

Dichiarazione di veridicità

Dichiarazione sostitutiva di certificazioni ai sensi dell'art. 46 del D.P.R. 445 del 28/12/2000

Dichiarazione sostitutiva dell'atto di notorietà ai sensi dell'art. 47 del D.P.R. 445 del 28/12/2000

Il sottoscritto Federico Grasselli, nato a Reggio Emilia il 15/09/1989, residente a Reggio Emilia in via B. Corti 1, DICHIARA, sotto la propria responsabilità e consapevole delle sanzioni penali previste agli artt. 75 e 76 del D.P.R. 445/2000 in caso di dichiarazione mendace, che quanto contenuto nel presente curriculum vitae et studiorum è corrispondente al vero, nonché di essere in possesso di tutti i titoli in esso riportati.

Extended Curriculum Vitae (updated May 2026)

1. PERSONAL INFORMATION

- 1.1. First name: Federico
- 1.2. Family Name: Grasselli
- 1.3. Date of Birth: 15/09/1989
- 1.4. Place of Birth: Reggio Emilia (RE), Italy
- 1.5. Nationality: Italian
- 1.6. ORCID: <https://orcid.org/0000-0003-4284-0094>
- 1.7. Scopus Author ID: [56531789400](https://scopus.com/authid/detail.uri?authorid=56531789400)
- 1.8. ResearcherID: [V-6384-2019](https://www.researcherid.com/rid/V-6384-2019)
- 1.9. Google Scholar: <https://scholar.google.com/citations?user=fdq93WkAAAAJ&hl=it>

2. SHORT PRESENTATION

- 2.1. My academic education focused on Theoretical Condensed Matter Physics, including quantum scattering in reduced dimensional systems, quantum theory of solids, and theoretical nanosciences.
- 2.2. During my PhD, supervised by Prof. G. Goldoni at the University of Modena and Reggio Emilia, and lying within the Marie Curie INDEX ITN-Project, I studied the unitary evolution of Coulomb bound electron-hole pairs in semiconductor nano-devices by a time-dependent Schrödinger approach. This activity included high-performance software deployment for massively parallel architectures, implementation of quantum chemistry approaches, and the validation of an original self-energy approach whereby internal degrees of freedom are embodied in an energy dependent potential, dramatically reducing the computational load.
- 2.3. I have also enforced my aptitude for working with experimental teams, specifically G. Rossi's group at Elettra/Fermi and TASC –Trieste Synchrotron and FEL facility–, and L.V. Butov's group at the University of California – San Diego.
- 2.4. My research activity in Prof. S. Baroni's group at SISSA, Trieste (IT), within the MAX EU Centre of Excellence for HPC applications, focused on the investigation of transport properties in electronic insulating systems within the framework of the Green-Kubo (GK) theory of linear response. I exposed how to combine the topological charge-transport quantization and the gauge invariance of transport to develop a simple, yet ab-initio accurate estimates for the electrical conductivity of insulating liquids. More recently, I contributed to calculating the heat and charge conductivities of water under planetary pT conditions, and to developing an evolution model of Uranus able to explain its anomalous low luminosity.
- 2.5. My research in the Laboratory of Computational Science and Modelling (COSMO), headed by Prof. M. Ceriotti at EPFL, Lausanne (CH), is focusing on a machine learning approach to finite temperature molecular dynamics simulations of metals. During the last year, I supervised a group project on uncertainty estimation for machine-learning committee models. From June 2021 to May 2023, I have been a Marie Skłodowska-Curie fellow in COSMO, with a project aimed at including nuclear quantum effects in transport coefficients.
- 2.6. I have organized several workshops on atomistic simulations and machine learning, after recognizing the importance of disseminating methods and code, establishing common standards, and fostering collaboration among computational materials science groups. Additionally, I co-initiated a European COST Action on data-driven techniques for functional materials engineering, where I currently serve as a Management Committee member, Science Communication Coordinator, and vice-leader of the Training, Dissemination, Exploitation, and Outreach working group.
- 2.7. I am currently Assistant Professor (Ricercatore Tenure Track) in the Department of Physics, Informatics and Mathematics of the University of Modena and Reggio Emilia.

