coworkers will take care of the *ab initio* modelling of the quantum dots.
- 2020: H2020-INFRAEDI (05-2020) grant to build TREX, a new European Center of Excellence in Exascale computing. TREX (`https://trex-coe.eu/`) is a multi-center project for the development of new algorithms and libraries based on stochastic approaches to the electronic structure problem in physics and chemistry, such as quantum Monte Carlo (QMC), in order to harvest the highly-parallel infrastructures offered by future exascale high-performance computing (HPC) machines. M. Casula is the coordinator of the Sorbonne-CNRS node, and will lead the demostration work pakage, which plans to apply the newly developed QMC libraries to cutting-edge problems in condensed matter physics and materials science.

Bibliometric data and scientific production

60 published papers, among them:
1 Nature Physics;
1 Nature Communications;
2 Proceedings of the National Academy of Sciences;
6 Physical Review Letters;
1 Europhysics Letters;
2 Journal of Chemical Theory and Computation;
2 Physical Review Research;
23 Physical Review B;
2 Physical Review A;
2 Physical Review Materials;
1 Chemical Physics Letters;
12 Journal of Chemical Physics.

Source: Publons Web of Science, September 2022.
Web page: `http://www.webofscience.com/wos/author/record/GSJ-1096-2022`
Total number of citations: 2450
H factor: 26

Source: Google Scholar, September 2022.
Web page: `https://scholar.google.fr/citations?hl=en&user=npgAMMMAAAAJ&cstart=20&pagesize=20`
Total number of citations: 3485
H factor: 29

Teaching experience
Teaching "Computational Materials Science" at the Master 2 level of SMNO (Sciences des Matériaux et Nano-Objets), Université Pierre et Marie Curie (UPMC) / Sorbonne Université (SU) (academic years: 2014-2015, 2015-2016, 2016-2017, 2017-2018, 2018-2019);
Teaching "Introduction to many-body physics of fermions and bosons" at the Master 2 level of ICFP (International Centre for Fundamental Physics), Ecole Normale Supérieure (academic year: 2017-2018, 2018-2019, 2019-2020, 2020-2021).
Teaching "Electronic structure theory" at the Master 2 level of ICFP (International Centre for Fundamental Physics), Ecole Normale Supérieure (academic year: 2021-2022, 2022-2023).

Advising and mentoring

- Thesis director of Doctoral students at SU:
  - Félix Mouhat, "Combining Quantum Monte Carlo with Langevin Molecular Dynamics to study water clusters", October 2014 - October 2018 (co-directed with Marco A. Saitta).
  - Romain Taureau, "Hydrides high-temperature superconductors by quantum Monte Carlo", started in October 2019.
  - Miha Srdinšek, "Efficient numerical methods for efficient Rényi entropy evaluation based on path integrals", started in October 2020 (co-directed with Rodolphe Vuilleumier).
  - Matteo Peria, "Machine learning methods to describe water clusters", started in November 2021 (co-directed with Marco A. Saitta).
  - Francesco Cassol, "Non-local correlations in extended dynamical mean field methods", started in December 2021 (co-advised with B. Lenz).
  - Damian Contant, "Electron correlation and lattice dynamics in quantum solids", started in September 2022 (co-advised with Maria Hellgren);
  - Codirection of a SISSA PhD student, Giacomo Tenti, started in September 2022.
- Principal advisor of Doctoral students at UPMC:
  - Nicolas Devaux, "Étude par Monte Carlo quantique de la transition α-γ du Cérium" ("Quantum Monte Carlo study of the α-γ transition in Cerium"), October 2012 - October 2015; thesis director: Frédéric Decremps;

- Nicolas Dupuy, "Corrélations électroniques des acènes vers la limite de longue taille : Étude par Monte Carlo quantique" ("Electronic correlations in the acenes towards the long-size limit: a Monte Carlo study"), October 2012 - April 2016; thesis director: Francesco Mauri; note: this thesis has been funded by the 2012 national campaign for students with disabilities;
- Mario Dagrada, "Improved quantum Monte Carlo simulations: from open to extended systems", October 2013 - October 2016; thesis director: Francesco Mauri.

- Thesis co-advisor of Doctoral students:
  - Luke Shulenburger (UIUC), "Correlation in the one-dimensional electron gas", co-advised during the period January 2006 - July 2008; thesis director: Richard M. Martin;
  - Todd Beaudet (UIUC), "Quantum Monte Carlo Study of Hydrogen Adsorption on Carbon and Transition Metal Systems", co-advised during the period January 2006 - July 2008; thesis director: Richard M. Martin;
  - Henri Hay (UPMC), "Étude de la structure et des propriétés des polymorphes de SiO_2 et B_2O_3 par méthodes ab initio" ("Structural properties of SiO_2 and B_2O_3 polymorphs by ab initio methods"), October 2013 - October 2016; thesis director: Guillaume Ferlat.

