

Elisa Molinari - Curriculum Vitae

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CV & POSITIONS

2001-now	Full Professor of Condensed Matter Physics, University of Modena and Reggio Emilia (Department of Physics, Informatics and Mathematics)
2010-now	Research associate, CNR-Nano (Consiglio Nazionale delle Ricerche - Istituto Nanoscienze), Modena
2015-now	Founding Director, MaX European Center of Excellence in Materials Modelling, Simulation and Design
2007-2010	Director of INFM-CNR (Istituto Nazionale per la Fisica della Materia del CNR), comprising 21 Research Centers in Italy
2002-2007	Founding Director; S3 Research Center of INFM "nanoStructures and bioSystems at Surfaces", Modena (now part of CNR-Nano)
2001-2007	Research associate, INFM (Istituto Nazionale per la Fisica della Materia)
1992-2001	Associate Professor, University of Modena
1985-1992	Research staff member, Istituto "Corbino" of CNR, Roma
1983-1985	'Post-doctoral scientist', Max-Planck-Institut für Festkörperforschung, in Stuttgart and Grenoble
1981-1983	Post-lauream fellow (supported by an industry) at the University of Modena
1981	Laurea cum laude in Physics, University of Modena

RESEARCH PROFILE

My research focuses on nanoscience and the understanding of fundamental physical phenomena that characterize matter and underpin technologies; on the design of future materials and nano-(bio-)devices; on the development of computational methods based on quantum physics, including applications in chemistry and biology.

The approach is highly interdisciplinary: starting from theoretical quantum physics, it sits at the interface between the physical and chemical sciences of materials, biophysics, computational sciences (large-scale codes and data), and applications, particularly in information technologies, energy, and the environment. We have always maintained a focus on close collaborations with experimental research, working to design and understand new experiments and observations. I have a continuing interest also in scientific imaging and communication. Coordinator of several European and international projects in these fields.

Research topics addressed by my group include:

- Coherence in natural and artificial organic nano(bio) systems
- Quantum materials and novel correlated phases in matter
- Computational spectroscopies and applications to materials for information and energy technologies
- Biomolecular systems and bio-inspired nanodevices
- Semiconductor structures: electron correlations, vibrations and electron-phonon interactions
- Algorithmic and computational developments

For further details and references, see Annex 1.

I am a Fellow of the American Physical Society, elected in 1999 "for her contribution to the theory of semiconductors and their interfaces, in particular, her fundamental work on electron-electron and electron-phonon interaction in nanostructures; and for her involvement in the training of young theorists from many countries."

Publications

- Over 300 papers in leading international journals. Over 16500 citations (*h*-index 68, Google Scholar, July 2025).
- For the full publication list see [Google Scholar](#); ORCID ID 0000-0002-0692-6096; Web of Science ResearcherID: Q-9199-2019.
- A selection of publications organized by research topic is listed in Annex 1.

Conferences

- Invited/plenary speaker at over 200 international conferences and workshops, including the major meetings in physical and chemical sciences of matter, as well as high-performance scientific computing. Selected conferences include: International Conference on the Physics of Semiconductors (ICPS), March Meeting of the Condensed Matter Division of the American Physical Society (APS), March Meeting of the Condensed Matter Division of the German Physical Society, Annual Meeting of the American Chemical Society (ACS), Spring Meeting of the Materials Research Society (MRS), European Conference on Surface Science (ECOSS), International Conference on Modulated Semiconductor Structures (MSS), Nanotube Conference (NT), Platform for Advanced Scientific Computing (PASC).
- Chair, co-chair, organizer of major workshops. Selected examples include: Excitonic and competing orders in low-dimensional materials (Milan CMD30); Excitonic insulator: New perspectives in long-range interacting systems (Lausanne 2018); Materials Design at the Exascale: High-performance and High Throughput Computing (Trieste 2018); Synergy between quantum computing and high-performance computing (ETH Zurich 2017); High performance computing for 2D materials research (Graphene Week Helsinki 2019). Chair of several national conferences in these fields.
- Scientific Committees of the main conferences in my research field. Recent examples include AI4AM-2024 (Barcelona 2024, 2026); ICPS (Ottawa 2024); Chem2DMat (Bologna 2021); Electronic Properties of Two-Dimensional Systems (Genova 2007); and several editions of ICPS and MSS.

