IL PRESENTE ALLEGATO COSTITUISCE UNO SCHEMA-TIPO, NEL QUALE SONO INDICATE ALCUNE VOCI A MERO TITOLO ESEMPLIFICATIVO, PERTANTO PUO' ESSERE MODIFICATO/INTEGRATO DAL CANDIDATO ADATTANDOLO ALLE PECULIARITÀ DELLA PROPRIA ATTIVITÀ SCIENTIFICO-PROFESSIONALE

Decreto Rettore Università di Roma "La Sapienza" n 2084/2025 del 09.07.2025

Simone Meloni
Curriculum Vitae

Ferrara
21 Agosto 2025

Part I – General Information

Full Name	Simone Meloni
Spoken Languages	Italian, English, French

Part II – Education

Type	Year	Institution	Notes (Degree, Experience,…)
University graduation	1997	Sapienza University of Rome	Degree in Chemistry, Summa Cum Laude
PhD	2000	Sapienza University of Rome	Degree in Chemical Sciences

Part III – Appointments

IIIA – Academic Appointments

Start	End	Institution	Position
2022	-	University of Ferrara (IT)	Associate Professor
2019	2022	University of Ferrara (IT)	Assistant Professor
2016	2016	Sapienza University of Rome (IT)	Research Professor
2013	2015	EPFL - École Polytechnique Fédérale de Lausanne (CH)	Senior Researcher
2011	2012	University College Dublin (IE)	MSCA Fellow at the UCD School of Physics
2009	2011	University College Dublin (IE)	Postdoctoral researcher at the UCD School of Physics
2001	2013	CASPUR/CINECA Supercomputing centre (IT)	Permanent staff member Materials' Science Group – 2009-2012 on leave of Absence
2001	2001	Princeton University (USA)	Visiting postodoctoral researcher of the group of Prof. Car
1999	2000	Max-Planck Institut für Festkörperforschung (GE)	Visiting PhD student of the group of Prof. Parrinello

IIIB – Other Appointments

Start	End	Institution	Position
2019	-	Daresbury Lab, SFTC (UK)	Visiting professor

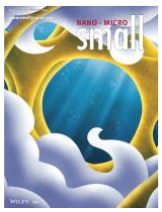
2012	2013	CINECA/Sapienza University of Rome (IT)	On secondment at the Dept. of Physics, Sapienza University of Rome
2012	2013	University College Dublin (IE)	Visiting researcher

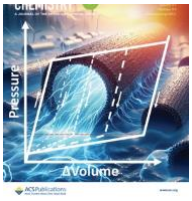
Part IV – Teaching experience

Year	Institution	Lecture/Course
2022 -	University of Ferrara (IT)	8 credits/56h. "Chemistry" for BSc in Phy.sics
2022 -	University of Ferrara (IT)	8 credits/48h. "Chemistry of Materials" for MScs in Chemistry and Physics
2020 -	University of Ferrara (IT)	"General and Inorganic Chemistry" 8 credits/48h. BSc in Agricultural Technologies and Po River Aquaculture
2019 -	University of Ferrara (IT)	"General and Inorganic Chemistry" 1 credits/8h. BSc Biotechnology for Medicine (2019-2020 ~1800 students; 2020 – 600 Students).
2019 - 2020	University of Ferrara (IT)	"General and Inorganic Chemistry" 8 credits/48h. BSc Biotechnology
2016-2019	Sapienza University of Rome	"Laboratory of atomistic and microfluidic simulations" 4 credits/24h for MSc in Nanotechnologies
2012	University College Dublin	"Theory and computational techniques to study rare events in atomistic and molecular simulations." PhD schools in Physics and Chemistry
2012	University College Dublin	"Theory and computational techniques to study rare events in atomistic and molecular simulations." PhD schools in Physics and Chemistry
2007-2009	Erasmus Mundus Atosim, partnership among ENS Lyon, FR, "La Sapienza" Rome and Universiteit van Amsterdam and Vrije Universiteit Amsterdam, NL	"Molecular Simulations", 1 credit/6h+lab

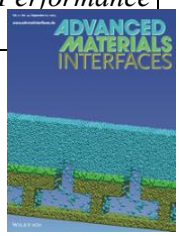
Part V - Society memberships, Awards and Honors

