Curriculum vitae of Professor Alfonso Pedone (updated 22/04/2026)

Personal data: Born in Atripalda (AV), June 26, 1980
Present Position: Associate Professor in Physical Chemistry at the Department of Chemical and Geological Sciences of the University of Modena and Reggio Emilia since 31 October 2015.
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EDUCATION

- **July 2004** Degree in Chemistry (summa cum laude) at the University of Modena and Reggio Emilia (UniMORE) with a thesis entitled '*Development of algorithms for the rationalization of data coming from Molecular Dynamics Simulations*', under the supervision of Prof. Ulderico Segre and Prof. Maria Cristina Menziani.
- **March 2008** Ph. D. in Chemistry at the UniMORE with a thesis entitled '*Computational Modelling of physical-chemical properties of inorganic amorphous materials*' under the supervision of Prof. Ulderico Segre.

VISITING SCIENTIST

- **May 2005** Visiting scientist at the laboratories headed by Prof. S. Coluccia and Prof. P. Ugliengo at the University of Turin;
- **Sept.-Dec. 2006** Visiting scientist at the lab of Prof. A. N. Cormack at the Alfred University, Alfred, NY, USA
- **April 2008**. Visiting scientist at the lab of Prof. V. Barone at University of Naples.
- **May 2013**. Visiting scientist at the Interdisciplinary Department on Molecular Systems and Materials of the IRAMIS Institute at the Commissariat à l'énergie atomique et aux énergies alternatives (CEA) in Saclay, France.
- **February 2015.** Visiting Scientist at The School of Biological and Chemical Sciences, Queen Mary University College of London, UK.
- **June 2016.** Visiting Scientist at the 'L'école Nationale Superéure de Chimie de Paris, Chemie ParisTech, FR.

PREVIOUS POSITIONS AND FELLOSHIPS

- **From April 2008 to April 2009.** Postdoctoral position at the Department of Chemistry of UniMORE granted by Fondazione Cassa di Risparmio di Modena on a project entitled '*Mechanical and Spectroscopic Properties of silica-based glasses for biomedical applications through computational chemistry methods*'.
- **From April 2009 to December 2010**. Fellowship in theoretical and computational chemistry at the Scuola Normale Superiore of Pisa. The position was granted by Telecom Italia.
- **From December 2010 to 30 October 2015.** Researcher at the Department of Chemical and Geological Sciences of the University of Modena and Reggio Emilia.

NATIONAL SCIENTIFIC ENABLING (ASN):

2012: I got the enabling for the position of Associate Professor in the sector **03/A2** Models and Methodologies for Chemical Sciences and the sector **03/B1** Fundamentals of chemical sciences and inorganic systems.

2013: I got the enabling for the position of Associate Professor in the sector **03/A2** Models and Methodologies for Chemical Sciences and the sector **03/B1** Fundamentals of chemical sciences and inorganic systems.

2017: I got the enabling for the position of Full Professor in the sector **03/A2** Models and Methodologies for Chemical Sciences.
2020: I got the enabling for the position of Full Professor in the sector **03/B1** Fundamentals of chemical sciences and inorganic systems.
2022: I renewed the enabling for the position of Full Professor in the sector **03/A2** Models and Methodologies for Chemical Sciences.

MEMBERSHIPS AND APPOINTMENTS

- Member of the Division of Theoretical and Computational Chemistry (DTCC) of the Italian Chemical Society.
- I have been elected in the governing council of the DTCC for the years 2014-2017.
- Member of the Interuniversity Consortium for Science and Technology of Materials (INSTM)
- Member of the CECAM (Centre Européen de Calcul Atomique et Moléculaire) node of the Scuola Normale Superiore of Pisa.
- Member of the "Virtual Integrated Laboratory for Large-scale Applications in a Geographically distributed Environment" (M3-VILLAGE; http://m3village.sns.it), which is a virtual network with nodes in several University Departments for High Performance Computing.
- Member of the PhD juries of Italian (University of Torino, University of Trieste, Scuola Normale Superiore di Pisa) and Foreign (ChemieParisTech, University of Copenhagen, University of Montpellier, Aalborg University) doctorate schools.
- 2025 Member of the Technical Committee on Atomistic Modelling and Simulations of Glasses of the International Commission of Glass

APPOINTMENTS AT UNIMORE

- Member of the Quality Committee of the Department of Chemical and Geological Sciences from 2016 to 2022.
- Member of the Research Committee of the Department of Chemical and Geological Sciences from 2021 to 2024.
- Member of the Department Council of Chemical and Geological Sciences from 2025 to 2028.
- Coordinator of the PhD School "M3ES" (Models and Methods for Materials and Environmental Sciences) at the Department of Chemical and Geological Sciences, University of Modena and Reggio Emilia, from November 2019 to 2022.
- Member of the University Research Observatory as the representative for the Chemistry area from 2019 to 2023.
- VQR (Research Quality Assessment) representative for the Department of Chemical and Geological Sciences for the periods 2010-2014 and 2015-2019.
- Member of the Doctorate School 'Multiscale Modelling, Computational Simulations and Characterization in Materials and Life Science' of the University of Modena and Reggio Emilia (from the academic years 2010/2011 to 2012/2014)
- Member of the Doctorate School in 'Models and Methods for Materials and Environmental Sciences' of the University of Modena and Reggio Emilia (from 2013/1014)

ORGANISATION OF SCIENTIFIC MEETINGS

- Main/Principal Organizer of the workshop Winter Modeling 2014 in Modena (http://wintermodeling.sns.it/). Winter Modeling is an annual meeting on different topics of

Theoretical and Computational Chemistry allowing young Italian scientist to meet international leading experts in the field.

- Member of the Scientific committee of the XXV National Congress of the Società Chimica Italiana – Division of Theoretical and Computational Chemistry, Rende (CS), 2014
- Member of the Scientific committee of the III National Congress of the Division of Theoretical and Computational Chemistry of the Italian Chemical Society, Roma (RM), 7-12 Settembre 2015
- Member of the Scientific committee of the IV National Congress of the Division of Theoretical and Computational Chemistry of the Italian Chemical Society, Pisa (Pi), 3-5 Ottobre 2016.
- Review editor della rivista open access Frontiers in Materials –Section Glass Science.
- Guest editor of International Journal of Applied Glass Science for the special Issue 'Predicting Glass Structure, Properties and Behaviour: advancements in experimental and computational techniques.' Deadline for submission July 2022.
- Member of the Scientific committee of the XIII Convegno Nazionale sulla Scienza e Tecnologia dei Materiali entitled 'Advanced Materials and Green Processes for a Sustainable Society'. Chair of the session "Material modelling: data sources and computational methods". Sestriere (Italy) 23-26 January 2022.
- Member of the Organizing committee of the 2022 Glass and Optical Materials Division (GOMD) Meeting of the American Ceramic Society, 22-26 May Baltimore, MD (USA).
- Member of the scientific committee and Chair of the Symposium Computational Glass Science del 26° International Congress on Glass, Berlin (Germany), 3-8 July 2022
- Organizing commitee of the VII congress of the Theoretical and Computational Chemistry division of the Italian Chemistry Society. Modena 21-22 September 2022
- Member of the Scientific Committee and Chair of the Symposium 'Atomistic Simulations and Predictive Modeling of Glasses' 2023 Glass and Optical Materials Division (GOMD) Meeting of the American Ceramic Society, 4-9 June, New Orleans, LA (USA).
- Member of the Scientific Committee and Chair of the Symposium 'Atomistic Simulations and Predictive Modeling of Glasses' 2024 Glass and Optical Materials Division (GOMD) Meeting of the American Ceramic Society, 19-23 Maggio, Las Vegas, NE (USA).
- Member of the Scientific Committee and Chair of the Symposium 'Atomistic Simulations and Predictive Modeling of Glasses' 2025 Glass and Optical Materials Division (GOMD) Meeting of the American Ceramic Society, 4-9 Maggio, Vancouver, Canada.
- Member of the Scientific Committee and Chair of the Symposium 7: Computer simulation, machine learning and predictive modeling of the Glass Lyon 2026 conference, which joins together the International Conference of Glass (ICG) - Annual Meeting and the 18th European Society of Glass (ESG) Conference. 13th April - 17th April 2026 at Palais des Congrès in Lyon, France

EDITORIAL ROLES

2018-now Associate Editor of of *Frontiers in Materials* – Section: Glass & Ceramics**,**
2023-now Associate Editor of *Glass Europe Journal*
2023 Guest Editor, *Special Issue of the International Journal of Applied Glass Science* titled **"Glass For Tomorrow"** (2023)
2024-now Editorial Advisory Board **of** *Journal of Non-Crystalline Solids (JNCS) & JNCS-X* (open access companion journal to JNCS)
2026-now Associate Editor of Journal of American Ceramic Society

FUNDING AND PROJECTS

I have actively contributed to the development of several Italian and Europen projects.