3. PROFESSIONAL EXPERIENCE AND FELLOWSHIPS

- 3.1. Starting 01/06/2024 – “Ricercatore Tenure Track” (Assistant Professor) in Condensed Matter Physics, Department of Physics, Informatics, and Mathematics, University of Modena and Reggio Emilia, Italy.
- 3.2. 01/06/2023 – 31/05/2024 – Postdoc (Collaborateur Scientifique Postdoctoral) in Prof. Michele Ceriotti's group at Laboratory of Computational Science and Modelling (COSMO), IMX, École Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland.
- 3.3. 01/06/2021 – 31/05/2023: Marie Skłodowska Curie fellowship in Prof. Michele Ceriotti's group at Laboratory of Computational Science and Modelling (COSMO), IMX, École Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland.
- 3.4. 01/06/2020 – 31/05/2021 – Postdoc (Collaborateur Scientifique Postdoctoral) in Prof. Michele Ceriotti's group at Laboratory of Computational Science and Modelling (COSMO), IMX, École Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland.
- 3.5. 16/05/2020 – 31/05/2020 – Visiting scientist in Prof. S. Baroni's group at Scuola Internazionale Superiore di Studi Avanzati (SISSA), Condensed Matter Theory Group, Trieste (IT).
- 3.6. 16/05/2017 – 15/05/2020 – Postdoc (Assegnista di Ricerca Postdoc) in Prof. S. Baroni's group at Scuola Internazionale Superiore di Studi Avanzati (SISSA), Condensed Matter Theory Group, Trieste (IT). The fellowship was funded by the EU Centre of Excellence “MaX: Driving the Exascale Transition”
- 3.7. A. Y. 2018/2019, 2019/2020, 2020/21: Graduate Teaching Assistant for the laurea (BSc) course “Fisica Statistica” (Statistical Physics) – Department of Physics, University of Trieste (IT).
- 3.8. 06/03/2017 – 05/04/2017 - Collaborator (“collaborazione occasionale”) for an activity of scientific communication and management for “Laboratorio Nanoscienze” of CNR Nano S3 within the project of Fondazione Cassa di Risparmio di Modena “Into the Future”, guidance project aimed at high-school student from the province of Modena (Prot. CNR Nano n. 0000953, dated March 3, 2017)
- 3.9. 01/01/2014 – 31/12/2016 – PhD National fellowship (“Borsa ministeriale di Dottorato di Ricerca”) in Physics and Nanosciences at School of Graduate Studies in Physics and Nanosciences, Università degli Studi di Modena e Reggio Emilia. The public defense of the thesis dates 03/03/2017
- 3.10. A.Y. 2016/17, 2015/16, 2014/15, 2013/2014 – Graduate Teaching Assistant for the laurea (BSc) course “Termodinamica Statistica” (Statistical Thermodynamics) – Department of Physics, Informatics, and Mathematics, University of Modena and Reggio Emilia (IT)
- 3.11. A.Y. 2016/17, 2015/16, 2014/15, 2013/14: Training lectures as experienced external collaborator “Collaboratore esterno: Esperto” for local, national and international stages of the Physics Olympiads. The activity has been partially funded by the Italian Government through the action “Piano Lauree Scientifiche”.

4. EDUCATION

- 4.1. 03/03/2017 – Dottore di Ricerca (PhD) in Physics and Nanosciences (XXIX Cycle) (cum laude), School of Graduate Studies in Physics and Nanosciences, Università degli Studi di Modena e Reggio Emilia, Italy. Title of the thesis: “*Time-dependent propagation of quantum complexes: the case of indirect excitons in semiconductor heterostructures*”. Supervisor: Prof. Guido Goldoni. Field of study: Theoretical Condensed Matter Physics. The PhD activity was lying within, and partially funded by, the Marie Skłodowska-Curie INDEX ITN action on indirect excitons.
- 4.2. 29/10/2013 - Laurea Magistrale degree (MSc) in Physics (110/110 cum laude), Università degli Studi di Modena e Reggio Emilia, Italy. Title of the thesis: “*Coherent propagation schemes for spatially indirect excitons*” (in Italian). Supervisor: Prof. Guido Goldoni. Field of study: Theoretical Condensed Matter Physics.
- 4.3. 28/10/2011 - Laurea degree (BSc) in Physics (110/110 cum laude), Università degli Studi di Modena e Reggio Emilia, Italy. Title of the thesis: “*Analysis of FePc, adsorbed on Au(110), via STM, STS, and break-junction techniques*” (in Italian). Supervisor: Prof. Giorgio Rossi. Field of study: Experimental Condensed Matter Physics
- 4.4. 2008 - High School Diploma (100/100 cum laude), Liceo Classico-Scientifico "Ariosto-Spallanzani", Reggio Emilia, Italy.

5. EUROPEAN PROJECTS

- 5.1. 2023: COST Action CA22154: “Data-driven Applications towards the Engineering of functional Materials: an Open Network (DAEMON)”. <https://www.cost.eu/actions/CA22154/>. Grade 45/50. Starting Date: 26.09.2023. Roles:
 - 5.1.1. Secondary Proposer of the action

- 5.1.2. Management Committee Member
- 5.1.3. Scientific Communication Coordinator
- 5.2. 2021: Marie Skłodowska-Curie Individual Fellowships: European Action 2020 –“TRANQUIL: TRANsport with QUantum nuclei in Ionic Liquids”. Proposal number: 101018557. Score 97.00/100.00

6. AWARDS

- 6.1. 25/02/2026: IoP trusted reviewer certificate
- 6.2. 07/03/2025: Abilitazione Scientifica Nazionale II Fascia (National Habilitation Associate Professorship)
- 6.3. 09/09/2021: Runner-up prize at the 5th Psi-K Volker Heine Young Investigator Award, <https://www.psik2020.net/volker-heine-young-investigator-award>
- 6.4. A.Y. 2012-13, 2010-11, 2009-10, 2008-09 – University award for academic merit "Premio di Studio" granted by the University of Modena and Reggio Emilia
- 6.5. A.Y. 2012-13, 2011-12, 2010-11, 2009-10, 2008-09 – University award "Fondo Sostegno Giovani" (50% refund of University fees for the students who gained merit and honors in Chemistry, Physics, and Mathematics BSc/MSc courses)
- 6.6. 2008 - National award for obtaining the Diploma "cum laude" (2008)
- 6.7. 2008 - High-School award "A. Iona" Liceo Classico-Scientifico "Ariosto-Spallanzani" for reaching the highest evaluation in Mathematics, Physics and Natural Sciences (S.Y. 2007-08)