Year	Title
From 2024	Member of the "Excellence" calls panel of the EU EuroHPC joint undertaken
2025	**Cover**: "Crystallite Size Effects on the Heat of Water Intrusion/Extrusion into/from Metal-organic Frameworks", J. Phys. Chem. Lett. 16, 2089 (2025)
2024	**Cover**: *"Counterintuitive trend of intrusion pressure with temperature in hydrophobic MOF", Small 2024, 20, 2402173 (Inspired by the Centenary of Surrealism).*
2024	**Cover**: *"Partial intrusion and extrusion in hydrophobic nanopores for mechanical energy dissipation", J. Phys. Chem. C 2024, 128, 12036*
2023	Winner of the prize awarded by the H2020 European Innovation Council 112CO2 "Opportunities for integrating methane decomposition with other processes" (https://www.112co2.eu/open-calls/monetary-prize/) with the proposal "PROCEED - upstream integration of 112CO2 with green methane production".
From 2022	Member of the Physics and Materials panel of the EuroHPC joint undertaken





From 2020	Member of the Internation Experts Panel in Physics and Materials of the Polish National Science Foundation NCN for calls of several classes (Master, OPUS, …)
2019	Reviewer of the French Science Foundation ANR
2024	**ESI "Highly Cited Papers",** articles within the top 1% in a given field in the publication year: *""Highly efficient and stable perovskite solar cells via a multifunctional hole transporting material", Joule 8, 1691 (2024)*
2017	**"Highlights 2017" della rivista the Journal of Physics:** *Condensed Matter: "Intrusion and extrusion of a liquid on nanostructured surfaces", http://iopscience.iop.org/journal/0953-8984/page/Highlights-2017*
2016	**ESI "Highly Cited Papers",** articles within the top 1% in a given field in the publication year: *"Entropic Stabilization of Mixed A-Cation ABX3 Metal Halide Perovskites for High Performance Perovskite Solar Cells", Ener Environ Sci 9, 656 (2016),*
2016	**ESI "Highly Cited Papers",** articles within the top 1% in a given field in the publication year: *"Ionic polarization-induced current-voltage hysteresis in CH3NH3PbX3 perovskite solar cells", Nat. Commun. 7, 10334 (2016)*
2016	**ESI "Highly Cited Papers",** articles within the top 1% in a given field in the publication year: *"Origin of unusual bandgap shift and dual emission in organic-inorganic lead halide perovskites", Science Adv. 2, e1601156 (2016)*



2015	**Cover:** *"Superhydrophobicity: Unraveling the Salvinia Paradox: Design Principles for Submerged Superhydrophobicity", Adv. Mater. Interf. 2, 1500248 (2015)*
2012	Prize "Ireland's Champions of EU research", assigned by the President of the Republic of Ireland.

Part VI - Funding Information [grants as PI-principal investigator or I-investigator]

Year	Title	Program	Grant value
2025	Horizon Europe European Research Council Advanced Grant (~2500000€ in 5 years) submitted as PI on August 28th 2025: COOL-SCW - Engineering Nanoconfined Mild-Condition Supercritical Water for Fundamental Insights and Next-Generation Technologies.		
2025	5 Horizon Europe Pathfinder Open submitted for the May 21st 2025 deadline, one as PI and four as CoI (unit leader), each with a budget of ~4000000€ in 4 years: - (PI) NoLongerPFAS: complete degradation of "forever chemicals" PFAS by confined supercritical water oxidation. - (CoI) Nauca - Metal organic frameworks as nanoscale non-linear ultrasound contrast agents for biomolecular imaging - (CoI) ANUBI: Active Nanoheterojunctions for Ultralight Biomedical Infection-Control - (CoI) Unveiling the Power of Carbon Molecular Sieve Membranes: A Game-Changing Approach for New and Relevant Gas Separations - (CoI) EcoTES: ENABLING COMPOSITE THERMAL ENERGY STORAGE VIA NANO-WETTABILITY CONTROL		
2022	"Perovskite-Inspired materials-based iNdoor PhotovOltaics for powering the Internet of Things – PINPOINT"	PRIN-PNRR	Total ~240000€ in 36 months; UNIFE unit led by me ~74000 € in 3 years.
2022	"MEDUSA – therModynamic anomaliEs in liquiDsUsing computer simulAtions"	Supervisor of Bernadeta Maria Jasiok, PRELUDIUM call of the Polish Science Foundation (Narodowe Centrum Nauki).	Budget ~210000 PLN (~45000€) in 3 years.