- **COFIN2006** (prot. 2006032335) entitled: *Interfacial phenomena in nanostructured biocompatible materials based on silica in contact with biological systems*. (Duration: 2006-2008, Role: member of a local research unit)
- **COFIN2006** (prot. 2006033728) entitled: *Integrated computational strategies for the interpretation of structural and dynamic properties of nanostructured systems through probes spectroscopically active*. (Duration: 2006-2008, Role: member of local research unit)
- **PRIN2008** (prot. 2008J9RNB3) entitled: *Temporal integration for Molecular Evolution*. (Duration: 2008-2010, Role: member of local research unit)
- Internal Project of the Scuola Normale Superiore di Pisa intended for Young researchers (GR PEDONE2010) entitled *Embedded Approaches to Evaluate the Magnetic Parameters of Free Radicals in Condensed Phases*. (Duration: 1 year, Role: coordinator, budget: 5500 €)
- **COST ACTION CM1002** – *CODECS: Converged Distributed Environment for Computational Spectroscopy* (Duration: 22/07/2010 – 24/05/2014, Role: participant of the action). Coordinated by Professor Vincenzo Barone, Scuola Normale Superiore di Pisa.
- Regional Project Emilia Romagna **SPINNER 2013** for PhD. Title: '*Optimization of the crystalline forms of drugs in relation to, bioavailability, patentability and design of solvated polymorphs and co-crystals with low environmental impact methods*'. (Duration: 2012-2015, Role: co-investigator, budget: 48750 €)
- **PRIN 2010** (prot. 2010C4R8M8) entitled: *Functional Organization at the nanoscopic level of (bio)molecules and hybrids for applications in the field of sensors, medicine and biotechnology*. (Duration: 2012-2015, Role: member of research unit)
- **FIRB 2012** (prot. 2012RBFR1248UI) entitled: *New Theoretical/Computational Multiscale Strategies for the Design of Photo and Thermo-responsive Hybrid Organic - Inorganic compounds for nanoelectronic circuits*. (Duration: 2012-2015, Role: coordinator of a local research unit, budget: 313.000 €)
- Bilateral **Project Galileo 2012** of the University Italo-Francese for the mobility of Young researchers. Title of the project: *Investigation of Mo-99 environment in Nuclear Waste Glasses: A synergic computational and experimental approach*. (Duration: 1 January 2013 – 31 December 2013, Role: Coordinator, budget: 2900 €)
- Grant Fondazione Cassa di Risparmio di Modena for the organization of the workshop Winter Modeling 2014 (Role: Coordinator, budget: 3910 €)
- E4 Computer Engineering Spa, Sponsorship to the Workshop Winter Modeling 2014 (900 €).
- **Internal Reseach Grant of UNIMORE – Strategic-Nano** - "The role of cerium oxidation state in bioactive glasses employed as biomaterials for third generation" - Years 2013-2014 Coordinator: Gianluca Malavasi (Role: partecipant, total budget 50.000 €)
- **Internal Research Grant of UNIMORE (FAR 2014)**: "Role of modular phyllosilicates for the capture and storage of CO_2: an experimental and computational investigation". (Role: principal investigator, total budget 28.000 €)
- **PRIN 2015** (prot. 2015XBZ5YA_002) entitled: Toward quantum photovoltaic: ultrafast energy and charge transport in hybrid nanomaterials (Duration: 2016-2018, Role: coordinator of a local research unit, budget: 40167 €)
- **Internal Research Grant of UNIMORE (FAR 2016)**: Innovative (oxide-based) materials and methods for fuel cell electrodes implementation. (Role: partecipant, budget 80.000 €, Coordinator Sergio Valeri)
- **COST ACTION COST CA21109 "Cartan geometry, Lie, Integrable Systems, quantum group Theories for Applications "** (Duration: 14/10/2022 – 13/10/2026, Role: participant of the action). Coordinated by Professor Rita Fioresi.
- **3 INDUSTRIAL PROJECTS** granted by Ashai Glass Co. Japan (starting date January 2019 to June 2023, **206000 €**)
- **Internal Grant of UNIMORE (FAR2020)** for large instrumentation (PI, Budget 45k€)
- **1 IDUSTRIAL PROJECT** granted by SCHOTT Glass (Germany) (PI, 36 k€)

- **PNRR 'ECOSYSTEM FOR SUSTAINABLE TRANSITION IN EMILIA-ROMAGNA'** Spoke 6 - Ecological transition based on HPC and Data Technology (Member of the Spoke Total Budget 2 M€, My budget was 80k€).
- **Internal Research Grant of UNIMORE** on the Strategic Line 'HPC digital design of sustainable materials' (acquisition of a position of Associate Professor of Physical Chemistry, equivalent budget of 78 k€/year)
- **Internal Research Grant of UNIMORE (FAR Interdisciplinare 2024)** Title 'Revolutionizing All-Solid-State Sodium Batteries with Advanced Computational Tools and Mixed Glass Former Effects' (PI, starting date 1/12/2024 – ending date 2/12/2026, budget 80 k€)

HPC Projects

- **CN HPC – Account ID: 1662286.** *Modelling Solid State Electrolytes*
  Host: **LEONARDO_B** Resources: **700,000 GPU hours.** Year: **2025**
- **ISCRA-C6 – Account ID: MLP-SSE** (Origin ID: HP10CQN3S1) *Machine Learning Potentials for Amorphous Solid Electrolytes Based on Sodium for All-Solid-State Batteries*
  Host: **LEONARDO_B.** Resources: **56,000 GPU hours.** Year: **2025**
- **ISCRA-C1 – Account ID: AmElAiML** (Origin ID: HP10C4SSMV) *Modelling Amorphous Solid-State Electrolytes for Sodium-Based All-Solid-State Batteries through Ab Initio and Machine Learning Molecular Dynamics*
  Host: **LEONARDO_B.** Resources: **80,000 GPU hours.** Year: **2024**
- **ISCRA-C – Account ID: ECPASIM** (Origin ID: HP10CLTYQ2) *Exploring Crystallization Pathways in Silicate Melts.*
  Host: **MARCONI100.** Resources: **2,000 node hours.** Year: **2020**
- **ISCRA-C – Account ID: ORAGCEO2** (Origin ID: HP10CPNFM4) *O_2 Reactivity on Clean and Ag-Decorated CeO_2(111)*
  Host: **MARCONI.** Resources: **400,000 CPU hours.** Year: **2019**
- **ISCRA-C11 – Account ID: AUNANMR** (Origin ID: HP10CJ027S) *Size Effects of Gold Nanoparticles on ^{13}C NMR of Bonded Ligands*
  Host: **FERMI.** Resources: **200,000 CPU hours.** Year: **2014**
- **ISCRA-B01 – Account ID: FuSiNBA** (Origin ID: HP10BMIQLW) *Functionalized Silica Nanoparticles for Biomedical Applications*
  Host: **SP6.** Resources: **100,000 CPU hours.** Year: **2011**