COORDINATION AND ADVISORY PROFILE

- **Director of MaX – Materials Design at the Exascale European Centre of Excellence (2015 – now):** Founded in 2015 and coordinated in Modena (CNR-NANO), MaX involves multiple leading Italian and European research groups: www.max-centre.eu. The Centre ensures that the European open-source scientific software for materials design —currently world-leading— maintains and extends its capabilities amid disruptive scientific supercomputing technologies and AI advances. MaX is a European e-infrastructure funded through three successive Horizon 2020 and Horizon Europe-EuroHPC projects (2015–2026), renewed for 2027-29.
- **Director of INFM – National Institute for the Physics of Matter of CNR (2007 – 2010):** Comprising 21 INFM research structures merged into CNR: 2 National Laboratories (TASC in Trieste and MDM in Agrate at STMicroelectronics), 10 Research Centers (Milan, Trieste, Trento, Modena, Pisa, Rome2, Naples, Lecce, Catania), 9 Regional Laboratories, and a central management unit in Genoa. INFM comprised over 420 employees and 650 associates (~430 professors/researchers, ~220 PhD students and postdocs).
- **Director of the INFM S3 Research Center in Modena (2002 – 2007):** Coordinated the founding 5-year competitive project for S3 (*nanoStructures and bioSystems at Surfaces*). S3 later merged into CNR and is now one of the two main sites of the Nanoscience Institute (alongside NEST at Scuola Normale Superiore, Pisa).

Selected scientific, advisory and evaluation boards: Europe and international

- ESRF – European Synchrotron Radiation Facility, Grenoble: Council, Head of Italian Delegation (2014-now)
- ICN2 – Institut Català de Nanociència i Nanotecnologia, Barcelona: International Advisory Board (2023-now)
- SeRC – Swedish e-Science Research Center: International Advisory Group (2024-now)
- Fritz-Haber-Institute of the Max-Planck Gesellschaft, Berlin: Scientific Board (2015-23)
- Max-Planck Institute for the Structure and Dynamics of Matter, Hamburg: Scientific Board (2016-23)
- JARA – Jülich-Aachen Research Alliance, Center for Simulation & Data Science: Advisory Board (2018-now)
- Europhysics Prize Committee (2024-now)

- EuroHPC Joint Undertaking: RIAG Research and Innovation Advisory Board (2019-21)
- Psi-k Network: Board of Trustees, Scientific Advisory Committee (2019-now)
- HPC3 – High Performance Computing Centres of Excellence Council: vice-president (2019-23)
- EU High Level Group on Materials (2018-22)
- Helmholtz Program on Nano & Microsystems, KIT Karlsruhe Institute of Technology: Advisory Board (2010-16)
- EU Program Committee “Nanotechnologies, Advanced materials, Biotechnology, Advanced manufacturing and processing” (NMBP) within Horizon2020: Expert Member, Italian Delegation (2014-20)
- EU Program Committee “Cooperation: Nano-, Materials, Production Systems” (NMP) within the 7th Framework Program: Member, Head of Italian Delegation (2007-14)
- EU European Research Council (ERC): Advanced Grants Evaluation Panels (2009-11)
- OECD Working Party on Nanotechnology, Member (2007-14)
- EU Advisory Group on “Nanosciences, Nanotechnologies, Materials and New Production Materials” - 7th Framework Program (2002-07)
- APS American Physical Society, Forum on International Physics: Executive Committee (2017-19)
- IUPAP - International Union for Pure and Applied Physics: Scientific Secretary of the Semiconductor Commission (1999-2002); Associate Secretary General (2002-03); Working Group on Women in Physics (2002-03)
- AI for Science – IOP Institute of Physics Publishing, Editorial Board (2025-now)
- Scientific Reports – Nature Publishing Group, Editorial Board (2014-17)
- Solid State Communications – Pergamon / Elsevier, Editorial Board (1990 – 2008)