2020	"Electro-Intrusion - Simultaneous transformation of ambient heat and undesired vibrations into electricity via nanotriboelectrification during non-wetting liquid intrusion-extrusion into-from nanopores"	H2020, call H2020-FETPROACT-2020-2. Grant No. 101017858.	Total € 3651381.25 for 48 months; UNIFE unit led by me € 558000 in 30 months.
2017	"Porous Lyophobic Crystalline Materials for Mechanical Energy Storage".	"Sapienza" Univesrity of Rome (IT), progetti "Grandi", n. RG11715C81D4F43C.	~ € 39000 in 1 year.
2015	CoI (PI Prof. U. Roethlisberger) of the R'Equip project for renewing the equipment of the lab.	Swiss Science National Foundation R'Equip call	270000 CHF (~250000€)
2010	"Clathrates hydrates and non-Hydrates: functional materuals for energy applications".	MIUR Fondo per gli Investimenti della Ricerca di Base – FIRB.	~324000€ in 5 years.
2009	"Advanced Molecular Simulations"	PI-GRANT Science Foundation Ireland. Grant 08-IN.1-I1869.	~850000€ in 4 years.

Part VII – Research Activities

Keywords	Brief Description
Energy materials	Investigation of materials of interest for energy applications
Perovskites and perovskite-inspired materials	3rd generation PV materials: defect-tollerant materials combining high-performance and facile deposition methods. Recently I started investigating materials for indoor PV, for powering the internet of things. These materials have more stringent requisite on zero toxicity, easy and safe disposal, and low costs, especially concerning hole/electron extracting layers and back contacts.
Porous materials and confined fluids	Porous materials and fluids confined within them. These materials can be used for energy recovery, energy storage storage and energy dissipation. These materials are at the base of the H2020 Electro-Intrusion project. Within this research we discovered interesting novel applications, such as technologies for mild conditions confined supercritical water (in 2025 we have shown that we can achieve confined supercritical water at 380K) and contrast agents for ultrasound imaging.
Molecular Sieve Membranes	Developing porous materials for gas separation, avoiding the expensive processes. Such as Cryogenic Distillation, or absorption and chemical methods, and improving over present ineffective membrane separation approaches.

Part VIII – Summary of Scientific Achievements

Product type	Number	Data Base	Start	End
Papers [international]	118	SCOPUS	1998	Aug. 21th 2025

Total Impact factor	792.423
Average Impact factor	6.951
Total Citations	5721
Average Citations per Product	48.5
Hirsch (H) index	35
Normalized H index*	1.84, excluding years when I worked out of academia; 1.25 from graduation

Part IX – Organization, coordination and participation to National and/or international research groups.

2019 -	Leader of the Laboratory of Advanced Modelings and Materials simulations of the Uinversity of Ferrara. The group runs several Italian and EU projects, leading the corresponding research units: i) "Electro-Intrusion - Simultaneous transformation of ambient heat and undesired vibrations into electricity via nanotriboelectrification during non-wetting liquid intrusion-extrusion into-from nanopores"; ii) "Perovskite-Inspired materials-based iNdoor PhotovOltaics for powering the Internet of Things – PINPOINT"; iii) "MEDUSA – therModynamic anomaliEs in liquiDsUsing computer simulAtions"; iv) "112CO2 - Low temperature catalytic methane decomposition for COx-free hydrogen production"
2016-2019	Member of the FLUMACS research group within the Department of Mechanical and Aerospace Engineering of the Sapienza University of Rome. During his staying, Prof. Meloni was involved in the ERC Advanced grant "BIC – Bubble Cavitaion from Inception to Collapse" led by Prof. Casciola. Prof. Meloni was responsible of the unit focusing on cavitation at the atomistic scale.
2014	Member of the LCBC group led by Prof. Roethlisberger at the EPFL. Prof. Meloni contributed to the National Centres for Competence in Research (NCCR) MARVEL (nccr-marvel.ch/) and MUST (https://www.nccr-must.ch/).
2009-2013	Member of the group of Advanced Simulations of the School of Physics of the University College Dublin, led by Prof. Ciccotti. Prof. Meloni led the unit of Nanomaterials. Additionally, Prof. led its own Maria-Sklodowska Curie Intraeuropean Fellowing SimDePro.