- Thesis supervisor of Master (M2) students at UPMC:
  - Samira Bouaouli, "Quantum Monte Carlo characterization of energetics and structural properties of the anthracene and phenanthrene molecules", February 2012 - June 2012;
  - Nicolas Devaux, "Caractérisation ab initio de la phase alpha du cérium" ("Ab initio characterization of the α phase of cerium"), February 2012 - June 2012;
  - Mario Dagrada, "The study of the problem of proton transfer barrier using density fuctional theory and quantum Monte Carlo methods", February 2013 - June 2013.
  - Alexandra Byba, "Machine learning modeling of CO_2 dynamics", September 2019 - February 2020 (coadvised with Marco Saitta).
  - Raghavendra Meena, "Magnetism in graphene nanoribbons by quantum Monte Carlo", September 2019 - May 2020.
  - Matteo Peria, "Machine learning water clusters from quantum Monte Carlo", April 2021 - June 2021 (coadvised with Marco Saitta).
  - Damian Contant, "Electron correlation in high-pressure solid hydrogen phases", March 2021-July 2021 (coadvised with Maria Hellgren).
  - Francesco Cassol, "Interplay of Spin Orbit Coupling and electron correlation in Sr_2IrO_4 ", March 2021- September 2021 (coadvised with Benjamin Lenz).

- Thesis supervisor of Master (M1) students at UPMC/SU:
  - Honghao Li, "Spin Hall effect in Rashba crystals: application to the $BaNi_2$ case", March 2017 - July 2017;
  - Mourad Mezaguer, "Modélisation du magnétisme dans le fer à haute pression par un Hamiltonien de spins classiques", February 2018 - June 2018 (coadvised with Tommaso Gorni).

Other activities

- Dissemination and outreach activity
  Speaker at the following schools:
  - "Quantum Monte Carlo, From Minerals and Materials to Molecules", July 2007, UIUC, USA;
  - "Advanced School on Quantum Monte Carlo Methods in Physics and Chemistry", January 2008, ICTP, Trieste, Italy;
  - "École de simulation numérique à Jussieu", June 2012, UPMC, Paris, France;
  - "PISACMS: Paris International School on Advanced Computational Materials Science" (`http://pisacms.sciencesconf.org/`), UPMC, Paris, France, which was held in August of the following years: 2015, 2016, 2017, 2019, 2021, 2022;

- "SJSACMS: Sorbonne-JNCASR school on Advanced Computational Material Science" (`https://sites.google.com/view/sjsacms/`), JNCASR, Bangalore, India, February 2018;
- CECAM "Summer School on Classical and Quantum Monte Carlo methods for Material Science, Nanotechnology and Biophysics", Sissa, Trieste, Italy, 26 June - 13 July 2018 (invited lecture series and computer lab sessions);
- "QMC Hands-on Summer Workshop", Hotel Kaštiel' Mojmírovce, Slovakia, 20-23 June 2022 (invited lecture series).

- Organization of workshops
  - Organizer of the CECAM workshop "Quantum Monte Carlo meets Quantum Chemistry: new approaches for electron correlation" together with Ali Alavi and Sandro Sorella, Lugano, Switzerland, 15-18 June 2010;
  - Organizer of the Mini-Colloque "Green's function methods from first principles: GW, dynamical mean field theory and beyond" together with C. Martins, for the French condensed matter meeting JMC15 (`http://jmc15.sciencesconf.org/`), Bordeaux, 22-26 August 2016;
  - Local organizing committee for the Quantum Many-Body Physics session of the IUPAP XXIX Conference on Computational Physics, July 9-13, 2017, Paris (CCP2017);
  - Organizer of the E-CAM/CECAM/PsiK workshop "Improving the accuracy of ab initio predictions for materials", together with Carlo Pierleoni, Dario Alfé, and David Ceperley, Paris, France, 17-20 September 2018;
  - Organizer of the parallel session "Propriétés remarquables des matériaux topologiques : de la théorie à la réalisation expérimentale" together with T. Cren and C. Brun, for the SFP General Congress (`https://indico.in2p3.fr/event/16792/`), Nantes, 8-12 July 2019;
  - Organizer of the SISSA/PsiK "Summer School on Quantum Monte Carlo methods for ab-initio electronic simulations" together with S. Sorella and K. Nakano; the school was held online from 12 to 16 July 2021. M. Casula acted also as speaker in this school;
  - Organizer of the "Cérémonie de remise des prix Ancel 2018-2021" together with H. Mariette and C. Hivert, Orsay, June 2022;
  - Organizer of the parallel session "Lattice vibrations: lifetime, transport and (quantum) thermodynamics" together with F. Finocchi, Ph. Depondt and L. Paulatto, for the SFP Journées de la Matière Condensée JMC18, Lyon, 22-26 August 2022;
  - Organizer of the symposium "Strongly correlated materials" at the Psi-K conference, Lausanne, 22-25 August 2022.