AGREEMENTS WITH NATIONAL AND INTERNATIONAL INSTITUTIONS

- **2011** Erasmus Trainsheep with the 'Institut Rayonnement-Matière de Saclay' Centre for the Energy and Commissariat à l'énergie atomique et aux énergies alternatives (IRAMIS-CEA Saclay) for **6 months** period of a Master Student in Chemistry (Elisa Gambuzzi).
- **2014** Erasmus Trainsheep with IRAMIS-CEA Saclay for **9 months** research period of a PhD Student of the M3ES Doctorate (Elisa Gambuzzi).
- **2018** Erasmus Trainsheep with IRAMIS-CEA Saclay for **6 months** period of a Master Student in Chemistry (Federica Lodesani).
- **2019** Erasmus Trainsheep with IRAMIS-CEA Saclay for **6 months** period of a Master Student in Chemistry (Marco Bertani).
- **2022** Erasmus Trainsheep with IRAMIS-CEA Saclay for **6 months** research period of a PhD Student of the M3ES Doctorate (Marco Bertani).

- **2022** Erasmus Trainsheep with IRAMIS-CEA Saclay for **6 months** research period of a PhD Student of the M3ES Doctorate (Federica Lodesani).
- **2024** Erasmus Trainsheep with IRAMIS-CEA Saclay for **6 months** period of a Master Student in Chemistry (Matilde Benassi).
- **2019-now** Erasmus Agreement between UniMORE & University of Strasbourg for exchange of students and researchers.
- **2020-2025** Erasmus Agreement between UniMORE & University of Montpellier for exchange of students and researchers.
- **2025-2028** Agreement for the Joint-Tutoring of PhD Thesis in 'Physics and Chemistry-Physics' stipulated between the University of Modena and Reggio Emilia and the University of Strasbourg.
- **2019-now** Cooperation Agreement between UniMORE and the Universite de Lille for the Implementation of Double PhD Degree between the Models and Methods for Materials and Environmental Sciences (DSCG) and the Ecole Doctorale Sciences de la Matière, du Rayonnement et de l'Environnement (Faculté des Sciences et Technologies).
- **2026** Erasmus+ Agreement for Student Mobility for Trainsheep with Max-Plank Institute for 6 month period of a PhD Student (Matilde Benassi). Host: Prof. Gàbor Csany

VISITING PROFESSORS HOSTED

- **2018 Prof. Gilles Lemercier, Université de Reims Champagne-Ardenne (FR).**
- **2024 Prof. Carlo Adamo, ChiemeParisTech, (FR).**
- **2027 Prof. Steve Martin, Iowa State University (USA).**

ACTIVITIES IN REFERRED SCIENTIFIC JOURNALS.

The candidate is referee of several international scientific journals such as: J. Chem. Theor. Comp., Chem. Mater., J. Phys. Chem. A/B/C, J. Mater. Chem., Phys. Chem. Chem. Phys., Nanoscale, J. Non-Cryst. Solids, Solid State Ionics, Chem. Phys. Lett., Org. Lett., Comp. Mater. Sci, Dalton Transactions, Appl. Surf. Sci., Sensor Actuator.

SELECTED INVITED PRESENTATIONS

1. VIII National Convention Environment Young Research (ARG) Ferrara 19-23 November 2007. '*A new Self-Consistent Interatomic potential model for oxides, silicates and silica based glasses*'
2. 37° Congress of Physical Chemistry of the Italian Chemical Society, Camogli (Genova) 24-29 February 2008. '*Computer Simulations of Chemical Physical Properties of Amorphous Inorganic Materials*'
3. Seminar at the centre of excellence S3 CNR-Nano Department of Physics, University of Modena and Reggio Emilia. 13 March 2008 '*A new Self-Consistent Interatomic potential model for oxides, silicates and silica based glasses*'
4. Workshop Winter Modeling 2011, Scuola Normale Superiore, Pisa, 13-14 January 2011. *Modeling of Novel Nanostructured Materials for Biomedical Applications.*
5. CECAM Workshop 'Brittle Fracture at the atomic scale'. CECAM-HQ-EPFL, Lausanne, Switzerland. 16-19 May 2011. *Modelling structural, elastic and spectroscopic properties of Silica-Based Glasses*
6. XXIV Congress of the Italian Chemical Society, Lecce, 11-16 September 2011 '*The Vincenzo Caglioti Prize and Computational Chemistry*'
7. Workshop Meeting of the COST action CODECS **'**Holistic Computational Spectroscopy: innovative concepts, modern tools, strategic vision and challenges', Pisa, 16-18 November 2012. '*Optical Properties of Dye-Doped Silica Nanoparticles via QM/MM Simulations*'

8. Workshop Winter Modeling 2012, Scuola Normale Superiore, Pisa, 14 February 2012. *Toward The Realistic Modelling of Dye-Doped Silica Nanoparticles.*
9. CECAM Conference: "Energy from the Sun: Computational Chemists and Physicists Take up the Challenge" Chia Laguna resort, Cagliari, Italia, 10-14 September 2012 Excited state properties of solar energy conversion devices based on dye-doped silica nano-structures.
10. 2° Congress of the Theoretical and Computational Chemistry division of the ICS, Padova, 20-22 February 2013. *Computational simulations of solid-state NMR spectra: a new era in structure determination of oxide glasses.*
11. Seminar at the Doctorate School in Chemistry of the University of Padova, 06 June 2013. Excited state properties of dye-doped silica nano-structures.
12. Kyenote al NIS colloquia 'Advances in Biomaterials: combining simulations with experiments' 27-28 November 2013, Torino. *Computational NMR spectroscopy applied to Bioglasses*
13. ElecMol 2014, '7th International Conference on Molecular Electronics' Strasbourg, France 24-29 August 2014. *Effect of the Organic Ligands on the Optoelectronic Properties of Undecagold Nanoclusters.*
14. XXV Congress of the Italian Chemical Society 2014, Rende (CS), Italy 7-12 September 2014. *Effect of the Organic Ligands on the Optoelectronic Properties of Undecagold Nanoclusters.*
15. Workshop Winter Modeling, VIII edition, Scuola Normale Superiore, Pisa, 1-2 December 2014 Structural and Optical Properties of Organically Protected Gold and Silver Nanoclusters
16. Seminar at The School of Biological and Chemical Sciences, Queen Mary University College of London, UK. Data: 04/02/2015 Title: *Toward the realistic modeling of dye-doped silica nanoparticles and organically protected metal nanoclusters*.
17. 2nd International Workshop on Challenges of Atomistic Simulations of Glasses and Amorphous Materials**.** Wuhan, China, June 22-24, 2015, title: *Molecular Dynamics Simulations of uniaxial tensile tests of silica based glasses: from bulk to nanowires.*
18. Workshop 'Nanostructured Metal Optics: from Theory to Enhanced Spectroscopies, Sensing, Imaging' Scuola Normale Superiore, Pisa, 1 April 2016
19. Seminar on the Frontier of the Chemistry at the Scuola Normale Superiore di Pisa for the students of the first years. Pisa, 25/05/2016. Title: 'Molecular Dynamics Simulations of Oxide Glass Structures and Properties'.
20. Plenary Lecture at the workshop Excited States in Complex Systems, ChemieParisTech, 21-23 Novembre 2016. Title: '*Excited State Dynamics of large-size fluorophores in water solvent and embedded in silica nanoparticles*'.
21. XXVI Congresso della Società Chimica Italiana, Paestum (SA), 10-14 September 2017. Title: From First-Principle Chemical Shift and EFG Tensors Calculations to Solid-State 1D and 2D NMR Spectra Simulations of Complex Systems.
22. Seminar at the Nano-Science Center of the University of Copenaghen, 13 October 2017. Title: *Computational NMR Spectroscopy applied to Material Science.*
23. Plenary Lecture at the 2018 Glass and Optical Materials Division (GOMD) Meeting of the American Ceramic Society, 20-24 May San Antonio, Texas (USA). Title: *Bioactive Glass Structure determination via Molecular Dynamics Simulations and NMR-DFT calculations*.
24. 25th International Congress on Glass (ICG2019). Title: Molecular Dynamics Simulations and DFT-GIPAW calculations of sodium borosilicate glasses. Boston, June 9-14, 2019.
25. Lecture at the GIDRM Conference 2019 entitled 'Computational methods and NMR Spectroscopy: a powerful synergy for chemistry, materials science and biology. Title of the presentation: Computational NMR spectroscopy as a new tool to probe materials structure. 10 December 2019, Pisa.
26. Seminar at the Scuola Normale Superiore di Pisa for the students of the first years. Pisa, 16/07/2021. Title: 'Molecular Modelling of Bioactive Glasses'. (online)
27. KeyNote Lecture at the XXVII Congress of the Italian Chemical Society. Title 'Exploiting Machine Learning Methods in Atomistic Simulations of Oxide Glasses'. 17 September 2021