Part X – Patents

2024	Together with Prof/Dr Yaroslav Grosu and Dr. of the CIC Energigune of the European Patent Application No. EP23382516.5 for "LOW-BIAS VOLTAGE INTRUSION-EXTRUSION ELECTRIC GENERATOR"

Part XI– Organization of Conferences and other Scientific International Events

2025 – "Multiscale Molecular Dynamics with MiMiC: Optimizing the Performance on Modern Supercomputers", Juelich (GE), June 2, 2025 – June 6, 2025

2024 – "From methods to applications: challenges and opportunities in contemporary simulations", Celebration of Giovanni Ciccotti's 80th birtday, Paris (FR), 13-15 June 2024

2023 – "Fluids in Porous Materials: from Fundamental Physics to Engineering Applications", Lausanne (CH), 19-21 June 2023

2022 - €MRS Fall Meeting Symposium "Breakthrough zero-emissions energy storage and conversion technologies for carbon-neutrality", 19-22 September 2022, Varsavia (PL)

2022 – Scuola CECAM su "Multiscale Modeling with MiMiC, Lausanna, 18-22 July 2022, Lausanne (CH)

2018 - "NanoGe Fall Meeting", simposio "Halide perovskites: when theory meets experiment from fundamentals to devices", Berlin (GE), 4-8 November 2019

2017 - "Addressing metastability in interfacial phenomena across multiple time and length scales", Lausanna (CH), 28 Agosto – 1 September 2017

2014 - "Binding free energy and kinetics: computation meets experiments", Genova (IT), 10-12 June 2014

2014 - "Superhydrophobicity, bubble stability, and heterogeneous nucleation", Rome (IT), 25-27 June 2014

2013 - "Five pieces and a do in computational physics, chemistry, biology, mathematics and engineering", Roma (IT), 18-20 December 2013

2013 - "Simulations and experiments on Materials for Hydrogen Storage", Dublino (IE), 11-13 October 2010

2008 - "standardization and databasing of classical and ab-initio atomistic simulations", ETH, Zurigo (CH), 18-19 September 2008

2008 - Scuola "Progress in simulating activated processes", Valle Capore (Roma, IT), 26-30 May 2008

Part XII – Talk to conference and other international scientific events

50 invited talk/lectures

76 – (Invited lectures) "Multiple timesteps IN molecular dynamics", "Introduction to Rare Events (Techniques)", "(Modern) Sampling Methods in Configuration and Trajectory space" – "Multiscale

Molecular Dynamics with MiMiC: Optimizing the Performance on Modern Supercomputers", Juelich (GE), June 2, 2025 – June 6, 2025

73 – (Invited) "Peculiar properties of water squeezed within nanoglasses", lecture at Alma Mater Studiorum, Bologna (IT), 13 May 2025

72 – (Invited) "Peculiar properties of water squeezed within nanoglasses", AQTIVATE Workshop, Jülich (GE), 3-5 February 2025

71 – (Invited) "Wetting and drying of nanocavities: stretching physics beyond the laws of classical (continuum) fluids", AQTIVATE Workshop, Jülich (GE), 3-5 February 2025

70 – (Invited) Round-table panellist, Symposium on sustainable energy vectors, 29th-30th October 2024, Valencia (ES).

69 – (Invited) "Theoretical insight into catalytic carbon nanostructure growth", Symposium on sustainable energy vectors, 29th-30th October 2024, Valencia (ES).

68 – (Invited) "Challenges in thermocatalytic degradation of methane: how simulations can help developing better processes and producing high added value byproducts", "Simulation assisted steps in research and technology in the hydrogen ecosystem" Webminar series, 17 October 2024

67 – (Invited Key Lecture) "Does nanoconfined water looks like bulk water?", CECAM Workshop "Computational chemistry across scales and disciplines", 1-3 October 2024, Lausanne (CH).

66 – (Invited Key Lecture) "Does nanoconfined water looks like bulk water?", Nanoinnovation, 9-13 September 2024, Rome (IT).