7. INTERNSHIPS AND VISITING ACTIVITIES

- 7.1. February and March 2023: Visiting scientist + PhD course on “Machine Learning Interatomic Potentials”. School of Graduate Studies “Physics and Nanosciences”, University of Modena and Reggio Emilia, Italy.
- 7.2. From 08/10/2022 to 14/10/2022 – Visiting scientist in Prof. Paul Erhart’s group, Chalmers University, Gothenburg, Sweden.
- 7.3. From 19/11/2018 to 02/12/2018, and from 14/06/2019 to 26/06/2019. Visiting period in L. Stixrude’s group at the University of California – Los Angeles (USA), as part of on-going collaborations
- 7.4. From 03/06/2015 to 03/07/2015. Visiting period in L. V. Butov’s group at the University of California – San Diego (USA), within the PhD internship activity
- 7.5. May – June, 2011. Visiting period in G. Rossi’s group at Elettra/Fermi and TASC at Trieste Synchrotron and FEL facility (IT), within the BSc internship activity.

8. INVITED PRESENTATIONS TO INTERNATIONAL CONFERENCES AND SCHOOLS

- 8.1. 03/10/2024, “*Simulating transport properties of superionic materials*”, TimeMan Seminar Series, Lille University (FR) (online).
- 8.2. 18/04/2024, “*Trustworthy machine learning for materials*”, ECT* Workshop - Bridging scales: At the crossroads among renormalisation group, multi-scale modelling, and deep learning – 15-19/04/2024, Trento.
- 8.3. 11/04/2024, “*An Introduction to DAEMON COST Action*”, EuMINE COST Action 1st General Meeting and Workshop, 10-12/04/2024, Bologna, IT.
- 8.4. 06/06/2023, “*Predicting the electronic free energy at finite temperature from ground state data*”, CMT@BRIXEN, The meeting of the condensed matter theory Italian community, 05-07/06/2023, Bressanone, IT.
- 8.5. 23/01/2023. “*Ab initio charge transport of ionic fluids: invariance principles and topological invariants*”, Lennard-Jones Centre Discussion Group (University of Cambridge), “Monday Seminar” Series.
- 8.6. 24/06/2022. “*Invariance principles of transport coefficients and thermal transport in super-ionic materials*”, Telluride Science Research Center’s Workshop “*Thermal Transport at the Nanoscale*”, 21-25/06/2022, Telluride, CO (USA).
- 8.7. 06/12/2021. “*The role of invariance principles and topology in the ab initio charge transport of ionic fluids*”, CECAM Workshop: Capturing Anharmonic Vibrational Motion in First-Principles Simulations.
- 8.8. 09/09/2021. “*Invariance principles and topology in the ab initio charge transport of ionic fluids*”, 5th Psi-K Volker Heine Award Ceremony (online).
- 8.9. 07/04/2020. “*Heat and charge transport in water at ice-giant conditions from ab initio MD simulations*”, ICTP Atomistic Webinar, Trieste (IT).
- 8.10. 24/07/2019. “*Topological quantisation and gauge invariance of charge transport in liquid insulators*”, CPMD Meeting 2019 - Pushing the Boundaries of Molecular Dynamics, CECAM Headquarters, Lausanne (CH)

- 8.11.21/05/2019. “*Topological quantization and gauge invariance of charge transport in liquid insulators*”, 2019 Workshop on Recent Developments in Electronic Structure, University of Illinois at Urbana-Champaign (USA)
- 8.12. 01/11/2019. “*Charge-transport quantization and gauge invariance of electrical conductivity in ionic fluids*”, International Conference “Games of Materials”, Dubrovnik (HR)
- 8.13. 03/10/2015. “*La discretitud del tiempo*”, International Conference “Ibn Arabi y Lull a la luz de la matemática y la física actuales”, Facultad de Ciencias – UNED, Madrid (ES).

9. OTHER CONTRIBUTIONS TO CONFERENCES

- 9.1. Oral: “*Predicting hot-electron free energies from ground-state data*”, APS March Meeting 2023, Las Vegas, Nevada (USA), 08/03/2023
- 9.2. Poster: “*Predicting hot-electron free energies from ground-state data*”, 21st International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods | (smr 3814) @ ICTP. Trieste (IT), 11-13/01/2023
- 9.3. Poster: “*Simulating transport coefficients of superionic conductors: Finite-size effects in ion dynamics and heat conduction*”, Psi-K Conference, 22-25/08/2022, SwissTech Center, EPFL, Lausanne (CH)
- 9.4. Web-presentation: “*Ab initio simulation of heat and charge transport in water at planetary pT conditions*”, APS March Meeting 2020, Denver, Colorado (USA) 03/03/2020 (physical meeting canceled due to COVID-19 emergency; web presentation at <http://meetings.aps.org/Meeting/MAR20/Session/J40.7>)
- 9.5. Poster: “*Charge-transport quantization and gauge-invariance of electrical conductivity in ionic fluids*”, 19th International Workshop on Computational Physics and Material Science: Total Energy and Force Methods | (smr 3266) @ICTP, Trieste (IT), 09/01/2019
- 9.6. Oral: “*Space-and-time coherent evolution of spatially indirect excitons: the role of the internal dynamics*”, Materials.it, Bologna (IT), 24/10/2018
- 9.7. Oral: “*Electrical conductivity and charge-transport quantization in ionic fluids*”, Materials.it, Bologna (IT), 22/10/2018
- 9.8. Oral: “*Quantum propagation of a correlated electron-hole pair in semiconductor heterostructures*” – FisMat, ICTP, Trieste (IT) October 2017
- 9.9. Oral: “*Space-and-time-dependent propagation of a composite particle*” – SISSA, Trieste (IT), February 16, 2017
- 9.10. Oral: “*Picosecond timescale scattering of an electron-hole pair in semiconductor heterostructures*”, 68th School in Solid State Physics: The Free Electron Laser for Ultrafast Imaging at the Nanoscale – Erice (IT), June 9, 2016
- 9.11. Oral: “*Time-dependent simulation of scattering of a quantum complex with internal excitations*”, at the International Conference on Mathematical Modeling in Physical Sciences (IC-MSQUARE) – Athens (GR), May 24, 2016
- 9.12. Oral: “*Time Dependent Quantum Dynamics of 2D Spatially Indirect Excitons*”, at Collective Electronic Excitations in 2D (CEE2D) Conference – Pisa (IT), September 24, 2015.
- 9.13. Oral: “*Time-Dependent Quantum Dynamics of 2D Spatially Indirect Excitons*” – UCSD Physics Department, San Diego, California (USA), June 12, 2015.
- 9.14. Poster: “*Time-dependent quantum dynamics of 1D indirect excitons*” in the “International Conference on Physics of Light-Matter Coupling in Nanostructures (PLMCN)” – Montpellier (FR), June 9-13, 2014