28. Seminar at the The State University of New Jersey, department of Materials Science and Engineering (New Jersey). Title of the Presentation 'New Advances in Atomistic Modelling of Oxide Glasses' 7 December 2021.
29. Keynote Lecture al 26° International Congress on Glass. Berlino 3-8 Luglio 2022. Titolo: '*Predicting Structure Properties and Behavior of Oxide Glasses Through Molecular Dynamics Simulations*'.
30. Keynote Lecture al 2° ELSICS Workshop 'Energy Landscapes and Structure of Ion Conducting Solids', Gottingen 26-28 Settembre 2022. Titolo: *Ionic Transport in Oxide Glasses'*
31. Invited talk al 'Winter Modeling 2023 - New frontiers in astrochemistry and astrobiology', Napoli, 23-24 Febbraio 2023. Titolo: *Modelling Structure and Properties of Oxide Glasses: the role of the interatomic potentials models.*
32. Invited Lecture at the Symposium 'Glass and Interactions with Its Environment' 2023 Glass and Optical Materials Division (GOMD) Meeting of the American Ceramic Society, 4-9 Giugno New Orleans, LA (USA). Titolo: *Unravelling the Structural Role of Doping Cations in Bioactive Glasses through Molecular Dynamics Simulations.*
33. 4th International Workshop on Challenges of Atomistic Simulations of Glasses and Amorphous Materials**.** Corning, NY (USA), July 13-15, 2023, title: *Interatomic Potentials Models for Oxide Glasses: Our Experience.*
34. MolSimEng 2023 Milan, October 6, 2023. Title: *Revolutionizing glass design: molecular dynamics simulations for multicomponent oxide glasses and challenges ahead.*
35. ICG Spring School 2024 : Glass for a sustainable future: How can glass scientists help meet the challenge? 29 Apr-3 May 2024 Lloret de Mar (Spain). Title: *Modern Computational Methodologies for Glass Developments*
36. 15th International Conference on the Structure of Non-Crystalline Materials. 15-19 July Cambridge (UK). Title: Unraveling the mysteries of glass structure: insights from atomistic simulations.
37. XXVIII Congresso Nazionale della Società Chimica Italiana, Milano, 26-30 agosto 2024. Title: *Enhancing Atomistic Simulations of Oxide Glasses Through the Power of Machine Learning*.
38. 51st National Congress on Magnetic Resonance, Firenze 4-6 Settembre 2024. Title: *Advancement in the simulation of Solid-State NMR Spectra of Oxide Glasses: Integrating ab initio calculations with Machine Learning*.
39. Invited Lecture at the Symposium 'Data-Driven Modeling and Machine Learning for Glass Science' 2025 Glass and Optical Materials Division (GOMD) Meeting of the American Ceramic Society, 4-9 Maggio Vancouver, Canada. Titolo: *Harnessing Machine Learning Potentials for Glass Science: From Oxide Glasses to Sodium-based Solid Electrolytes.*
40. 1st ACee-GISEL Joint Conference, Padova (Italy) 21-23 July 2025 title: *Structure and Properties of Sodium-Phosphorous Oxysulfides Electrolytes for Sodium All-Solid-State Batteries.*
41. 5th International Workshop on Challenges of Atomistic Simulations of Glasses and Amorphous Materials**.** *Yokohama, Japan, August 6-8, 2025, title: Exploring Glassy Materials with Machine Learning Potentials: From Oxide Networks to Sodium-based Solid Electrolytes*
42. Lecture at Aalborg University, Denmark, October 9*, 2025, title: Exploring Glassy Materials with Machine Learning Potentials: From Oxide Networks to Sodium-based Solid Electrolytes.*
43. Invited Talk at the conference 'Beyond the Quantum Year: Theoretical Chemistry Meets the Scuola Superiore Meridionale', Naples 4-6 February 2026. Title: *Machine Learning Interatomic Potentials for NaPSO glass electrolytes: Opportunities and limitations of Universal Models.*
44. Invited Talk at Glass Lyon 2026 conference 13th April - 17th April 2026 at Palais des Congrès in Lyon, France. Title: *Decoding Medium-Range Order in Sodium Oxysulfide Glasses: Dataset Sensitivity of Machine Learning Interatomic Potentials.*
45. Lecture at the FOURTH SÃO CARLOS SCHOOL ON GLASSES AND GLASS-CERAMICS April 27 – May 1, 2026. São Paulo and São Carlos, Brazil. Title: *ML potentials and glass simulation.*

46. Invited talk at 23rd International Symposium on Non-Oxide and new Optical Glasses (ISNOG) June 14-17, 2026. DGI Byen, Copenhagen, Denmark. Title: *Unraveling the Mixed Glass Former Effect in Sodium Thiophosphate Glass Electrolytes: A Molecular Dynamics Perspective.*
47. Invited talk at 40th Şişecam International Glass Conference Istanbul (Turkey) 18-19 June 2026. Title: *Challenges in Atomistic Simulations of Glasses and Amorphous Materials.*
48. Invited talk at 1st Chinese–Italian Symposium on Frontiers in Materials Chemistry Fuzhou (Cina) 24-27 June 2026. Title: *Challenges in Atomistic Simulations of Glasses and Amorphous Materials.*
49. Lecture at first school on "Chemistry through the eyes of AI and ML". Turin 7-11 September 2026. Title: "AI Methods for interatomic models and materials".

INTERNATIONAL PRIZES/ AWARDS/ACADEMY MEMBERSHIPS

- MODENA ROTARY CLUB prize titled "The best scientific brains in chemistry, physics and mathematics", **2005**.
- "*Primo Levi*" Prize for the best young Italian researcher in chemistry released by the Italian Chemical Society, **2006**.
- Best Poster award at the Winter Modeling workshop, Pisa, **2010**. Title of the poster: '*Modeling Optical Properties of Fluorophores in different Environments*'
- Best Poster award at the Congress of the Chemical Physics Division of the Italian Chemical Society, Stresa (Verbania), **2010**. Title of the poster:' *Absorption and Emission Spectra of Fluorophores encapsulated in nanoparticles*'.
- '*Vincenzo Caglioti*' Prize released by the Accademia Nazionale dei Lincei (Rome), for the best young Italian researcher in chemistry under 35 years old, **2011**.
- Medal 'Eolo Scrocco' released by the Computational and Theoretical Chemistry division of the Italian Chemical Society, **2012**.
- Prize 'Roetti' released by the Computational and Theoretical Chemistry division of the Italian Chemical Society, **2017**.
- **Top 2% Scientist Worldwide (Career Impact)** Ranked among the top 2% of scientists worldwide based on career-long citation impact, according to the Stanford University–Elsevier ranking for 5 consecutive years (**2020–present**).