65 – (Invited) "Materials and processes for the future challenges in the field of renewable energies", University of Porto, Oporto (PT), 1 February 2023

64 – "Intrusion mechanism of water in ZIF-8 hydrophobic MOF: capillary condensation or subnanoscopic front advancement?", 12th International Colloids Conference, Palma de Majorca (ES), 11-14 June 2023

63 – (Invited) siMol meeting, Oxfordshire (UK), 31 October-1 November 2023

62 – (Invited) Conference on Artificial Photosynthesis and Green Catalysis, Lausanne (CH), July 17-19 2023

63 – (Invited) "Wetting and drying of nanoporous systems: From theoretical modeling to design principles of novel energy materials", Seminar at the Valencia Polytechnique University (ES), 18 May 2023

60 – (Invited) "Intrusion of water in hydrophobic crystalline porous materials", Metastability and multiscale effects in interfacial phenomena, Lausanne (CH), 13-15 March 2023

59 – (Invited) "Getting liquids in and out porous materials: a theoretical point of view", Symposium on Materials for Emerging Energy Technologies, Madrid (ES), 19-20 May 2022

58 – (Invited) "Ab initio simulation to improve the resistance to inactivation and enhance recovery of nickel-based catalysts for methane dehydrogenation.", International Hydrogen Summer School, Porto (PT), 5-8 September 2022.

57 – (invited) "Mobile ionic species in halide perovskites: Thermodynamics, dynamics, energetics and unexpected consequences on the properties of the material from atomistic simulation", SimOEP'22, International Conference on Simulation of Organic Electronics and Photovoltaics, Winthertun (CH), 7-9 September 2022

56 – "Wetting and drying of nanoporous systems: From theoretical modeling to design principles of novel energy materials",ACS Fall meeting 2022, Chicago (USA), 21-25 August 2022.

55 – (Invited) Teaching to the School "Multiscale Molecular Dynamics with MiMiC", Lausanne (CH), July 18-22, 2022

53 – "What does Determines the Stability of Surface Nanobubbles?", Transnational Access Meeting (TAM) of HPC Europa 3, 3-4 November 2021, online

52 – (Invited) " The peculiar physics of liquids confined within complex porous solids", Phase transition at the nanoscale, S. Anna di Camprena, Pienza (IT) 23-26 June 2021.

51 – (Invited) "Phase stability and defects dynamics in halide perovskites: fundamental processes affecting the efficiency and stability of hybrid perovskites for solar cells applications", FIM-S3 seminar series, online 21 April 2021.

50 – "Interaction between Ionic Defects and Grain Boundaries in Metal Halide Perovskites", Atomic-level Characterization of Hybrid Perovskites (HPATOM), online 26-28 January 2021

49 – (Invited) “Liquid intrusion (and extrusion) in porous and textured materials”, Frontiers in ion channels and nanopores-theory, experiments, and simulation, online 2-5 February 2021

48 – (Invited) “From first principles to the simulations of complex systems”, series of 4 lectures, "Multiscale simulations and biological channels", Rome (IT) 14-16 September 2020

47 – “Scientific challenge for next generation photovoltaics”, Campus Party, Digital Edition, 2020

46 – (Invited) “Spatial and temporal multiscale simulations of nanofluidic systems: from physics and chemistry to engineering”, CECAM 50° - Italian celebration day, Bologna (IT) 9/7/2019

45 – “Dynamical Effects in Confined Nucleation”, Roma Tre Congress on Water under Extreme Conditions, Rome (IT), 12-14 June 2019

44 – (Invited) ”Lead-Halide Perovskites: theory and experiments to unveil a promising candidate for 3rd generation solar cells”, Daresbury Laboratory, Warringhton (UK), 29 June 2019

43 – (Invited) “Intrusion/Extrusion of Liquids in/from Porous Lyophobic Materials Beyond the Classical Picture”, Daresbury Laboratory, Warringhton (UK), 29 June 2019

42 – “Intrusion/Extrusion of Liquids in/from Porous Lyophobic Materials Beyond the Classical Picture”, Mainz Materials Simulation Days 2019, Mainz (GE), 5-7 June 2019

41 – (Invited) “Simulation of chemical reactions and physical processes in condensed phase with applications to energy materials.”, Department Seminar, Dept. of Chemistry, University of Napoli Federico II, May 30 2019

40 – (Invited) “Wetting of lyophobic textured surfaces and porous materials”, “Colloquium”, Trento University, 13 November 2018

39 – (Invited) “Liquid intrusion/extrusion in porous systems: atomistic and continuum rare event simulations with engineering applications”, Computer Simulation in the Physical & Life Sciences, Temple University in Roma (IT), 26 October 2018