- Scientific management
  - Head of the "Théorie Quantique des Matériaux" (TQM) team of the IMPMC;
  - Member of the CNRS Comité National Section 03;
  - Board member of the PsiK A3 working group on many-body non-perturbative methods;
  - President of the Condensed Matter Division of the French Physical Society (March 2020 - February 2022);
  - Board member of the French national research group "N-body" (`https://wiki.lct.jussieu.fr/gdrnbody/index.php/Accueil`);
  - Member of the scientific board ("Conseil Scientifique") of the IMPMC;
  - Former spokesperson of the Doctoral School ED397 "Physique et chimie des matériaux";
  - Former Member of the "Comité d'experts 28ème section" (UPMC recruitment and selection panel, condensed matter physics);
  - Former Board member of the French national research group "GDR Correl" (`http://gdrcorelec.ups-tlse.fr/index.php?title=Accueil`).

- External examiner/referee of the following PhD theses:
  - *Ab initio molecular dynamics of water by quantum Monte Carlo*, defended by Ye Luo at SISSA in October 2014;
  - *Spin-Fluctuation Spectra in Magnetic Systems, A Novel Approach Based on TDDFT*, defended by Tommaso Gorni at SISSA in November 2016;

- *Variational and auxiliary field Monte Carlo for the Hubbard and Hubbard-Holstein models: An accurate finite-size scaling and a "sign problem" solution*, defended by Seher Karakuzu at SISSA in October 2018;
- *From atoms to large multi-scale structures: modeling and simulations with ab-initio methods*, defended by Tommaso Morresi at the Department of Civil, Environmental and Mechanical Engineering of the University of Trento in May 2019;
- *Theoretical study of the many-body states of defects in diamond: the case of the NV center under high pressure*, defended by Mariya Romanova at the École Polytechnique in October 2019;
- *Quantum Monte Carlo Methods for electronic structure calculations: application to hydrogen at extreme conditions*, defended by Vitaly Gorelov at La Maison de la Simulation in September 2020;
- *Spectral and magnetic properties of copper oxides: towards a theoretical description from first principles*, defended by Benjamin Bacq-Labreuil at the Institut Polytechnique de Paris in September 2022.

- Peer-review activity
  - Referee of various high-impact International Scientific Journals (Nature, APS, ACS, AIP, IOP, Springer, and MDPI Journals);
  - IOP trusted reviewer status;
  - Reviewer for the ANR (Agence Nationale de la Recherche), ANVUR (Italian National Agency for the University and Research Evaluation), PRIN (Progetti di Rilevante Interesse Nazionale), the Polish National Science Centre, prématuration PSL and EuroTechPostdoc2 programs, for PRACE (Partnership for Advanced Computing in Europe) and for evaluating CECAM Flagship Workshop proposals.

- Recruitement
  - Member of the recruitement committee Comité de Sélection CNU 28 - IPR Rennes for hiring a Full Professor at the Institut de Physique de Rennes (2022).

Publications (peer-reviewed journal articles in reverse chronological order)
Blue color indicates publications arising from the work done during Master/PhD projects I supervised

1. T. Morresi, R. Vuilleumier and M. Casula, *Hydrogen phase-IV characterization by full account of quantum anharmonicity*, Physical Review B **106**, 054109 (2022);
2. M. Srdinšek, M. Casula, and R. Vuilleumier, *Quantum Rényi entropy by optimal thermodynamic integration paths*, Physical Review Research **4**, L032002 (2022);
3. M. Hellgren, D. Contant, T. Pitts and M. Casula, *High-pressure II-III phase transition in solid hydrogen: new insights from state-of-the-art ab initio calculations*, arXiv preprint arXiv:2205.01368, accepted on the Physical Review Research;
4. R. Meena, G. Li, and M. Casula, *Ground-state properties of the narrowest zigzag graphene nanoribbon from quantum Monte Carlo and comparison with density functional theory* The Journal of Chemical Physics **156**, 084112 (2022);
5. D. Santos-Cottin, M. Casula, L. de' Medici, F. Le Mardelé, J. Wyzula, M. Orlita, Y. Klein, A. Gauzzi, A. Akrap, R. P. S. M Lobo, *Optical conductivity signatures of open Dirac nodal lines*, Physical Review B **104**, L201115 (2021);
6. N. Nikolaj Bittner, D. Golež, M. Casula, Ph. Werner, *Photo-induced Dirac cone flattening in* $BaNiS_2$, Physical Review B **104**, 115138 (2021);
7. N. Nilforoushan, M. Casula, A. Amaricci, M. Caputo, J. Caillaux, L. Khalil, E. Papalazarou, P. Simon, L. Perfetti, I. Vobornik, P. K. Das, J. Fujii, D. Santos-Cottin, Y. Klein, M. Fabrizio, A. Gauzzi, M. Marsi, *Moving Dirac cones by chemical substitution*, Proceedings of the National Academy of Sciences **118** (33), e2108617118 (2021);
8. Tommaso Gorni, Pablo Villar Arribi, Michele Casula, and Luca de' Medici, *Accurate modeling of FeSe with screened Fock exchange and Hund's metal correlations*, Physical Review B **104**, 014507 (2021);