10. SCHOOLS ATTENDED

- 10.1. COST Academy Science Communicator Workshop, Bruxelles, 6-7/03/2024.
- 10.2. COST Academy Leadership Workshop, Bruxelles, 8/09/2023.
- 10.3. Workshop “*Thermal Transport at the Nanoscale*”, Telluride, CO (USA), June 21-25, 2022.
- 10.4. Joint ICTP-IAEA Workshop on *Fundamentals of Vittrification and Vitreous Materials for Nuclear Waste Immobilization* | (smr 3159) November 6-10, 2017.
- 10.5. CINECA school: “*Python for Scientific Computing*” – Modena (IT), January 25-27, 2016
- 10.6. “*Winter School on the Physics of Indirect Excitons*” – Les Houches (FR), March 16-20, 2015
- 10.7. CINECA school: “*Introduction to Parallel Computing with MPI and OpenMP*” – Casalecchio di Reno (IT), December 9-11, 2014
- 10.8. CINECA school: “*Introduction to HPC Scientific programming: Tools and Techniques*” – Casalecchio di Reno (IT), November 3-5, 2014
- 10.9. “*International School on Physics of Indirect Excitons*”, “Ettore Majorana” Foundation and Centre for Scientific Culture – Erice (IT), July 26-August 1, 2014

- 10.10. CINECA school: “*Introduction to the FERMI Blue Gene/Q, for users and developers*” – Casalecchio di Reno (IT), March 17, 2014

11. ORGANIZATION OF CONFERENCES/WORKSHOP

- 11.1.25-28/11/2025: CECAM-Psi-K Flagship Workshop “*Uncertainty quantification in atomistic modeling: From uncertainty-aware density functional theory to machine learning*”, Lausanne (CH). See: <https://www.cecaml.org/workshop-details/1380>
- 11.2.9-13/06/2025: CECAM-Psi-K Flagship School “*School on Machine Learning for Molecules and Materials Research*”, Zadar (HR). See: <https://www.cecaml.org/workshop-details/1379>
- 11.3.5-6/02/2024 DAEMON COST Action CA22154 General Meeting 2024, Binario F, Stazione Termini, Roma. See: https://cost-daemon.eu/?page_id=168
- 11.4.6-10/11/2023: CECAM-Psi-K Hybrid School “*School on Machine Learning Interatomic Potentials (ML-IP 2023)*”, Aalto University, Espoo, Finlandia. see: <https://www.cecaml.org/workshop-details/1213>
- 11.5.23-26/05/2023: CECAM-Psi-K Flagship School “*Young Researchers' School on Theory and Simulation in Electrochemical Conversion Processes*”, Ecole Normale Supérieure, Paris. see: <https://www.cecaml.org/workshop-details/1216>
- 11.6.15-18/11/2021: “*ML-IP 2021*”: Early-career oriented online workshop on Machine-Learning Interatomic Potentials, approved and funded by Psi-K, <https://www.mlip-workshop-2021.xyz/>.

12. REVIEWER FOR HIGH-PERFORMANCE-COMPUTATION (HPC) PROPOSALS

- 12.1. Reviewer for HPC projects ISCRA-LISA - CINECA; subject: computational condensed matter physics

13. REVIEWER FOR SCIENTIFIC JOURNALS

- 13.1. Reviewer for “*Proceedings of the National Academy of Sciences*” (PNAS, USA).
- 13.2. Reviewer for “*Nature Communications*” (Springer-Nature, UK)
- 13.3. Reviewer for “*Physical Review Letters*” (APS – American Physical Society, USA).
- 13.4. Reviewer for “*Physical Review Materials*” (APS – American Physical Society, USA)
- 13.5. Reviewer for “*The Journal of Chemical Physics*” (AIP – American Institute of Physics).
- 13.6. Reviewer for “*Journal of Physics Communications*” (IoP – Institute of Physics).