Selected scientific, advisory and evaluation boards: Italy

- IIT – Istituto Italiano di Tecnologia: Scientific Technical Committee (2024-now); Evaluation Committee (2025)
- CNR-DSFTM – Dipartimento Scienze Fisiche e Tecnologie della Materia of CNR: Scientific Council (2023-now)
- MUR Ministero Università e Ricerca, Italy – ‘Supervisory board’ of PNRR - Piano Nazionale di Ripresa e Resilienza (2021-25)
- Associazione Big Data: Board of directors (2015-26)
- Università di Trento – Board of Directors (Consiglio di amministrazione) (2012-18)
- Università di Modena e Reggio Emilia - Board of Directors (Consiglio di amministrazione) (2020-now); Senato Accademico (1994-99)
- CINECA & Italian Supercomputing Resource Allocation - ISCRA: Scientific Board (2010-15)
- [MUR Ministero Università e Ricerca, Italy – FIRB "Futuro in Ricerca" 2012 call – Chair of the Physical Sciences & Engineering \(PE\) general panel](#)
- High Technology Network of the Emilia-Romagna Region, CIMS I Scientific and Industrial Steering and Monitoring Committee: President (2011-14)
- Science Festival, Genova: Scientific Board (2003-12)
- Women and Science Association, Italy (Associazione Donne e Scienza): Steering Committee (2019-24); Founding Member (July 2006)

Selected Research Projects

Key projects as overall project coordinator (**) or local research unit leader (*):

- ** MaX: Materials Design at the eXascale – European Centre of Excellence (*Horizon Europe-EuroHPC*, 2023-26)
- * HANAMI: HPC alliance for applications and supercomputing innovation: the Europe - Japan collaboration (*Horizon Europe-EuroHPC*, 2024–26)
- * EUMaster4HPC: European Master for High Performance Computing (*Horizon Europe-EuroHPC*, 2020-25)
- * BIG-MAP: Novel methodologies for autonomous discovery of advanced battery chemistries (*EU-H2020*, Local budget: ~€240,000)
- ** MaX: Materials Design at the eXascale – European Centre of Excellence (*EU-H2020*, 2018-21, Total funding: ~€8,500,000; Local unit: €1,580,000)