38 – “Bubble Nucleation in Water Under Extreme Confinement: Modular Design of Hydrophobic Textured Surfaces to Enhance Self-Recovery of the Cassie-Baxter State”, WaterX exotic properties of water under extreme conditions, Maddalena Island (IT), 3-8 June 2018

37 – (Invited) “Homogeneous and Confined Nucleation of Vapor Bubbles”, ISR International Workshop Series II - The Fluid Dynamics of Bubbles across the Scales, Guangzhou (CN) 28-30 September 2017

36 – (Invited) “Rare Events: Theory and Methods”, ISR International Workshop Series II - The Fluid Dynamics of Bubbles across the Scales, Guangzhou (CN) 28-30 September 2017

35 – (Invited) “Nucleation mechanism of the sequential deposition process”, €-MRS, Warsaw (PL) 17-22 September 2017

34 – (Invited) “Mechanisms and Nucleation Rate of Methane-Hydrate by Dynamical Nonequilibrium Molecular Dynamics.”, Addressing metastability in interfacial phenomena across multiple time and length scales, Lausanne (CH), 29 August-1 September 1, 2017

33 – “Vapor nucleation under extreme confinement”, XXIX IUPAP Conference on Computational Physics (CCP2017), Paris (FR) 9-13 July 2017

32 – (Invited) “Unusual photoluminescence emissions in lead halide perovskites and their molecular origin”, 21 International Conference on Solid State Ionics, Padua (IT), 18-23 June 2017

31 – “Vapor nucleation under extreme confinement”, Congress on Water Under Extreme Conditions, 2017, Rome (IT), 14-16 June 2017

30 – (Invited) “Ab initio hydrodynamics”, 19h International Conference on Finite Elements in Flow Problems - FEF 2017, Rome (IT), 5-7 April 2017

29 – (Invited) “The Salvinia Paradox: how the hydrophilic patches help keeping the plants surface dry”, Workshop “Hybrid Methods in Molecular Simulation”, Cagliari (IT), 3-4 April 2017

28 – “The Salvinia Paradox: how the hydrophilic patches help keeping the plants surface dry”, CECAM/ESI Workshop “Water at interfaces: from proteins to devices”, Wien (AT), 29 November - 2 December 2016

27 – (Invited) “Superhydrophobicity recovery on complex surfaces”, Nanoinnovation 2016, Rome (IT), 20-23 September 2016

26 – “Dewetting of superhydrophobic surface”, mMAST, Brussels (BE), 6rd-8th September 2016

24 – “The Salvinia Paradox: how hydrophilic patches help keeping its surface dry”, Italian Soft Days, Milan (IT), 23rd-24th June 2016

23 – “Mechanism of the Cassie-Wenzel transition via the atomistic and continuum string methods”, 2nd Conference on Multiscale Modelling of Condensed Phase and Biological Systems, Manchester (UK), 13th - 15th April 2016

22 – “Hysteresis in perovskite solar cells: experimental and theore6cal evidence of its defect-related origin ”, Roma (IT), HOPV15, 10th-13th May 2015

21 – (Invited) “Wetting of textured surfaces by advanced atomistic and continuum simulations”, “Superhydrophobicity, bubble stability, and heterogeneous nucleation”, Rome (IT), Joint CECAM Workshop and Sapienza Conference, Rome (IT), 25th-27th June 2014

20 – (Invited) “Methane clathrate hydrate nucleation mechanism by advanced sampling techniques”, CECAM Workshop “Molecular-level understanding of nucleation”, Lausanne (CH), 23rd-25th June 2014

19 – (Invited) “Multiscale simulations to study structural and electronic properties of Si nanoparticles embedded in a-SiO2 and a-SiNx dielectrics.”, Conference “SiO2, Advanced Dielectrics and Related Devices”, Cagliari (IT), 16-18 June 2014

18 – (Invited) “Rare event methods: modern techniques and their application to challenging chemical and physical problems”, Physical and Theoretical Chemistry Colloquia, 23 April 2014, Univ. of Duisburg-Essen

17 – (Invited) “Superhydrophobicity lost: the Cassie-Baxter to Wenzel phase transition”, “Advanced Molecular Simulation Methods in the Physical Sciences”, Beijing (CH), 24th-30th July 2013