9. Tommaso Morresi, Lorenzo Paulatto, Rodolphe Vuilleumier, Michele Casula, *Probing anharmonic phonons by quantum correlators: A path integral approach*, J. Chem. Phys. **154**, 224108 (2021);

10. Kousuke Nakano, Tommaso Morresi, Michele Casula, Ryo Maezono, Sandro Sorella, *Atomic forces by quantum Monte Carlo: application to phonon dispersion calculation*, Phys. Rev. B **103**, L121110 (2021);

11. N. Nilforoushan, M. Casula, M. Caputo, E. Papalazarou, J. Caillaux, Z. Chen, L. Perfetti, A. Amaricci, D. Santos-Cottin, Y. Klein, A. Gauzzi, and M. Marsi, *Photoinduced renormalization and electronic screening of quasi-two-dimensional Dirac states in $BaNiS_2$*, Phys. Rev. Research **2**, 043397 (2020);

12. Kousuke Nakano, Claudio Attaccalite, Matteo Barborini, Luca Capriotti, Michele Casula, Emanuele Coccia, Mario Dagrada, Claudio Genovese, Ye Luo, Guglielmo Mazzola, Andrea Zen, and Sandro Sorella, *TurboRVB: A many-body toolkit for ab initio electronic simulations by quantum Monte Carlo*, J. Chem. Phys. **152**, 204121 (2020);

13. Blair W. Lebert, Tommaso Gorni, Michele Casula *et al.*, *Epsilon iron as a spin-smectic state*, Proceedings of the National Academy of Sciences **116** (41), 20280 (2019);

14. S. Klotz, M. Casula, K. Komatsu, S. Machida, T. Hattori, *High-pressure structure and electronic properties of YbD_2 to 34 GPa*, Physical Review B **100**, 020101 R (2019);

15. G. Ferlat, M. Hellgren, F.X. Coudert, H. Hay, F. Mauri, M. Casula, *van der Waals forces stabilize low-energy polymorphism in B_2O_3: Implications for the crystallization anomaly*, Physical Review Materials **3**, 063603 (2019);

16. D. Santos-Cottin, Y. Klein, Ph. Werner, T. Miyake, L. de' Medici, A. Gauzzi, R. P. S. M. Lobo, and M. Casula, *Linear behavior of the optical conductivity and incoherent charge transport in $BaCoS_2$*, Physical Review Materials **2**, 105001 (2018);

17. M. T. Entwistle, M. Casula, and R. W. Godby, *Comparison of local density functionals based on electron gas and finite systems*, Physical Review B **97**, 235143 (2018);

18. Jeongnim Kim, Andrew D. Baczewski *et al.*, *QMCPACK: an open source ab initio quantum Monte Carlo package for the electronic structure of atoms, molecules and solids*, Journal of Physics: Condensed Matter **30**, 195901 (2018);

19. Nicolas Dupuy, and Michele Casula, *Fate of the open-shell singlet ground state in the experimentally accessible acenes: A quantum Monte Carlo study*, The Journal of Chemical Physics **148**, 134112 (2018);

20. Yannick Klein, Michele Casula, David Santos-Cottin, Alain Audouard, David Vignolles, Gwendal Fève, Vincent Freulon, Bernard Plaçais, Marine Verseils, Hancheng Yang, Lorenzo Paulatto, and Andrea Gauzzi, *Importance of nonlocal electron correlation in the $BaNiS_2$ semimetal from quantum oscillations studies*, Physical Review B **97**, 075140 (2018);

21. Félix Mouhat, Sandro Sorella, Rodolphe Vuilleumier, Marco Saitta, and Michele Casula, *Fully Quantum Description of the Zundel Ion: Combining Variational Quantum Monte Carlo with Path Integral Langevin Dynamics*, Journal of Chemical Theory and Computation **13**, 2400 (2017);

22. Mario Dagrada, Seher Karakuzu, Verónica Laura Vildosola, Michele Casula, and Sandro Sorella, *Exact special twist method for quantum Monte Carlo simulations*, Physical Review B **94**, 245108 (2016);

23. Brian Busemeyer, Mario Dagrada, Sandro Sorella, Michele Casula, and Lucas K. Wagner, *Competing collinear magnetic structures in superconducting FeSe by first- principles quantum Monte Carlo calculations*, Physical Review B **94**, 035198 (2016);

24. Philipp Werner, and Michele Casula, *Dynamical screening in correlated electron systems – from models to realistic materials*, Journal of physics: Condensed Matter **28**, 383001 (2016);

25. David Santos-Cottin, Michele Casula, Gabriel Lantz, Yannick Klein, Luca Petaccia, Patrick Le Févre, François Bertran, Evangelos Papalazarou, Marino Marsi, and Andrea Gauzzi. *Rashba coupling amplification by a staggered crystal field*, Nature Communications **7**, 11258 (2016);