SUPERVISION OF PhD STUDENTS AND POSTDOCTORAL FELLOWS

- **2012-2014.** Supervisor of one Ph.D. Student, Dr. Elisa Gambuzzi working on a thesis entitled '*Computational Modeling of Oxide Glasses*'.
- **2012-2014.** Co-Tutor of one Ph.D. Student, Dr. Davide Presti who is working on a thesis entitled '*Computational strategies for the study of pharmaceutical molecular crystals*'
- **2013-2017.** Supervisor of one post-doctoral fellow, Dr. Francesco Muniz Miranda working on a project entitled '*Computational investigation of optoelectronic properties of organically protected gold nanoclusters*'.
- **2014-2016.** Co-tutor of a Ph.D. Student, Dr. Tavanti Francesco working on a thesis entitled '*Computational Modeling of Nanoparticle-Protein interactions*'.
- **2015-2016.** Supervisor of a post doctoral fellow, Dr. Elisa Gambuzzi. Title of the project: '*Development and application of new computational protocols for the investigation of hybrid nanomaterials*
- **2016-2017.** Supervisor of a post doctoral fellow, Dr. Davide Presti. Title of the project: '*Role of modular phyllosilicates for the capture and storage of CO_2: an experimental and computational investigation*'
- **2017-2019.** Co-Tutor of one Ph.D. Student, Dott. Luca Brugnoli working on a thesis entitled '*Computational study of fuel cell components'*.

- **2017-2018.** Tutor of post doctoral fellow, Dr. Mariagrazia Fortino. Title of the project: Computational investigation of the spectroscopic properties of organic molecules used in the hybrid-photovoltaic cells.
- **2019-2022.** Supervisor of one Ph.D. Student, Dott.ssa Federica Lodesani working on a thesis entitled '*Computer Simulation of nucleation and crystallization of silicate glasses'*.
- **2020-2023.** Supervisor of one Ph.D. Student, Dott. Marco Bertani working on a thesis entitled '*Exploiting machine learning techniques in computational simulations of oxide glasses*.
- **2020-2022.** Tutor of post-doctoral fellow, Dr. Luca Brugnoli. Title of the project: *Development of ReaxFF for Ceria/Silica interactions*.
- **2022-2025** Supervisor of a PhD student, Dott.ssa Annalisa Pallini. Title of the project: '*Understanding Composition-Structure-Property Relationships to Design Ultra Strong AluminoSilicate Glasses*.
- **2022-2023.** Supervisor of a post-doc, Dott.ssa Federica Lodesani. Title of the project '*Studio del meccanismo di nucleazione e cristallizzazione in silicati fusi*'.
- **2023-2025.** Supervisor of a Post-doc, Dr. Marco Bertani. Titolo progetto '*Verso la comprensione delle relazioni struttura-conduttività in elettroliti solidi amorfi per batterie a stato solido di nuova generazione*'.
- **2024-2026.** Supervisor of a PhD Student, Dott.ssa Matilde Benassi. Title '*Machine Learning Potentials for Amorphous Solid Electrolytes for All Solid State Batteries*'.
- **2025-2026.** Supervisor of a Post-doc, Dr. Marco Bertani. Title 'Development of Machine Learning Interatomic Potentials for sodium based solid electrolytes.**'**.
- **2025-2026.** Supervisor of a Post-doc, Dr Michael Alejandro Hernandez Bertran. Title of project 'Determination of the structure-properties relationships in sodium-based solid electrolytes through computational techniques.'
- **2025-2028** Supervision of PhD Student, Dott. Antonio Familiari. Title: Advanced first-principles and machine learning modelling of polyanionic glasses and glass-ceramics for energy storage applications. Thesis in co-tuturing with Prof. Guido Ori, CNRS Strasburg (FR).

TEACHING ACTIVITIES

- Teacher of the course: *Physical Chemistry 1 - Thermodynamics* (9 CFU) at the master of science in Chemistry, UniMORE (from the academic years 2015/2016 to now)
- Teacher of the course: *Physical Chemistry and Spectroscopy* (6 CFU) at the master of science in Chemistry, UniMORE (from the academic years 2016/2017 to now)
- Teacher of the course: *General Chemistry* (9 CFU) at the master of science in Natural Sciences, UniMORE (academic years 2011/2012 – 2012/2013 – 2013/2014 - 2014/2015)
- Teacher of the course*: Methods in modelling and Multiscale Simulations* at the doctorate school in Multiscale Modelling, Computational Simulations and Characterization in Materials and Life Science, UniMORE, since 2011.
- Teacher of the course: *Inorganic Environmental Chemistry* at the Master of Science in Natural Sciences, UniMORE (a.y. 2010/2011).
- Teacher of the course: *Computational Modeling of Bio- and Nano-systems* at the master course of Chemistry, Scuola Normale Superiore of Pisa (a.y. 2008/2009 and 2009/2010)

MAJOR COLLABORATIONS

The PI collaborates with research groups of other Italian and foreign universities and research institutes on scientific projects that fall within the goals of the new EU funding program for research, Horizon 2020.

(1) Prof. Steve Martin (Iowa University, USA) Topic: Solid State Electrolytes for All Solid State Batteries.

(2) Prof. Ashutosh Goel (Rutgers University, USA) Topic: Quantitative Structure Properties Relationships in Bioactive Glasses.
(3) Dr. Shingo Urata (AGC Inc., Japan) Topic: Simulation of Nucleation and Crystallization in Silicate Glasses, Mechanochemical Polishing of Glass Surfaces
(4) Prof. Vincenzo Barone (DREAMSLAB at Scuola Normale Superiore of Pisa, ITALY) Topic: Development of integrated computational strategies for computational spectroscopy.
(5) Prof. Luca Prodi and Dr. Marco Montalti (Photochemical Nanoscience Lab, Dept. of Chemistry of the University of Bologna, ITALY) Topic: Computational and Experimental Characterization of the photphysical properties of dye-doped silica nanoparticles.
(6) Prof. Angela Agostiano (University of Bari and Head of the Bari division of the Institute for physico-chemical processes of the Italian National Council of Research – IPCF-CNR) Topic: Investigation of protein-nanoparticles interactions.
(7) Dr. Thibault Charpentier (Commissariat à l'énergie atomique et aux énergies alternatives, Saclay, FRANCE) Topic: Experimental and Computational Solid-State NMR characterization of oxide glasses
(8) Prof. A. J. Salinas (Departamento de Quimica Inorganica y Bioinorganica, Facultad de Farmacia Universidad Complutense, 28040 Madrid, Spain) Topic: Experimental and computational investigation of Biomaterials.
(9) Dr. Antonio Tilocca (University College of London, UK) Topic: Car-Parrinello Molecular Dynamics Simulations of bioglasses
(10) Prof. A. N. Cormack (Kazuo Inamori School of Engeneering, Alfred University, Alfred, NY, USA). Topic: Simulation of Mechanical Properties of Oxide Glasses
(11) Prof. Carlo Adamo (Chemie ParisTech, France) Topic: Optical Properties of Photochromic Molecular Crystals
(12) Prof. Piero Ugliengo (University of Turin) Topic: Investigation of Drug-delivery systems based on the MCM-41.

This is a non-exhaustive list of all the ongoing collaborations established with other Italian and foreign institutions. (*see my web page for more information*)

SCIENTIFIC LEADERSHIP PROFILE

Research activity in the field of computer simulations based on classical, quantum mechanical and multiscale methods applied to the study of inorganic materials (zeolites, clays, glasses and glass-ceramics), organic molecular crystals and nanomaterials for applications in the field of nano medicine, biomaterials, nanoelectronics, energy conversion, and confinement of radioactive waste.