16 – (Invited) “Time-dependent Non-equilibrium Molecular Dynamics”, ”Lorentz center international workshop “Modelling the Dynamics of Complex Molecular Systems”, Leiden (NL) 13th-24th August 2012

15 – (Invited) “A pseudo-quantum description of vacancy diffusion in crystals”, CECAM Workshop “Free energy calculations: from theory to applications”, “Modeling the dynamics of complex molecular systems” Conference, Leiden (NL) 13-24 August 2012

14 – (Invited) “A pseudo-quantum description of vacancy diffusion in crystals”, CECAM Workshop “Free energy calculations: from theory to applications”, Paris 4-8 June 2012

13 – “A novel approach to study vacancy dynamics in crystals (by rare event techniques)”, SimBioMa Conference, Konstanz (DE) 28 September – 1 October

12 – (invited) “Nanotechnology in materials and fibers”, workshop on Science and technology for the third millennium sportswear, University “Foro Italico”, Rome (IT) 11 April 2011

11 - (Invited) “Data Management in Europe”, ZCAM-CECAM workshop on Databases in Quantum Chemistry, Zaragoza (ES) 21-24 September 2010

10 - “Study of nucleation by rare event methods”, LAM 14, Rome (IT) 11-16 July 2011

9 - (Invited): “Hydrodynamics from non-equilibrium statistical mechanics: evolution of a curved interface between immiscible liquids”, SIMAI 2010, Cagliari (IT) 21-25 June 2010

8 - “Dehydrogenation mechanism in sodium alanates”, CPMD 2008, Trieste (IT) 23-27 June 2008

7 - “Dehydrogenation mechanism in sodium alanates”, SimBioMa Conference, Konstanz (DE) 5-8 April 2008

6 - “Ab-initio simulation of carbon clustering on Ni(111) surface: the bonding mechanism between Na and C.”, Conference on Computational Physics 2007, Brussels (BE) 5-8 September 2007

5 - “ESF Forward Look for non-hardware aspects of Computational Science Infrastructure”, Conference on Computational Physics 2007, Brussels (BE) 5-8 September 2007

4 - “Hydrogen Diffusion in Sodium Alanates”, Conference on Computational Physics 2007, Brussels (IT) 5-8 September 2007

3 - “Computational Material Science Application Programming Interface (CMSApi): a tool for developing applications for atomistic simulations”, INTERNATIONAL SCHOOL OF SOLID STATE PHYSICS - 34th course: Computer Simulations in Condensed Matter: from Materials to Chemical Biology.

2 - “Ab-initio study of carbon clustering on Ni(111) surface”, Conference on Computational Physics 2004, Genoa (IT) 1-4 September 2004

1 - “Reduction on arrays: comparison of performances between different algorithms”, Fifth European Workshop on OpenMP (EWOMP), 22-23 September 2003, Aachen (GE)

Part XIII – Public Engagement (3rd mission)

Interviews on National Radio Broadcasts

27 January 2021: https://www.radio24.ilsole24ore.com/programmi/smart-city/puntata/trasmissione-27-gennaio-2021-210402-ADNEZBGB

30 May 2019: http://www.radio24.ilsole24ore.com/programma/smart-city/trasmissione-maggio-2019-210431-ACUiRkK

26 March 2018: http://www.radio24.ilsole24ore.com/programma/smart-city/effetto-loto-sanno-come-155552-gSLAYnz6cC

Articles/Interviews appeared on journals and magazine

https://www.ilrestodelcarlino.it/ferrara/cronaca/ridurre-le-masse-tumorali-un-metodo-non-invasivo-jucjkvrt

https://www.ilrestodelcarlino.it/ferrara/cronaca/tumori-ricerca-da-unife-una-nuova-strada-per-ridurre-la-massa-del-cancro-b4mw5pt0

https://www.ilrestodelcarlino.it/ferrara/cronaca/tumori-ricerca-da-unife-una-nuova-strada-per-ridurre-la-massa-del-cancro-b4mw5pt0

https://www.ilrestodelcarlino.it/ferrara/cronaca/dagli-ammortizzatori-dell-auto-si-può-produrre-energia-pulita-1.5918569

"Scenari" de Il Sole 24ore, article "Da energia di scarto a elettricità a zero emissione" ("from waste energy to zero emission electric energy"), February 28 2022

Online articles

PRACE grant success stories "Understanding And Improving The Tolerance Of Perovskites" https://prace-ri.eu/understanding-and-improving-the-tolerance-of-perovskites/

Public speaches

"From quantum mechanics to next-generation green energy materials" for "Venerdi dell'Universo", Ferrara 18 March 2022 (in Italian , https://www.youtube.com/watch?v=tqDOg6OK8t4)

School visits

2023- "Il laboratorio in un computer: dalla meccanica quantistica alla progettazione dei materiali del futuro."