26. David Santos-Cottin, Andrea Gauzzi, Marine Verseils, Benoit Baptiste, Gwendal Feve, Vincent Freulon, Bernard Plaçais, Michele Casula, and Yannick Klein, *Anomalous metallic state in quasi-2D BaNiS2*, Phys. Rev. B **93**, 125120 (2016);

27. F. Decremps, G. Morard, G. Garbarino, and M. Casula, *Polyamorphism of a Ce-based bulk metallic glass by high-pressure and high-temperature density measurements*, Phys. Rev. B **93**, 054209 (2016);

28. S. Sorella, N. Devaux, M. Dagrada, G. Mazzola, and M. Casula, *Geminal embedding scheme for optimal atomic basis set construction in correlated calculations*, J. Chem. Phys. **143**, 244112 (2015);

29. H. Hay, G. Ferlat, M. Casula, A. P. Seitsonen, and F. Mauri, *Dispersion effects in SiO2 polymorphs: An ab initio study*, Phys. Rev. B **92**, 144111 (2015);

30. N. Dupuy, Samira Bouaouli, Francesco Mauri, Sandro Sorella, and Michele Casula, *Vertical and adiabatic excitations in anthracene from quantum Monte Carlo: Constrained energy minimization for structural and electronic excited-state properties in the JAGP ansatz*, J. Chem. Phys. **142**, 214109 (2015);

31. N. Devaux, M. Casula, F. Decremps, S. Sorella, *Electronic origin of the volume collapse in Cerium*, Physical Review B **91**, 081101(R) (2015);

32. Ambroise van Roekeghem, Thomas Ayral, Jan M. Tomczak, Michele Casula, Nan Xu, Hong Ding, Michel Ferrero, Olivier Parcollet, Hong Jiang, Silke Biermann, *Dynamical correlations and screened exchange on the experimental bench: spectral properties of the cobalt pnictide* $BaCo_2As_2$, Physical Review Letters **113**, 266403 (2014);

33. Jan M. Tomczak, M. Casula, T. Miyake, and S. Biermann, *Asymmetry in band widening and quasiparticle lifetimes in SrVO3: Competition between screened exchange and local correlations from combined GW and dynamical mean-field theory GW + DMFT*, Phys. Rev. B **90**, 165138 (2014);

34. Gianluca Giovannetti, Michele Casula, Philipp Werner, Francesco Mauri, and Massimo Capone, *Downfolding electron-phonon Hamiltonians from ab initio calculations: Application to K3 picene*, Phys. Rev. B **90**, 115435 (2014);

35. Mario Dagrada, Michele Casula, Antonino M. Saitta, Sandro Sorella, and Francesco Mauri, *Quantum Monte Carlo Study of the Protonated Water Dimer*, J. Chem. Theory Comp. **10**, 1980 (2014);

36. Michele Casula, Sandro Sorella *Improper s-wave symmetry of the electronic pairing in iron-based superconductors by first-principles calculations*, Phys. Rev. B **88**, 155125 (2013);

37. V. Brouet, Ping-Hui Lin, Y. Texier, J. Bobroff, A. Taleb-Ibrahimi, P. Le Fèvre, F. Bertran, M. Casula, P. Werner, S. Biermann, F. Rullier-Albenque, A. Forget, and D. Colson, *Large Temperature Dependence of the Number of Carriers in Co-Doped* $BaFe_2As_2$, Phys. Rev. Lett. **110**, 167002 (2013);

38. Jan M. Tomczak, Michele Casula, Takashi Miyake, Ferdi Aryasetiawan, Silke Biermann, *Combined GW and dynamical mean field theory: Dynamical screening effects in transition metal oxides*, Europhysics Letters **100**, 67001 (2012);

39. M. Casula, Ph. Werner, L. Vaugier, F. Aryasetiawan, T. Miyake, A. J. Millis, and S. Biermann, *Low-Energy Models for Correlated Materials: Bandwidth Renormalization from Coulombic Screening*, Phys. Rev. Lett. **109**, 126408 (2012);

40. Michele Casula, Matteo Calandra, and Francesco Mauri, *Local and nonlocal electron-phonon couplings in* K_3 *picene and the effect of metallic screening*, Phys. Rev. B **86**, 075445 (2012);

41. Philipp Werner, Michele Casula, Takashi Miyake, Ferdi Aryasetiawan, Andrew J. Millis, and Silke Biermann, *Satellites and large doping and temperature dependence of electronic properties in hole-doped* $BaFe_2As_2$, Nature Physics **8**, 331 (2012);

42. Michele Casula, Alexey Rubtsov, and Silke Biermann *Dynamical screening effects in correlated materials: Plasmon satellites and spectral weight transfers from a Green's function ansatz to extended dynamical mean field theory*, Physical Review B **85**, 035115 (2012);