The main research topic is the simulation of multicomponent oxide glasses and glass-ceramics. In particular the development and application of methods to simulate the structure, transport properties (ionic conductibility, mobility, viscosity etc…), electronic properties, mechanical properties (elastic moduli and fracture mechanisms), thermodynamical properties, chemical durability (surface reactivity) and crystal nucleation.

I am also interested in computational spectroscopy in general, i.e. development of protocols and codes for the simulation of solid state NMR spectra, computation of NMR and EPR parameters of organic radicals embedded in different environments and hydrid organic-metal nanoparticles, simulation of UV-Vis absorption and emission spectra of dye molecules in solutions and embedded in different inorganic matrices.

The domain of competence includes: i) Density Functional Theory (DFT) and Time-Dependent DFT; ii) First principles Molecular Dynamics Simulations; iii) Molecular Mechanics, Classical Molecular Dynamics Simulations; iv) Hybrid QM/QM' and QM/MM methods; v) Metadynamics; vi) Development of accurate Force-Field parameters; vii) Coarse Grain Molecular Dynamics Simulations.

The scientific activity of Prof. Pedone and its leadership in the field of theoretical/computational chemistry is witnessed by the large number of contributions to the most important scientific journals in chemistry, with special reference to chemical physics, theoretical chemistry and material chemistry.
He has co-authored more than 160 papers published in international journals and seven book chapters. Moreover, he has delivered more than 40 invited lectures in Italian and foreign institutions.
His papers have received over 6500 citations on the Scopus database (over 7700 in Google Scholar) and he has h-index = 43 (49, Google scholar). Finally, I am consistently ranked among the top 2% of scientists worldwide since 2020, according to the Stanford University–Elsevier global ranking based on standardized citation metrics.

LIST OF SCIENTIFIC PUBLICATIONS ON INTERNATIONAL JOURNALS WITH IF.

		Quartile (Scopus)
1	Lusvardi, G.; Malavasi, G.; Menabue, L.; Menziani, M. C. **Pedone, A.** and Segre, U.. *A Computational Tool for the Prediction of Crystalline Phases Obtained from Controlled Crystallization of Glasses*. **J Phys. Chem. B** (2005), 109(46), 21586-21592, DOI: 10.1021/jp0546857	Q1
2	Malavasi, G.; Menziani, M. C.; **Pedone, A.** and Segre, U. *Void size distribution in MD-modelled silica glass structures.* **J. Non-Crys. Sol.** (2006), 352(3), 285-296. DOI: 10.1016/j.jnoncrysol.2005.11.022	Q1
3	**Pedone, A.**; Malavasi, G.; Menziani, M. C.; Cormack, A. N.; Segre, U. *A New Self-Consistent Empirical Interatomic Potential Model for Oxides, Silicates, and Silica Based Glasses*. **J. Phys. Chem. B** (2006) 110, 11780-11795. DOI: 10.102/jp0611018	Q1
4	Lusvardi, G; Malavasi, G; Menabue, L.; Menziani, M. C. **Pedone, A.** and Segre, U. *Density of multicomponent silica-based potential bioglasses: quantitative structure-property relationships (QSPR) analysis.* **J. Eur. Cer. Soc.** 27 (2007) 499-504. DOI: 10.1016/j.jeurceramsoc.2006.04.067	Q1
5	Malavasi, G; **Pedone A.** and Menziani M. C. *Towards a quantitative rationalization of multicomponent glass properties by means of Molecular Dynamics Simulations*. **Molecular Simulation** (2006) 32(10), 1045-1055. DOI: 10.1080/08927020600932793	Q2
6	Malavasi, G.; Menziani, M. C.; **Pedone, A.**; Civalleri, B., Corno, M. and Ugliengo P. *A computational multiscale strategy to the study of amorphous materials.* **Theor. Chem. Acc.** 2007, 117(5-6), 933-942. 10.1007/s00214-006-0214-1	Q3
7	**Pedone, A.**; Malavasi, G., Cormack, A. N., Segre, U. and Menziani, M. C.. *Insight into elastic properties of binary alkali-silicate glasses; prediction and interpretation through atomistic simulation techniques.* **Chem. Mater.** 2007, 19(13),3144-3154. DOI: 10.1021/cm062619r	Q1
8	**Pedone, A.**; Corno, M.; Civalleri, B.; Malavasi, G., Menziani, M. C.; Segre, U. and Ugliengo P. *An ab initio parameterized interatomic force field for Hydroxyapatite.* **J. Mater. Chemistry** 2007, 17, 2061-2068 DOI:1039/b617858h	Q1

9	Malavasi, G.; Lusvardi, G.; **Pedone**, A.; Menziani, M. C.; Doppiaggi, M.; Gualtieri, A.; Menabue, L.. *Crystallization Kinetics of Bioactive Glasses in the ZnO-Na2O-CaO-SiO2 System*. **J. *Phys. Chem A*** *(2007) 111(34), 8401-8408* DOI: 10.1021/jp071528u	Q2
10	Linati, L.; Lusvardi, G.; Malavasi, G.; Menabue, L., Menziani, M. C.; Mustarelli, P., **Pedone, A** and Segre U. *Medium range order in phospho-silicate bioactive glasses: insights from MAS-NMR spectra, Chemical durability experiments and Molecular Dynamics Simulations*. **J. Non- Cryst. Sol.** (2008) 354, 84-89 DOI: 10.1016	Q1
11	**Pedone**, **A.**; Malavasi, G.; Menziani, M. C.; Segre, U.; Musso, F.; Corno, M.; Civalleri, B.; Ugliengo, P. *FFSiOH: a new Force Fields for Silica Polymorphs and their Hydroxylated Surfaces based on Periodic B3LYP calculations*. **Chem. Mater.** 20 (7), 2522-2531, 2008.	Q1
12	**Pedone**, **A.**; Malavasi; G. Cormack, A. N.; Segre, U.; Menziani, M. C. *Elastic and dynamical properties of alkali silicate glasses from computer simulation techniques*. **Theor. Chem. Acc.** (2008) 120(4-6), 557-564. *DOI: 10.1007/s00214-008-0434-7*	Q3
13	Lusvardi, G.; Malavasi, G.; Menabue, L.; Menziani, M. C.; **Pedone**, A.; Segre, U.; Aina, V.; Petardi, A.; Morterra, C.; Boccafoschi, F.; Gatti, S.; Borsetti, M.; Cannas, M. *Properties of zinc releasing surfaces for clinical applications*. **Journal of Biomaterials Applications** (2008), 22(6), 505-526. DOI :10.1177/088532820?079731	Q2
14	Andreoli R.; Castellini E.; Malavasi, G.; **Pedone, A.** *Deflocculant effects on surface properties of Kaolinite investigated through malachite green adsorption*. **Colloids and Surfaces A: Physicochemical and Engineering Aspects** (2008), 329(1-2), 31-37. DOI:10.1016/j.colsurfa.2008.06.045	Q1
15	**Pedone**, **A.**; Malavasi, G.; Menziani, M. C.; Segre, U.; Cormack, A. N. *Role of Magnesium in Soda-Lime Glasses: Insight into Structural, transport and Mechanical Properties through computer simulations*. **J. Phys. Chem. C** (2008), 112(29), 11034-11041. DOI:10.1021/jp8016776	Q1
16	**Pedone**, **A.**; Malavasi, G.; Menziani, M. C.; Segre, U.; Cormack, A. N. *Molecular Dynamics studies of the stress-Strain Behaviour of Silica Glass under Tensile Load*. **Chem. Mater.** (2008) 20(13), 4356-4366. DOI:10.1021/cm800413v	Q1
17	Lusvardi, G.; Malavasi, G.; Cordata, M.; Menabue, L.; Menziani, M. C., **Pedone, A**.; Segre, U. *Elucidation of the Structural role of Fluorine Potential Bioactive Glasses by Experimental and Computational Investigation.* **J. Phys. Chem. B** (2008) 112(40), 12730-12739. DOI:10.1021/jp803031z	Q1
18	Corno, M.; **Pedone, A**.; Dovesi, R. and Ugliengo P. *B3LYP Simulation of the Full Vibrational Spectrum of 45S5 Bioactive Silicate Glass compared to v-Silica*. **Chem Mater.** (2008), 20(17), 5610-5621. DOI:10.1021/cm801164u	Q1
19	**Pedone, A**. ; Pavone, M. ; Menziani, M. C. and Barone, V. *Accurate First-Principle Prediction of ^{29}Si and ^{17}O NMR Parameters in SiO_2 polymorphs: The cases of zeolites Sigma-2 and Ferrierite.* **J. Chem. Theo. Comp.**. (2008), 4, 2130-2140. DOI:10.1021/ct8003035	Q1