14. MEMBER OF EVALUATION COMMITTEES

- 14.1. Since A.Y. 2025/2026: Member of the Council of PhD in Physics and NanoSciences, UNIMORE
- 14.2. Member of evaluation committee for the public selection of a research fellowship on “*Implementazione di tecniche avanzate di calcolo ad alte prestazioni (HPC) e ad alto flusso (“high-throughput”, HTC) al software di simulazione quantistica Quantum ESPRESSO*” Area Fisica della SISSA, atto di nomina: Prot. n. 26875-III/13 N.817/2022.
- 14.3. Member of evaluation committee for the public selection of a research fellowship on “*Proprietà topologiche e di trasporto di carica in conduttori ionici*” Area 02 – Scienze fisiche, settore concorsuale 02/B2 - (s.s.d. FIS/03), presso l’Area Fisica della SISSA, atto di nomina: Prot. n. 26874-III/13 N.816/2022.
- 14.4. Member of the evaluation committee for the public selection of a research fellowship on “*Proprietà di trasporto in liquidi e solidi disordinati*” Area 02 – Scienze fisiche, settore concorsuale 02/B2 - (s.s.d. FIS/03), presso l’Area Fisica della SISSA, atto di nomina: Prot. n. 26132-III/13 N.785/2022.
- 14.5. Member of the evaluation committee for the public selection of a research fellowship on “*High-performance computing on heterogeneous, modular, and scalable hardware architectures, based on GPU accelerators*” Area di Fisica della SISSA, atto : prot. n. 5894-III/12 N. 190/2020.
- 14.6. Member of the evaluation committee for the public selection of a research fellowship on “*Ab initio simulation of charge-transfer processes at the interface between metals and 2D overlayers*” Area di Fisica della SISSA, atto: prot. n. 4830-III/12 N. 164/2020.

15. APPROVED HPC PROJECTS

- 15.1. CSCS Production Project: “*A machine learning study of the dissociation of water on Li3PS4 surfaces*” (320,000 Node hours on CSCS Cray XC50 – Hybrid system), approved at Centro Svizzero di Calcolo Scientifico - CSCS (01/10/2023 – 30/09/2024).
- 15.2. HPC Project: “*Quantum Dynamics of COMposite Particles*”(acronym: QDCOMP), ISCRA C Project, approved and accepted at CINECA HPC systems, Tier-1 IBM NeXtScale supercomputing cluster ‘Galileo’ (2016-2017).

- 15.3. HPC Project: “*Fully QUantum Dynamics of 2D Indirect eXcitons*”(acronym: FUQUDIX), ISCRA C Project, approved and accepted at CINECA HPC systems, Tier-1 IBM NeXtScale supercomputing cluster ‘Galileo’ (2015-2016).

16. TEACHING AND MENTORING ACTIVITIES

- 16.1. February-May 2026: 48 h of lectures, “*Advanced Condensed Matter Theory*”, MSc in Physics, UNIMORE.
- 16.2. September 2025 - May 2026: 40 h of lectures, “*Laboratory of machine learning and advanced computing for physics*”. MSc in Physics, UNIMORE.
- 16.3. February-June 2025: 48 h of lectures, “Machine learning for scientific applications”, MSc in Physics, UNIMORE
- 16.4. September-December 2024: 24 hours of lectures, “*Solid State Physics*”, MSc in Physics, UNIMORE
- 16.5. March 2023: PhD course “*Machine Learning Interatomic Potentials - A short course*”. 12 hours of lectures. School of Graduate Studies “Physics and Nanosciences”, University of Modena and Reggio Emilia, Italy.
- 16.6. April-May 2020 and 2021: PhD-oriented on-line course on “*Theory and numerical simulation of heat, mass and charge transport in condensed matter*” (given together with Prof. Stefano Baroni, SISSA). Approx. 50 subscribers from international institutions.
- 16.7. A.Y. 2019/20, 2020/21: “Didattica Integrativa” (Supplementary Lectures) for the Laurea (BSc) Course “*Fisica Statistica*” (Statistical Physics) – Department of Physics, University of Trieste (IT).
- 16.8. A.Y. 2018/19: “Attività Formativa Complementare” (Graduate Teaching Assistant) for the Laurea (BSc) Course “*Fisica Statistica*” (Statistical Physics) – Department of Physics, University of Trieste (IT).
- 16.9. A.Y. 2016/17, 2015/16, 2014/15, 2013/14: Graduate Teaching Assistant for the Laurea (BSc) course “*Termodinamica Statistica*” (Statistical Thermodynamics) – Department of Physics, Informatics, and Mathematics, University of Modena and Reggio Emilia (IT).
- 16.10. A.Y. 2016/17, 2015/16, 2014/15, 2013/14: Training lectures for the Physics Olympiads, from Second-level- to International-stages of the competition. The activity was partially funded by the Italian Government through the programme “Piano Lauree Scientifiche”.

17. EDITORIAL WORK

- 17.1. I have accepted to serve as Guest Editor for Machine Learning Science and Technology (IoP), to soon publish a focus issue on uncertainty quantification in atomistic modeling.