43. Michele Casula, Matteo Calandra, Gianni Profeta, and Francesco Mauri, *Intercalant and Intermolecular Phonon Assisted Superconductivity in K-Doped Picene*, Physical Review Letters **107**, 137006 (2011);

44. N. Helbig, J.I. Fuks, M. Casula, M.J. Verstraete, M.A.L. Marques, I.V. Tokatly, A. Rubio, *Density functional theory beyond the linear regime: Validating adiabatic LDA*, Physical Review A **83**, 032503 (2011);

45. Sandro Sorella, Michele Casula, Leonardo Spanu, Andrea Dal Corso, *Ab-initio calculations for the beta-tin diamond transition in Silicon: comparing theories with experiments*, Physical Review B **83**, 075119 (2011);

46. M. Casula, S. Moroni, C. Filippi, S. Sorella, *Size-consistent variational approaches to non-local pseudopotentials: standard and lattice regularized diffusion Monte Carlo methods revisited*, Journal of Chemical Physics **132**, 154113 (2010);

47. B. Clark, M. Casula, D. M. Ceperley, *Hexatic and Mesoscopic Phases in a 2D Quantum Coulomb System*, Physical Review Letters **103**, 055701 (2009);

48. M. Marchi, S. Azadi, M. Casula, S. Sorella, *Resonating Valence Bond wave function with molecular orbitals: application to first-row molecules*, J. Chem. Phys. **131**, 154116 (2009);

49. M. Casula, M. Marchi, S. Azadi, S. Sorella, *A consistent description of the iron dimer spectrum with a correlated single-determinant wave function*, Chemical Physics Letters **477**, Issues 4-6, 255 (2009);

50. L. Shulenburger, M. Casula, G. Senatore, and R. M. Martin, *Spin resolved energy parametrization of a quasi-one-dimensional electron gas*, Journal of Physics A, Mathematical and theoretical **42**, Issue 21, 214021 (2009);

51. M. Casula, D. M. Ceperley, and Erich J. Mueller, *Quantum Monte Carlo study of one dimensional trapped fermions with attractive contact interactions*, Phys. Rev. A **78**, 033607 (2008);

52. L. Shulenburger, M. Casula, G. Senatore, and R. M. Martin, *Correlation effects in quasi one dimensional electron wires*, Phys. Rev. B **78**, 165303 (2008);

53. Todd D. Beaudet, Michele Casula, Jeongnim Kim, Sandro Sorella, and Richard M. Martin, *Molecular hydrogen adsorbed on benzene: insights from a quantum Monte Carlo study*, J. Chem. Phys. **129**, 164711 (2008);

54. S. Sorella, M. Casula, and D. Rocca, *Weak binding between two aromatic rings: feeling the van der Waals attraction by quantum Monte Carlo methods*, J. Chem. Phys. **127**, 014105 (2007);

55. M. Casula, S. Sorella, and G. Senatore, *Ground state properties of the one-dimensional Coulomb gas using the lattice regularized diffusion Monte Carlo*, Phys. Rev. B **74**, 245427 (2006);

56. M. Casula, *Beyond the locality approximation in the standard diffusion Monte Carlo method*, Phys. Rev. B **74**, 161102 R (2006);

57. M. Casula, and G. Senatore, *Charge and spin correlation of a one dimensional electron gas on the continuum*, Chem. Phys. Chem. **6**, 1902 (2005);

58. M. Casula, C. Filippi, S. Sorella, *Diffusion Monte Carlo with Lattice Regularization*, Phys. Rev. Lett. **95**, 100201 (2005);

59. M. Casula, C. Attaccalite and S. Sorella, *Correlated geminal wave function for molecules: an efficient resonating valence bond approach*, J. Chem. Phys. **121**, 7110 (2004);

60. M. Casula and S. Sorella, *Geminal wave function with Jastrow correlation: a first application to atoms*, J. Chem. Phys. **119**, 6500 (2003).

Peer-reviewed conference proceedings

1. M. Casula, S. Yunoki, C. Attaccalite, S. Sorella, *Resonating Valence Bond Wave Function: from lattice models to realistic systems*, for the proceedings of the "Conference on Computational Physics, CCP 2004", Computer Physics Communications **169**, Issues 1-3, 386 (2005).