- * EXC-INS: Excitonic insulator in two-dimensional long-range interacting systems (*PRIN*, 2018-22, Total funding: ~€940,000; Local unit: ~€405,000)
- * IQBITS: Integrated Qubits Towards Future High-Temperature Silicon Quantum Computing Hardware Technologies (*EU-H2020 FET-Open*, 2019-22, Local unit: ~€400,000)
- * MUSIQ: Multiphoton Microscopy and Ultrafast Spectroscopy: Imaging meets Quantum (*EU-H2020 MSCA-ITN*, 2018-22, Local unit: ~€260,000)
- * SUPER: Supercomputing unified platform (*POR-FESR Emilia-Romagna*, 2019-21, Local unit: ~€357,000)
- ** MaX: Materials Design at the eXascale – EU Centre of Excellence (*EU-H2020 e-INFRA*, 2015-18)
- ** PROSURF: Computational toolbox for protein-surface docking (*FP6-EU STREP*, 2006-09)
- * EXCITING: First-principles approach to Optical Properties of Solids (*FP6-EU TMR Network*, 2002-05)
- * SAMBA: Single protein biomolecular transistor (*FP6-EU IST-FET*, 2001-04)
- * DNA-wires: DNA-based nanowires (*FP6-EU IST-FET*, 2003-05)
- * NOMADE: Nanomolecular devices (*FIRB*, 2002-06)
- ** Blow-up: Images from the nanoworld (*CRMo Foundation*, 2006)
- ** Nanolab: 5 projects for new research instrumentation at the S3 Center (*CRMo Foundation*, 2002-07)
- * SQID: Semiconductor Implementation of Quantum Information Devices (*FP6-EU IST-FET*, 2000-02)
- * SSQI: Mesoscopic Implementation of Quantum Information Processing Devices (*INFM PRA*, 1999-2001)
- ** S3: nanoStructures and bioSystems at Surfaces – R&D Center (*INFM CRS*, 2002-06)
- ** Marie Curie Research Training Grant UH (*FP4-Marie Curie*, 1998-99)
- * OLIGO-LED: Properties of modified oligothiophenes for organic LEDs (*PRIN*, 1999–2001)
- * ULTRAFast: Ultrafast quantum optoelectronics (*FP5-EU TMR Network*, 1997-01)
- * NANOSCI-ERA: Nanoscience in the European Research Area – EU ERAnet (*FP6*, 2005-10)
- * NANOPT: NANometre Structures for Future OPToelectronic Applications (*FP5-EU ESPRIT*, 1992-99)
- ** NANOWIRES: Joint with Weizmann Institute of Science, IL (M. Heiblum) (*International FIRB*, 2007-10)
- ** Italy-Columbia University Partnership on Carbon-based nanoscience (A. Pinczuk) (*MAE*, 2008-09)
- * DOTS: Quantum phenomena in dots, with NRC Ottawa (P. Hawrylak) (*International FIRB*, 2007-10)
- ** QCCS: Quantum Control of Charge & Spin: Next Generation Nanodevices, with Tokyo University (S. Tarucha) (*MAE*, 2003-04)
- ** OOM: Optics of Organic Materials, with University of S. Paulo, Brazil (M.J. Caldas) (*MAE*, 2002)
- ** WIP: Europe for the 1st Int. Conference on Women in Physics – UNESCO, Paris, 2002 (*EU FP6*, 2001)

TEACHING AND MENTORSHIP

Courses taught the University of Modena and Reggio Emilia:

- Nanoscience and Quantum Materials – Master's Degree in Physics
- Good Practices in Research – Master's Degree in Physics
- General Physics – Bachelor's Degree in Vehicle Engineering / Information Engineering
- Elements of Quantum Physics – Master's Degree in Mathematics

Previously taught courses: Fundamentals of Nanoscience, General Physics, and Modern Physics across various Engineering and Life Science programs.

Doctoral & Postdoctoral Supervision:

- Board Member of the PhD School in *Physics and Nanoscience*.
- Directed and delivered lectures in numerous national and international PhD and postdoctoral schools.
- Supervised at least 16 PhD students and 20 young researchers and postdocs; female representation in the group has consistently exceeded the field average.
- At least 8 alumni have built successful independent scientific careers and are now Full Professors (in Italy at PoliTo, SISSA, UniBo, UniPd, and internationally; 3 are women).
- Two former group members were awarded ERC Starting Grants; a third was selected as eligible.