20	Lusvardi, G.; Malavasi, G.; Tarsitano, F., Menabue, L.; Menziani, M. C., **Pedone, A**. *Quantitative Structure-Property Relationships of Potentially Bioactive Fluoro Phospho-Silicate Glasses.* **J Phys Chem B**, (2009) 113, 10331-10338. DOI:10.1021/jp809805z	Q1
21	Corno, M., **Pedone, A.** *Vibrational features of phosphor-silicate glasses: Periodic B3LYP Simulations*. **Chemical Physics Letters**, (2009), 476, 218-222. DOI:10.1016/j.cplett.2009.06.039	Q2
22	**Pedone, A.**; Malavasi, G.; Menziani, M. C. *Computational Insight Into the Effect of CaO/MgO Substitutions on the Structural Properties of Phospho-silicate Bioactive Glasses.* **J. Phys. Chem. C**, (2009), 113, 15723-15730. DOI:10.1021/jp904131t	Q1
23	**Pedone, A**. *Properties Calculations of Silica-Based Glasses by Atomistic Simulations Techniques: A review*. **J. Phys. Chem. C**, (2009), 113, 20773-20784. DOI:10.1021/jp9071263	Q1
24	Pota, M.; **Pedone, A.**, Malavasi, G.; Durante, C.; Cocchi, M.; Menziani, M. C. *Molecular Dynamics Simulations of Sodium Silicate Glasses: Optimization and Limits of the Computational Procedure.* **Computational Materials Science and Engineering**. (2010), 47, 739-751 DOI:10.1016/j.commatsci.2009.10.017	Q1
25	**Pedone, A**.; Bloino, J.; Monti, S.; Prampolini, G.; Barone, V. *Absorption and Emission UV-Vis Spectra of the TRITC Fluorophore molecule in solution: a quantum mechanical study*. **Phys. Chem. Chem. Phys. (**2010) 12, 1000-1006, DOI:10.1039/b920255b	Q1
26	**Pedone**, **A**.; Barone, V. *Unraveling Solvent Effects on the Electronic Absorption Spectra of TRITC Fluorophore in Solution: a Theoretical TD-DFT/PCM study*. **Phys. Chem. Chem. Phys.** 2010, 12, 2722-2729. DOI:10.1039/b923419e	Q1
27	Cimino, P.; **Pedone, A**.; Stendardo, E.; Barone, V. *Interplay of stereo-electronic, environmental, and dynamical effects in determining the EPR parameters of aromatic spin-probes: INDCO as a test case.* **Phys. Chem. Chem. Phys.** 2010, 12, 3741-3746.	Q1
28	**Pedone, A.;** Biczysko, M.; Barone, V. *Environmental Effects in Computational Chemistry: Accuracy and Interpretations.* **ChemPhysChem** (2010)**,** 11, 1812. DOI:10.1002/cphc.200900976	Q1
29	**Pedone, A**.: Charpentier, T.; Menziani, M. C. *Multinuclear NMR study of the $CaSiO_3$ Glass: Simulation from first principles.* **Phys. Chem. Chem. Phys.** (2010), 2010, 12, 6054 – 6066, DOI: 10.1039/b924489a	Q1
30	Barone, V.; Bloino, J.; Monti, S.; **Pedone, A**.; Prampolini, G. *A Theoretical Multi-level Approach for the Study of Optical Properties of Organic Dyes in Solution*. **Phys. Chem. Chem. Phys.** 12, 2010, 10550–10561**,** DOI: 10.1039/c002722g	Q1
31	Barone, V.; Cimino, P.; **Pedone, A.** *An integrated computational protocol for the accurate prediction of EPR and PNMR parameters of nitroxide radicals in solution.* **Magnetic Resonance in Chemistry,** 2010, 48, S11-S22. DOI 10.1002/mrc.2640	Q2
32	Stendardo, E.; **Pedone, A**.; Cimino, P.; Menziani, M. C.; Crescenzi, O.; Barone, V. *Extension of the AMBER Force-Field for the Study of Large Nitroxides in*	Q1

	Condensed Phases: An ab initio Parameterization. **Phys. Chem. Chem. Phys.** 2010, 12, 11697 – 11709	
33	**Pedone, A.**; Charpentier, T.; Malavasi, G.; Menziani, M. C. *New Insights into the Atomic Structure of 45S5 Bioglass by means of Solid-State NMR Spectroscopy and Accurate First-Principles Simulations.* **Chem. Mater. ,** 2010, 22, 5644-5652 **DOI:** 10.1021/cm102089c	Q1
34	Barone, V.; Bloino, J.; Monti, S.; **Pedone, A.**; Prampolini, G. *Fluorescence Spectra of Organic Dyes in Solution: A Time Dependent Multilevel Approach* **Phys. Chem. Chem. Phys.**, 2011, 13, 2160-2166. DOI: 10.1039/c0cp01320j.	Q1
35	Christie, J. K.; **Pedone, A**.; Menziani, M. C.; Tilocca, A. *The fluorine environment in bioactive glasses: ab initio molecular dynamics simulations.* **J. Phys. Chem. B,** 2011**,** 115, 2038-2045, DOI:10.1021/jp110788h.	Q1
36	Ori, G.; Montorsi, M.; **Pedone, A**.; Siligardi, C. *Insight into the Structure if Vanadium containing Glasses: a Molecular Dynamics Study.* **J. Non-Crys. Sol.,** 2011 357**,** 2571–2579 DOI:10.1016/j.jnoncrysol.2011.02.002.	Q1
37	**Pedone, A.**; Prampolini, G.; Monti, S.; Barone, V**.** *Absorption and Emission Spectra of Fluorescent Silica Nanoparticles from TD-DFT/MM/PCM calculations.* **Phys. Chem. Chem. Phys. 2011, 13, 16689–16697** DOI:10.1039/C1CP21475F.	Q1
38	**Pedone, A**.; Prampolini, G.; Monti, S.; Barone, V.*; Realistic Modelling of fluorescent Dye-Doped silica nanoparticles: A Step Toward the Understanding of their Enhanced Photophysical Properties.* **Chem. Mater.** 2011, 23, 5013-5023**.**	Q1
39	**Pedone, A**.; Gambuzzi, E.; Malavasi, G.; Menziani M. C. *First-Principles Simulations of the ^{27}Al and ^{17}O Solid State NMR spectra of the $CaAl_2Si_3O_{10}$ glass.* **Theor Chem Acc** 2012, 131, 1147, DOI: 10.1007/s00214-012-1147-5	Q3
40	Biczysko, M.; Bloino, J.; Brancato, G.; Cacelli, I.; Cappelli, C.; Ferretti, A.; Lami, A.; Monti, S.; **Pedone, A.**; Prampolini, G.; Puzzarini, C.; Santoro, F.; Trani, F.; Villani, G. *Integrated computational approaches for spectroscopic studies of molecular systems in the gas phase and in solution: pyrimidine as a test case.* **Theor Chem Acc** 2012, 131,1201, DOI: 10.1007/s00214-012-1201-3	Q3
41	**Pedone, A.**; Charpentier, R.; Menziani, M. C. *The structure of fluorine containing Bioactive Glasses: new insights from First-Principles Calculations and Solid State NMR Spectroscopy***. J. Mater. Chem.** 2012, 22, 12599-12608 DOI: 10.1039/C2JM30890H.	Q1
42	**Pedone, A**.*;* Presti, D.; Menziani, M. C. *On the ability of Periodic Dispersion-Corrected DFT Calculations to Predict Molecular Crystal Polymorphism in para-diiodobenzene.* **Chem. Phys. Lett.** 2012**,** 541, 12-15.	Q2
43	**Pedone, A**.; Gambuzzi, E.; Menziani M. C. *Unambiguous description of the oxygen environment in multicomponent aluminosilicate glasses from ^{17}O Solid State NMR computational spectroscopy.* **J. Phys. Chem. C**. 2012, 116, 14599-14609	Q1
44	Salvadori, E.; Di Valentin, M.; Kay, C. M. W.; **Pedone, A**.; Barone V.; Carbonera D. *The Electronic Structure of the Lutein Triplet State in Plant Light-Harvesting Complex II.* **Phys. Chem. Chem. Phys**. 2012, **14**, 12238–12251	Q1