Invited Speaker at Workshops and Conferences

1. *Quantum Monte Carlo in the next Decade* workshop at the Flatiron Institute CCQ, invited talk: "Structural properties and phase transitions of hydrogen and hydrogen-rich compounds by quantum Monte Carlo", September 2022, New York City, (New York, USA);

2. *Recent developments on QMC* workshop organized for the 60th birthday anniversary of Saverio Moroni, invited talk: "Phase diagram of high-pressure hydrogen including nuclear quantum effects", October 2021, Rome (Italy);

3. *HPC Online Lectures on Quantum Computational Materials Science* international web workshop, invited talk: "Quantum Materials: A quantum Monte Carlo approach", November 2020, Singapore;

4. *New Generation in Strongly Correlated Electron Systems* international workshop, keynote talk: "From Dirac to Mott physics: the fascinating properties of $BaNi_xCo_{(1-x)}S_2$", September 2019, Pescara (Italy);

5. *Congrès Général de la SFP*, French national congress, invited introductory talk: "Hydrides superconductors and insulator-to-metal transition in high-pressure YbH_2", July 2019, Nantes (France);

6. *TSRC workshop on Stochastic Electronic Structure Methods* international workshop, invited talk: "Ubbelhode effect in protonated water clusters", June 2019, Telluride (Colorado, USA);

7. *Alumni colloquium of the Physics Department, University of Trieste*, invited talk: "A journey through superconductivity: from the origins to the latest developments", May 2018, Trieste (Italy);

8. *TSRC workshop on Stochastic Electronic Structure Methods* international workshop, invited talk: "Fully Quantum Description of Water Clusters: Combining Variational Quantum Monte Carlo with Path Integral Langevin Dynamics", July 2017, Telluride (Colorado, USA);

9. Indo-French workshop on material science, invited talk "Strong spin-orbit coupling in low-Z materials: avenues of spintronic applications in $BaNiS_2$", November 2016, Bangalore (India);

10. CECAM workshop *Computational methods towards engineering novel correlated materials*, invited talk "From dynamically screened Hubbard U to Holstein phonons in extended dynamical mean-field theory: application to K_3Picene", October 2016, Lausanne (Switzerland);

11. Workshop on *Matériaux, États Électroniques, Interactions et Couplages non-Conventionnels*, invited talk "Quantum Monte Carlo methods for strongly correlated systems from first principles", June 2016, Paris (France);

12. *GdR Mico French workshop*, invited talk "Improper s-wave symmetry of the electronic pairing in iron-based superconductors from ab-initio quantum Monte Carlo calculations", November 2015, Paris (France);

13. *International workshop " TSRC workshop on Stochastic Electronic Structure Methods"*, invited talk "Electronic origin of volume collapse in Cerium", June 2015, Telluride (Colorado, USA);

14. *CECAM workshop "Stochastic wavefunction methods in quantum chemistry, electronic structure theory and condensed matter physics"*, invited talk " Electronic origin of volume collapse in Cerium", April 2015, Lausanne (Switzerland);

15. *Fifth RIKEN-AICS international symposium*, invited talk "Probing structural, magnetic, and superconducting properties of iron selenide (FeSe) by quantum Monte Carlo methods", December 2014, Kobe (Japan);

16. *New Frontiers in Multiscale Modelling of Advanced Materials - MAM1*, invited talk "Electron-phonon coupling in potassium-doped superconducting picene", June 2014, Trento (Italy);

17. *International Symposium on Superconductivity 2013 (ISS2013)*, invited talk "Improper s-wave symmetry of pairing in iron-pnictides from ab-initio quantum Monte Carlo calculations", November 2013, Tokyo (Japan);

18. *International workshop "Total Energy"*, invited talk "Dynamical screening effects from first principles: implications for low-energy models and application to the iron pnictides", January 2013, Trieste (Italy);

19. *International conference on Computational Physics CCP2012*, invited talk "Variational Monte Carlo approaches as a route to describe strongly correlated materials from a fully ab-initio perspective", October 2012, Kobe (Japan);

20. *International symposum "Quantum Simulation and Design (ISC-QSD)"*, invited talk "Electron-phonon coupling in potassium-doped superconducting picene", Octobre 2012, Osaka (Japan);

21. *French workshop "Théorie de la matière condensée en Ile de France"*, invited talk on "Variational quantum Monte Carlo calculations of solids: state-of-the-art and open issues", November 2010, Institut Henri Poincaré, Paris (France);

22. *PsiK-2010 international conference*, invited talk on "Jastrow correlated geminal wave functions in variational quantum Monte Carlo calculations of solids", September 2010, Berlin (Germany);

23. *Advanced School on Quantum Monte Carlo Methods in Physics and Chemistry*, invited talk on "One dimensional trapped fermions with attractive contact interactions", January 2008, Trieste (Italy);

24. *International Workshop on Computational Physics and Materials Science: "Progress in Computational Electronic Structure Theory"* invited talk on "Diffusion Monte Carlo methods with non-local potentials", January 2008, Bonn (Germany);

25. *Advances in continuum quantum Monte Carlo methods*, invited talk on "Diffusion Monte Carlo methods with non-local potentials", September 2007, Lyon (France);

26. *ISSP international workshop on "Foundations and applications of the density functional theory"*, introductory lecture on variational and diffusion Monte Carlo methods, and lecture on "Non-local pseudo-potentials in the diffusion Monte Carlo framework", July 2007, Kashiwa, Tokyo (Japan);

27. *March Meeting 2007*, invited talk on "Lattice regularized diffusion Monte Carlo method", March 2007, Denver CO (USA);