Annex 1: Main Research Topics and Selected Publications

Overview of Main Topics

1. **Coherence in Natural and Artificial Organic Nano(bio) Systems:** Processes leading to sub-100 ps charge separation following photo-excitation in molecular systems remain incompletely understood. We proposed and analyzed model systems representative of photosynthetic aggregates, relevant to artificial organic photovoltaic materials. Our simulations predicted significant roles for quantum coherence and vibronic coupling, leading to ultrafast spectroscopy experiments that confirmed coherent phenomena across complex materials. [1–5]
2. **Quantum Materials and Novel Correlated Phases in Matter:** Long-range electronic interactions exhibit striking effects in low-dimensional (1D/2D) systems—such as van der Waals materials, nanowires, and nanotubes—due to reduced electronic screening. Walter Kohn and others hypothesized over 50 years ago the existence of an excitonic insulator phase. Our group predicted several 1D and 2D materials as ideal candidates and identified technological implications e.g. in ferroelectrics. Combining first-principles descriptions of excitons, dielectric screening, and topological properties with appropriate effective models, we inaugurated an active field of theoretical and experimental inquiry worldwide. [6–10]
3. **Materials for Information, Energy and Quantum Technologies, and their Computational Spectroscopies:** Low-dimensional carbon-, graphene-, and quasi-2D materials serve as key components in nanotechnology and as testbeds for electronic correlations. We were among the first to show how spectral signatures depend fundamentally on spectroscopy-specific electron-electron interactions. We developed methods and codes for optical, electron energy loss, photoemission, and tunneling spectroscopies. Current work targets materials for next-generation batteries and photovoltaics, including controlling graphene nanostructure growth on surfaces, quantifying nanoplasmonics, and designing optoelectronic devices. Machine-learning based studies of electrode-electrolyte interfaces allow us to track the degradation mechanisms in Li-based batteries. [11–19]
4. **Biomolecular Systems and Bio-Inspired Nanodevices:** Electron transfer in biomolecules is poorly described by conventional molecular dynamics. Using first-principles quantum simulations, we elucidated the electronic properties of biomolecules (G4-DNA, metalloproteins) and proposed bio-inspired nanodevices. We pioneered first-principles modeling of protein-surface interactions. Notably, in collaboration with experimentalists across biology, chemistry, and engineering, we demonstrated the first ‘nanobiotransistor’ utilizing the electron-transfer capability of azurin. [20–25]
5. **Semiconductor Structures: Electron Correlations, Vibrations and Electron-Phonon Interactions:** Phonon modes and interactions differ sharply at interfaces and in nanostructures compared to bulk media. Upon the introduction of semiconductor heterostructures, our group provided pioneering predictions of vibrational spectra in superlattices, interface electron-phonon scattering, and their roles in electronic relaxation and transport. Early work on quantum dots laid the theoretical foundation for single electron spectroscopies and devices, and for all-optical quantum computing implementations. [26–31]
6. **Algorithmic and Computational Developments:** Our group develops electronic structure algorithms and open-source codes for condensed matter physics, leading major European initiatives such as MaX (www.max-centre.eu). Methodological developments directly support our research via high-throughput automated workflows and machine learning approaches. [32–33]

Selected Publications

Coherence in Natural and Artificial Organic Nano(bio) Systems:

1. V. Petropoulos et al., Vibronic Coupling Drives the Ultrafast Internal Conversion in a Functionalized Free-Base Porphyrin, *J. Phys. Chem. Lett.* 15, 4461 (2024).
2. A. De Sio et al., Intermolecular conical intersections in molecular aggregates, *Nature Nanotech.* 16, 63 (2021).
3. S.M. Falke et al., Coherent ultrafast charge transfer in an organic photovoltaic blend, *Science* 344, 1001 (2014).
4. A. De Sio et al., Tracking the coherent generation of polaron pairs in conjugated polymers, *Nature Communications* 7, 13742 (2016).
5. C. Rozzi et al., Quantum coherence controls the charge separation in a prototypical artificial light-harvesting system, *Nature Communications* 4, 1602 (2013).

Quantum Materials and Novel Correlated Phases in Matter:

6. M. D’Alessio et al., Stabilization of sliding ferroelectricity through exciton condensation, *Nature Communications* 17, 5345 (2026).
7. B. Sun et al., Evidence for equilibrium exciton condensation in monolayer WTe₂, *Nature Physics* 18, 94 (2022).

8. S. Ataei et al., Evidence of ideal excitonic insulator in bulk MoS₂ under pressure, *Proc. Natl. Acad. Sci. USA* 118, e2010110118 (2021).
9. D. Varsano et al., A monolayer transition-metal dichalcogenide as a topological excitonic insulator, *Nature Nanotechnology* 15, 367 (2020).
10. D. Varsano et al., Carbon nanotubes as excitonic insulators, *Nature Communications* 8, 1461 (2017).