45	**Pedone, A**.*;* Bloino, J.; Barone, V. *Role of Host-Guest Interactions in Tuning the Optical Properties of Coumarin Derivatives Incorporated in MCM-41: A TD-DFT Investigation.* **J. Phys. Chem. C,** 2012, 116, 17807−17818	Q1
46	Grubisic, S.; Brancato, G.; **Pedone, A.**; Barone, V. *Extension of the AMBER force field to cyclic α, α dialkylated peptides*. **Phys. Chem. Chem. Phys.,** 2012**,** 14, 15308-15320 **DOI:** 10.1039/C2CP42713C	Q1
47	Malavasi, G.; **Pedone, A.**; Menziani, M. C. *The study of the structural role of gallium and aluminium in 45S5 Bioactive glasses from computer simulations.* **J. Phys. Chem. B**, 2013, 117, 4142-4150. DOI: 10.1021/jp400721	Q1
48	Berardo, E.; **Pedone, A.**; Ugliengo, P.; Corno, M. *DFT modeling of 45S5 and 77S soda-lime phospho-silicate glass surfaces: clues on different bioactivity mechanism*. **Langmuir**, 2013, 29, 5749-5759. DOI: 10.1021/la304795w	
49	Charpentier, T.; Menziani, M. C.; **Pedone, A.** *Computational simulations of solid state NMR spectra: a new era in structure determination of oxide glasses*. **RSC Advances.** 2013, 3 (27), 10550 – 10578 DOI: 10.1039/C3RA40627J	Q1
50	**Pedone, A.;** Gambuzzi, E.; Barone, V.; Bonacchi, S.; Genovese, D.; Rampazzo, E.; Prodi, L.; Montalti, M. *Undestanding the photophysical properties of coumarin-based Pluronic-Silica (PLUS) silica nanoparticles by means of time-resolved emission spectroscopy and accurate TDDFT/stochastic calculations.* **Phys. Chem. Chem. Phys.,** 2013**,** 15, 12360-12372	Q1
51	Malavasi, G.; Menabue, L.; Menziani, M. C.; **Pedone, A**.; Salinas, A.; Vallè-Regi, M. *The bioactivity of SiO_2–CaO and SiO_2–CaO–P_2O_5 glasses explained by molecular dynamic simulations.* **J. Sol-Gel Sci. Technol.** 2013, 67:208-219 DOI 10.1007/s10971-011-2453-4**.**	Q2
52	**Pedone, A.** *The Role of the Solvent on Charge Transfer in 7-aminocoumarin dyes: new hints from TD-CAM-B3LYP and State Specific PCM calculations***. J. Chem. Theo. Comp.** 2013, 9, 4087-4096 DOI: 10.1021/ct4004349	Q1
53	Ferrara, C.; Tealdi, C.; Mustarelli, P.; **Pedone, A.**; Menziani, M. C. *Local versus average structure in $LaSrAl_3O_7$: a NMR and DFT investigation*. **J. Phys. Chem. C** 2013, 117 (45), 23451–23458	Q1
54	Presti, D.; **Pedone, A.**; Menziani, M. C.; Civalleri, B.; Maschio, L. *Oxalyl Dihydrazide Polymorphism: a Periodic Dispersion-Corrected DFT and MP2 Investigation.* **CrystEngComm.** 2014, 16, 102-109. DOI: 10.1039/C3CE41758A	Q1
55	Gambuzzi, E.; **Pedone, A.**; Menziani. M. C.; Angeli, F.;Caurant, D.; Charpentier, T. *Probing the silicon and aluminium chemical environments in silicate and aluminosilicate glasses by solid state NMR spectroscopy and accurate first-principles calculations.* **Geochim. Cosmochim. Ac.** 2014, 125, 170-185	Q1
56	Muniz-Miranda, F.; Menziani, M. C**.; Pedone, A.** *Assessment of Exchange-Correlation Functionals in reproducing the Structure and Optical Gap of Organic-protected Gold Nanoclusters.* **J. Phys. Chem. C.** 2014, 118, 7532-7544	Q1
57	Barone, V.; Biczysko, M.; Bloino, J.; Carta, L.; **Pedone, A.** *Environmental and dynamical effects on the optical properties of molecular systems by time-independent and time-dependent approaches: coumarin derivatives as test cases.*	Q2

	Comp. Theor. Chem. 2014, 1037, 35-48. http://dx.doi.org/10.1016/j.comptc.2014.03.027	
58	Presti, D.; **Pedone, A.**; Menziani, M. C. *Unravelling the polymorphism of [(p-cymene)Ru(kN-INA)Cl_2] through dispersion-corrected DFT and NMR GIPAW calculations.* **Inorg. Chem.** (**2014**) 53(15) 7926-7935 **DOI:** 10.1021/ic5006743	Q1
59	Muniz-Miranda, F.; Menziani, M. C**.; Pedone, A.** O*n the Optoelectronic Properties of Phosphine and Thiolate Protected Undecagold Nanoclusters* **Phys. Chem. Chem. Phys.** 2014, **16**, 18749-18758, **DOI:** 10.1039/C4CP02506G.	Q1
60	Gambuzzi, E.; Charpentier, T.; Menziani, M. C.; **Pedone, A.** *Computational interpretation of ^{23}Na 3QMAS NMR Spectra: a thorough investigation of the Na environment in silicate glasses.* **Chem. Phys. Letters (2014)** 612, 56-61, DOI: 10.1016/j.cplett.2014.08.004.	Q2
61	Gambuzzi, E.; **Pedone, A.** *Core-Shell Molecular Dynamics Simulations of Ce-containing Silicophosphate Glass Structures.* **Phys. Chem. Chem. Phys. (2014)** 16 (39), 21645 - 21656 **DOI:** 10.1039/C4CP02577F	Q1
62	Delle Piane, M.; Corno, M.; **Pedone, A.**; Dovesi, R.; Ugliengo, P. *MCM-41 mesoporous silica as drug delivery system: adsorption of ibuprofen simulated by large-scale hybrid density functional calculations.* **J. Phys. Chem. C** 2014, 118 (46), pp 26737–26749 **DOI:** 10.1021/jp507364h	Q1
63	Presti, D.; Labat, F.; **Pedone, A.**; Ciofini, I.; Menziani, M. C.; Adamo C. *In silico study of thermochromic molecular crystals: a DFT QM/QM' approach for the description of solid Salicylidene Aniline.* **J. Chem. Theor. Comput.** 2014, 10 (12), pp 5577–5585 **DOI:** 10.1021/ct500868s	Q1
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