28. *QMC 2006 workshop on "New Developments in Quantum Monte Carlo"*, invited talk on "Lattice regularized DMC", May 2006, Tempe AZ (USA);

29. *CECAM workshop, Ab-Initio Simulation methods beyond Density Functional Theory*, invited talk on "Lattice Regularized Diffusion Monte Carlo Simulations of iron dimer", September 2005, Lyon (France);

Contributed Talks and attended Workshops: 23 contributions

1. *Psi-K conference*, poster: "Manipulating the Dirac states by varying the strength of electron correlation in BaNi(Co)S_2", August 2022, Lausanne (Switzerland);

2. *Journées de la matière condensée JMC 2022*, August 2022, Lyon (France);

3. *Remise des prix Ancel 2018-2021 et des grands prix de la SFP*, June 2022, Orsay (France);

4. *Journées de la matière condensée JMC 2021*, August 2021, on-line participation;

5. *Cutting-Edge Topics in Quantum Materials* international workshop, contributed talk: "Linear behavior of the optical conductivity and incoherent charge transport in $BaCoS_2$", September 2019, Paris (France);

6. *Congrès Général de la SFP*, French national congress, contributed talk: "$BaNiS_2$ monolayer as possible Z2 topological insulator", July 2019, Nantes (France);

7. *GDR Meeticc workshop, Techniques avancées : Focus sur les oxydes, supraconducteurs 2D et dichalcogénures*, poster: "Dirac cones, Rashba splittings and electron correlation in $BaNiS_2$", 15-16 October 2018, Versailles (France);

8. *Journées de la matière condensée JMC 2018*, poster: "Efficient fully-quantum first-principles dynamics: application to protonated water clusters", August 2018, Grenoble (France);

9. *WaterX workshop: exotic properties of water under extreme conditions*, June 2018, La Maddalena (Italy);

10. *CCP2017* conference, contributed talk: "Absence of spin edge polarization of acenes in the long-chain limit by quantum Monte Carlo methods", July 2017, Paris (France);

11. *CECAM-FR-MOSER* workshop on "Practical problems with dynamical nuclear quantum effects through semi-classical methods", oral contribution: "Coupling Quantum Monte Carlo with stochastic dynamics", June 2017, Paris (France);

12. *Journées de la matière condensée JMC15*, contributed talk "Fully quantum dynamics of proton transfer in aqueous systems: the case study of the Zundel ion", August 2016, Bordeaux (France);

13. *PsiK international conference*, contributed talk "From dynamically screened Hubbard U to Holstein phonons in extended dynamical mean-field theory: application to K_3Picene", September 2015, San Sebastian (Spain);

14. *International workshop "EXS2014 Exotic Superconductors and Superfluids"*, oral contribution "Downfolding electron-phonon Hamiltonians from ab-initio calculations: application to K_3 picene", October 2014, Trieste (Italy);

15. *International workshop "Condensed Matter in Paris 2014"*, oral contribution "Improper s-wave symmetry of the electronic pairing in iron-based superconductors from ab-initio quantum Monte Carlo calculations", August 2014, Paris (France);

16. *APS March Meeting 2014*, oral contribution "Improper s-wave symmetry for the electronic pairing in iron-based superconductors by first-principles calculations", March 2014, Denver, CO (United States);

17. *International workshop "Superconductivity 100 Years Later, a Computational Approach"*, contributed poster on "Superconductivity in K_3Picene", September 2011, Alghero (Italy);

18. *International workshop "Strong correlation from first principles"*, oral contribution "Satellites and large doping- and temperature-dependence of electronic properties in hole-doped $BaFe_2As_2$", September 2011, Seeon Monastery (Germany);

19. *French workshop on strongly correlated systems: GDR-MICO*, accepted talk on "Screening effects in correlated materials", October 2009, Aspet (France);

20. *International Conference on Strongly Coupled Coulomb Systems*, accepted talk on "Correlation effects in quasi-one-dimensional electron wires", July 2008, Camerino (Italy);

21. *March Meeting 2008*, oral contribution on "One dimensional trapped fermions with attractive contact interactions", March 2008, New Orleans, LA (USA);

22. *March Meeting 2006*, oral contribution on "Lattice Regularized Diffusion Monte Carlo Simulations of iron dimer", March 2006, Baltimore, MD (USA);

23. *March Meeting 2005*, oral contribution on "Correlated geminal wave function: a resonating valence bond approach for quantum chemistry", March 2005, Los Angeles, CA (USA);

24. *CCP2004, Conference on computational physics*, September 2004, Genova (Italy);

25. *Scuola Internazionale di Fisica "Enrico Fermi" - CORSO CLVII: The electron liquid paradigm in Condensed Matter Physics*, July 2003, Varenna (Italy);

26. *CECAM-ESF/PsiK workshop: The diffusion quantum Monte Carlo method*, September 2002, Lyon (France).