Materials for Information, Energy and Quantum Technologies, and their Computational Spectroscopies:

11. M. Hernandez Bertran et al, Tracking the Lithiation State of LiSi from Machine-Learned XPS Binding Energies, *npj Computational Materials*, DOI: 10.1038/s41524-026-02302-8, in press (2026).
12. M. Hernandez Bertran et al, Understanding the irreversible lithium loss in silicon anodes using multi-edge X-ray scattering analysis, *Chemistry of Materials* 37, 3648 (2025).
13. M. Zanfrognini et al., Distinguishing Different Stackings in Layered Materials via Luminescence Spectroscopy, *Phys. Rev. Lett.* 131, 206902 (2023).
14. M.G. Betti et al., Dielectric response and excitations of hydrogenated free-standing graphene, *Carbon Trends* 12, 100274 (2023).
15. R. Denk et al., Exciton-dominated optical response of ultra-narrow graphene nanoribbons, *Nature Communications* 5, 4253 (2014).
16. G. Levita et al., Sliding properties of MoS₂ layers: Load and interlayer orientation effects, *J. Phys. Chem. C* 118, 13809 (2014).
17. J. Maultsch et al., Exciton binding energies in carbon nanotubes from two-photon photoluminescence, *Phys. Rev. B* 72, 241402 (2005).
18. P. Ruffieux et al., Electronic Structure of Atomically Precise Graphene Nanoribbons, *ACS Nano* 6, 6390 (2012).
19. E. Chang et al., Excitons in carbon nanotubes: An ab initio symmetry-based approach, *Phys. Rev. Lett.* 92, 196401 (2004).

Biomolecular systems & bio-inspired nanodevices:

20. H. Wu et al, Laterally π -Extended Polyhelicenes, *Journal of the American Chemical Society* 147, 43842 (2025).
21. R. Di Felice et al., DFT study of cysteine adsorption on Au(111), *J. Phys. Chem. B* 107, 1151 (2003).
22. F. Iori et al., GoIP: the Interaction of Proteins With Au(111) Surfaces in Water, *J. Comp. Chem.* 30, 1465 (2009).
23. G. Maruccio et al., Towards Protein Field-Effect Transistors: Report and Model of a Prototype, *Adv. Mater.* 17, 816 (2005).
24. R. Rinaldi et al., Solid-State Molecular Rectifier Based on Self-Organized Metalloproteins, *Adv. Mater.* 14, 1453 (2002).
25. A. Calzolari et al., G-quartet biomolecular nanowires, *Appl. Phys. Lett.* 80, 3331 (2002).

Semiconductor Structures: Electron Correlations, Vibrations & Electron-Phonon Interactions:

26. A. Debernardi et al., Anharmonic phonon lifetimes in semiconductors from density-functional perturbation-theory, *Phys. Rev. Lett.* 75, 1819 (1995).
27. H. Rücker et al., Microscopic calculation of the electron-phonon interaction in quantum-wells, *Phys. Rev. B* 45, 6747 (1992).
28. A. Hartmann et al., Few-particle effects in semiconductor quantum dots: Observation of multicharged excitons, *Phys. Rev. Lett.* 84, 5648 (2000).
29. F. Troiani et al., Exploiting exciton-exciton interactions in semiconductor quantum dots for quantum-information processing, *Phys. Rev. B* 62, R2263 (2000).
30. S. Kalliakos et al, A molecular state of correlated electrons in a quantum dot, *Nature Physics* 4, 467 (2008)
31. R. Zhang et al., How to Identify Plasmons from the Optical Response of Nanostructures, *ACS Nano* 11, 7321 (2017).

Algorithmic & Computational Developments:

32. M. Bonacci et al., Towards high-throughput many-body perturbation theory: efficient algorithms and automated workflows, *npj Comput. Mater.* 9, 74 (2023).
33. D. Leon et al., Efficient full frequency GW for metals using a multipole approach for the dielectric screening, *Phys. Rev. B* 107, 1551 (2023).