18. TUTOR AND SUPERVISION ACTIVITIES

- 18.1. Supervisor of Filippo Montorsi’s PhD programme, PhD School in Physics and Nanosciences, UNIMORE. Tentative title: “*Quantum effects on the transport properties of liquids and their uncertainty estimation*”.
- 18.2. Co-supervisor of Luoxuan Peng’s PhD programme, PhD School in Physics and Nanosciences, UNIMORE. Tentative title: “*Machine learning for simulation in quantum materials discovery*”
- 18.3. Supervisor of Paolo Dugoni’s MSc Thesis in Physics, UNIMORE (defended on April 14th, 2026). Title: “*Uncertainty quantification in symbolic regression for modelling ion diffusion in electrolytes*”.
- 18.4. Co-supervisor of Alessia Bortolazzi’s MSc Thesis, UNIMORE (defended on April 14th, 2026). Title: “*Ab initio & Machine Learning Combined Study of the Lattice Thermal Conductivity of Boron Arsenide including Anharmonic Effects*”.
- 18.5. Co-supervisor Paolo Pegolo’s PhD thesis, SISSA (defended on January 5th, 2023). Title: “*Charge and heat transport in ionic conductors*” <https://iris.sissa.it/handle/20.500.11767/130672>.
- 18.6. Tutor in PhD programme of Chiheb Ben Mahmoud at EPFL (supervisor: Prof. Michele Ceriotti). Thesis defended on 20.03.2023, title “*Machine-learning the electronic density of states: electronic properties without quantum mechanics*” <https://infoscience.epfl.ch/record/301314> See Publication: Ben Mahmoud, Grasselli, Ceriotti, Phys. Rev. B., 106 (12), L121116 (Letter), 2022.
- 18.7. Tutor in PhD programme of Giulio Imbalzano at EPFL (supervisor Prof. Michele Ceriotti). Thesis defended on 12.11.2021, title: “*Transferable machine-learning models of complex materials: the case of GaAs*” <https://infoscience.epfl.ch/record/290022>. See Publication: Imbalzano et al., Journal of Chemical Physics, 154(7), 074102 (Editor’s pick), 2021.

19. LANGUAGE SKILLS

- 19.1. Italian (mother language)
- 19.2. English (C1)

19.3. French (C1)

19.4. Spanish (B1)

20. COMPUTATIONAL SKILLS

- 20.1. Extensive experience on Car-Parrinello simulations and electronic structure calculations, specifically through the codes of the Quantum ESPRESSO package
- 20.2. Experience in classical molecular dynamics and nudged-elastic-band calculations through the software package LAMMPS and GPUMD
- 20.3. Machine learning techniques to fit interatomic potentials and materials properties
- 20.4. Molecular structure visualization software: VMD, xcrysden, VESTA
- 20.5. Operating systems: Unix (Linux), Windows
- 20.6. Programming languages: Fortran, Mathematica, Matlab, Bash (Unix Shell), Python; fundamentals of C, Basic and Processing (mainly for Arduino board applications)
- 20.7. Parallel programming: MPI, OpenMP
- 20.8. Markup languages: LaTeX, HTML
- 20.9. Content Management System: WordPress

21. OUTREACH ACTIVITIES

- 21.1. Since December 2025: activities promoted as the Communication Coordinator of the Dept. of Physics, Informatics and Mathematics, UNIMORE.
- 21.2. Since June 2025: Admin of the webpage of the Theory and Simulations of Materials group, UNIMORE: <https://www.theomat.unimore.it/>.
- 21.3. May 20, 2026: Outreach event “Research Shots”, following the style of Pint of Science, at Binario 49 café (Reggio Emilia), in collaboration with the Dept. of Science and Methods of Engineering, UNIMORE.
- 21.4. Organization of Open Day of the Dept. of Physics, Informatics and Mathematics (February 2025 and 2026), with pedagogical activities to high-school students.
- 21.5. March 11, 2026: Topical Seminar, High School (Liceo Scientifico Statale) Wiligelmo, Modena. “*In minimis maxima: Calcoli su scala atomica per predire l’evoluzione dei pianeti*”.
- 21.6. European Researchers’ Night 2025, Modena. Activity: “*Matter of Matching: Un gioco di carte tra memoria e scienza dei materiali*” see: <https://www.nottedellaricerca.unimore.it/2025/evento.html?e=112>
- 21.7. September 5, 2024: Topical Seminar (Training for Physics Olympiads to students of Emilia-Romagna and Marche) “*In minimis maxima: Calcoli su scala atomica per predire l’evoluzione dei pianeti*”.
- 21.8. 26 April 2024: Oral contribution (online) aimed at young researchers interested in writing a proposal, Marie Skłodowska-Curie Action Info Day, University SS Cyril e Methodius, North Macedonia.
- 21.9. Spring-Summer 2022 and 2023: Lectures (in French) on solid-state batteries aimed at high school students “College Voltaire”, Geneva, Switzerland.
- 21.10. November 2021 – Contribution as a researcher in *Science is Wonderful!* (SiW), 2021 edition, a EU funded project of outreach aimed at pupils of first and secondary schools, lying within the Marie Skłodowska Curie Action.
- 21.11. August 2020 – Contribution on *All About Space* magazine on the internal structure of Uranus and Neptune; title: “What is the interior of an ice giant planet likely to be?”.
- 21.12. August 2020 – Participation in a RAI radio program (“Radar”) and in a web-radio podcast (“Co.Scienza”) to speak of charge and heat transport at planetary conditions, main results of the recent research of the ER.
- 21.13. September 2019 – collaboration with SISSA and ICTP for the outreach event “Trieste-Next”.
- 21.14. September 2019 – collaboration at SISSA for a “street science” project to be performed during the European Researchers’ Night 2019.
- 21.15. March 6 – April 5, 2017 – Collaboration (“collaborazione occasionale”) for an activity of management and science communication on Nanoscience, within the project “Into the Future” (CNR Nano and Fondazione Cassa di Risparmio di Modena), a guidance project aimed at high-school student from the province of Modena (Prot. CNR Nano n. 0000953), now at its 3rd Edition (<https://www.fondazione-crmo.it/intothefuture3/>)
- 21.16. February – April, 2017 - Participation to the project “Into the Future”, as CNR associate researcher (activity on double slit experiment)
- 21.17. From 2014 - Seminars and workshops on Modern Physics, given for an audience of high-school students, and general public
- 21.18. From 2012 - Activities on science communication within the project “Inco.Scienza” (<https://www.inco-scienza.org/>)

- 21.19. A.Y. 2011-12 - Outreach activity on the Physics of Semiconductors, with lectures given at the planetarium of Modena (Civico Planetario “F. Martino”) and at the High-School (Liceo Scientifico) “Ariosto-Spallanzani”, Reggio Emilia.

22. PUBLICATIONS

- 22.1. M. A. Hernandez Bertran, D. Tisi, F. Grasselli, M. Ceriotti, E. Molinari & D. Prezzi, “Tracking the Lithiation State of Li_xSi from Machine-Learned XPS Binding Energies” arXiv preprint [arXiv:2602.23028](https://arxiv.org/abs/2602.23028) (2026).
- 22.2. S. Chong, T. Jiang, M. Domina, F. Bigi, F. Grasselli, J. Lee & M. Ceriotti, “Resolving the body-order paradox of machine learning interatomic potentials”, *J. Chem. Phys.* **164**(6), 064121 (2026).
- 22.3. F. Grasselli, K. Rossi, S. de Gironcoli & A. Grisafi, “Long-range electrostatics in atomistic machine learning: a physical perspective”. arXiv preprint [arXiv:2602.11071](https://arxiv.org/abs/2602.11071) (2026).
- 22.4. W. Zhou, B. Tang, Z. Fan, F. Grasselli, S. Baroni & B. Song, “Heat transport in superionic materials via machine-learned molecular dynamics”, arXiv preprint [arXiv:2512.04718](https://arxiv.org/abs/2512.04718) (2025).
- 22.5. L. Benić, F. Grasselli, C. Ben Mahmoud, D. Novko & I. Lončarić, “Machine learning model for efficient nonthermal tuning of the charge density wave in monolayer NbSe₂”, *Journal of chemical theory and computation*, **21**(16), 8130-8141 (2025).
- 22.6. P. Pegolo, E. Drigo, F. Grasselli & S. Baroni, “Transport coefficients from equilibrium molecular dynamics”, *J. Chem. Phys.*, **162**(6), 064111 (2025).
- 22.7. F. Grasselli, S. Chong, V. Kapil, S. Bonfanti & K. Rossi, “Uncertainty in the era of machine learning for atomistic modeling”, *Digital Discovery*, **4**(10), 2654-2675 (2025).
- 22.8. W.B. How, S. Chong, F. Grasselli, K. Huguenin-Dumittan & M. Ceriotti, “Adaptive energy reference for machine-learning models of the electronic density of states” *Phys. Rev. Materials*, **9**, 1, 013802 (2025).
- 22.9. S. Chong, F. Bigi, F. Grasselli, P. Loche, M. Kellner & M. Ceriotti, “Prediction rigidities for data-driven chemistry”, *Faraday Discussions*, **256**, 322-344 (2025).
- 22.10. F. Bigi, S. Chong, M. Ceriotti & F. Grasselli, “A prediction rigidity formalism for low-cost uncertainties in trained neural networks”, *Machine Learning: Science and Technology*, **5**(4), 045018 (2024).
- 22.11. D. Tisi, F. Grasselli, L. Gigli, and M. Ceriotti, “Thermal transport of Li₃PS₄ solid electrolytes with *ab initio* accuracy”. *Phys. Rev. Materials* **8**, 6, 065403 (2024).
- 22.12. P. Pegolo and F. Grasselli, “Thermal transport of glasses via machine learning driven simulations”, *Front. Mater.* **11**:1369034 (2024).
- 22.13. L. Gigli, D. Tisi, F. Grasselli, and M. Ceriotti, “Mechanism of charge transport in lithium thiophosphate”, *Chemistry of Materials* **36**, 3, 1482 (2024).
- 22.14. S. Chong, F. Grasselli, Ch. Ben Mahmoud, J. D. Morrow, V. L. Deringer, and M. Ceriotti, “Robustness of local predictions in atomistic machine learning models”, *J. Chem. Theory Comput.*, **19**(22), 8020 (2023).
- 22.15. P. Pegolo, S. Baroni and F. Grasselli, “Self-interaction and transport of solvated electrons in molten salts”, *J. Chem. Phys.* **159**, 094116 (2023).
- 22.16. A. Grisafi and F. Grasselli, “Effect of a temperature gradient on the screening properties of ionic fluids”, *Phys. Rev. Materials* **7**, 045803 (2023).
- 22.17. Ch. Ben Mahmoud, F. Grasselli, M. Ceriotti, “Predicting hot-electron free energies from ground-state data”, *Phys. Rev. B. Lett.*, **106**(12), L121116 (2022).
- 22.18. P. Pegolo, S. Baroni, F. Grasselli, “Topology, Oxidation States, and Charge Transport in Ionic Conductors” *Annalen der Physik*, **2200123** (2022) (Invited; on the cover page of the journal)
- 22.19. F. Grasselli, “Investigating finite-size effects in molecular dynamics simulations of ion diffusion, heat transport, and thermal motion in superionic materials” *J. Chem. Phys.* **156**, 134705 (2022)
- 22.20. P. Pegolo, S. Baroni and F. Grasselli, “Temperature- and vacancy-concentration-dependence of heat transport in Li₃ClO from multi-method numerical simulations”, *npj Computational Materials* **8**, 24 (2022)
- 22.21. L. Stixrude, S. Baroni and F. Grasselli, “Thermal and Tidal Evolution of Uranus with a Growing, Frozen Core”, *the Planetary Science Journal* **2**, 222 (2021)
- 22.22. F. Grasselli and S. Baroni, “Invariance principles in the theory and computation of transport coefficients”, *Eur. Phys. J. B* **94**, 160 (2021) (invited)
- 22.23. G. Imbalzano, Y. Zhuang, V. Kapil, K. Rossi, E.A. Engel, F. Grasselli, and M. Ceriotti, “Uncertainty estimation for molecular dynamics and sampling”, *Journal of Chemical Physics*, **154**(7), 074102 (Editor’s pick, 2021)

- 22.24. P. Pegolo, F. Grasselli, and S. Baroni, “Oxidation States, Thouless’ Pumps, and Nontrivial Ionic Transport in Nonstoichiometric Electrolytes”, [Phys. Rev. X **10**, 041031](#) (2020)
- 22.25. F. Grasselli, L. Stixrude, and S. Baroni, “Heat and charge transport in H_2O at ice-giant conditions from *ab initio* molecular dynamics simulations”, [Nature Commun. **11**, 3605](#) (2020)
- 22.26. F. Grasselli and S. Baroni, “Topological quantization and gauge invariance of charge transport in liquid insulators”, [Nature Phys. **15**, page 967](#) (2019)
- 22.27. R. Bertossa, F. Grasselli, L. Ercole, S. Baroni, “Theory and Numerical Simulation of Heat Transport in Multicomponent Systems”, [Phys. Rev. Lett. **122**, 255901](#) (2019)
- 22.28. S. Baroni, R. Bertossa, L. Ercole, F. Grasselli, A. Marcolongo, “Heat transport in insulators from *ab initio* Green-Kubo theory”, Handbook of Materials Modeling. Applications: Current and Emerging Materials, edited by W. Andreoni and S. Yip, 2nd ed., [Chap. 12-1](#) (Springer), and arXiv:1802.08006v1 [cond-mat.stat-mech] (2018)
- 22.29. F. Grasselli, A. Bertoni, and G. Goldoni, “Classical and quantum dynamics of indirect excitons driven by surface acoustic waves”, [Phys. Rev. B **98**, 165407](#) (2018)
- 22.30. F. Grasselli, “Variational approach to the soft-Coulomb potential in low-dimensional quantum systems”, [American Journal of Physics **85**, p. 834](#) (2017)
- 22.31. F. Grasselli, A. Bertoni, G. Goldoni, “Exact long-wavelength plasmon dispersion on a ring with soft Coulomb interactions”, [Physica Scripta **92**, p. 095802](#) (Aug. 2017)
- 22.32. F. Grasselli, A. Bertoni, and G. Goldoni, “The role of internal dynamics in the coherent evolution of indirect excitons”, Superlattices and Microstructures, special issue devoted to “[Indirect Excitons: Physics and Applications](#)” **108**, p. 73 (2017) (invited)
- 22.33. T. Pincelli, F. Grasselli, V. N. Petrov, P. Torelli, and G. Rossi “Performance of photoelectron spin polarimeters with continuous and pulsed sources: from storage rings to free electron lasers”, [Journal of Synchrotron Radiation **24**, 175](#) (2017)
- 22.34. F. Grasselli, A. Bertoni, and G. Goldoni, “Time-dependent scattering of a composite particle: A local self-energy approach for internal excitations”, [Phys. Rev. B **94**, 125418](#) (2016)
- 22.35. F. Grasselli, A. Bertoni, and G. Goldoni, “Two-body quantum propagation in arbitrary potentials”, [Journal of Physics: Conference Series, Vol. **738**, p. 012028](#), Article for the Proceedings of the 5th International Conference on Mathematical Modeling in Physical Sciences (IC-MSQUARE 2016)
- 22.36. F. Grasselli, A. Bertoni, G. Goldoni, “Exact two-body quantum dynamics of an electron-hole pair in semiconductor coupled quantum wells: A time-dependent approach”, [Phys. Rev. B **93**, 195310](#) (2016)
- 22.37. F. Grasselli, A. Bertoni, and G. Goldoni, “Space- and time-dependent quantum dynamics of spatially indirect excitons in semiconductor heterostructures”, [J. Chem. Phys. **142**, 034701](#) (2015)

23. RESEARCH MONOGRAPHS AND CHAPTERS IN VOLUMES

- 23.1. S. Baroni, R. Bertossa, L. Ercole, F. Grasselli, A. Marcolongo, “Heat transport in insulators from *ab initio* Green-Kubo theory”, Handbook of Materials Modeling. Applications: Current and Emerging Materials, edited by W. Andreoni and S. Yip, 2nd ed., Chap. 12-1 (Springer), and arXiv:1802.08006v1 [cond-mat.stat-mech] (2018)

24. OTHER INTERESTS

- 24.1. Musicology and Early Music, with one article published in the field: F. Grasselli, “*Ipotesi di ricostruzione degli automatismi del nuovo organo a Pratolino (1766)*”, *Informazione Organistica (Italian Journal of Organology)*, Vol. **32** (2012)
- 24.2. Live musical performance, singing in a choral ensemble, and playing the harmonica and the guitar in clubs, music festivals and happenings around Italy