2024 U.T.E.F, Univeristà per l'Educazione Permanente. "Un futuro elettrizzante: le sfide scientifiche per le energie rinnovabili del 21° secolo e oltre", Portomaggiore (FE), 24 Ottobre 2023.

Part XIV – Management and Administrative Activities

Since 2023 – Member of the Quality Assurance Committee of the Doctoral School in Chemical Sciences, University of Ferrara.

2023 – Member of selection committees: twice for the awarding of a research fellowship (assegno di ricerca) and once for the recruitment of a tenure-track researcher (RTD-A), Department of Chemical, Pharmaceutical and Agricultural Sciences (DOCPAS), University of Ferrara.

2023 – Member of the Admission Committee for the 39th cycle of the PhD Program in Chemical Sciences, University of Ferrara.

2022 – Member of the Admission Committee for the 38th cycle of the PhD Program in Chemical Sciences, University of Ferrara.

2022 – Member of the Evaluation Committee for the extension of a RTD-A position, Department of Chemical, Pharmaceutical and Agricultural Sciences, University of Ferrara.

2021 – Member of the selection committee for the awarding of research fellowships on three occasions, Department of Chemical, Pharmaceutical and Agricultural Sciences, University of Ferrara.

Since 2022 – Coordinator of internal internship activities for the BSc program in Chemistry, University of Ferrara (approximately 200 students).

2022 – Member of the committee responsible for drafting and, following approval, implementing a high-performance computing infrastructure at UNIFE (budget: €400,000).

Since 2022 – Member of the UNIFE team implementing the PNRR project "Research Ecosystems": ECOSISTER – Emilia-Romagna Innovation Ecosystem.

2022 – Coordinator of UNIFE's activities in the preparation of a PNRR "Extended Partnerships" project proposal for Topic 4: Quantum Sciences and Technologies.

Since 2022 – Member of the internal committee for the allocation of departmental research funding (DOCPAS), University of Ferrara.

2022 – 2025. Coordinator of cross-disciplinary tutoring activities in General Chemistry for the BSc programs in i) Biology, ii) Biotechnology, iii) Agricultural and Aquaculture Technologies of the Delta, University of Ferrara.

Since 2021 – Coordinator for Communication, Dissemination and Exploitation activities of the H2020 FET project Electro-Intrusion.

2020–2022 – Responsible for coordinating and supporting the use of remote teaching infrastructure within DOCPAS during the COVID-19 crisis.

Since 2020 – Member of the "Research and Third Mission" Committee of the Department of Chemical, Pharmaceutical and Agricultural Sciences (DOCPAS).

Since 2020 – Member of the Faculty Board of the Doctoral School in Chemical Sciences, University of Ferrara.

2011–2020 – Member of the Faculty Board of the Doctoral School in Theoretical and Applied Mechanics, Sapienza University of Rome.

2006–2009 – Coordinator of the Scientific and Technical Computing course program at the CASPUR Supercomputing Center.

2006–2009 – Scientific Secretary of the European Science Foundation's "Forward Look Initiative": EUROPEAN COMPUTATIONAL SCIENCE: THE LINCEI INITIATIVE – FROM COMPUTERS TO SCIENTIFIC EXCELLENCE.

Part XV– Mentoring and Supervisioning

Here I report only the starting year of Mentoring/Supervisining. For example, Dr. Le Donne is reported only on 2021 despite he still part of my group

2025- Gianmarco Sigolo (MSc student), Matteo Bragagnolo (MSc student), Gianmarco Lapenna (BSc student), Leonardo Gnesato Anselmi (BSc student), Alice Piantavigna (MSc student)

2024 – L. Brugnati (BSc student), R. Verni (BSc student) Università di Ferrara;

2023 – M. S. Barro (BSc student) Università di Ferrara; N. Verziaggi (PhD student) , Università di Ferrara;

2022 – S. Buzzoni (BSc student), M. Alvelli (BSc student), GianMarco Sigolo (BSc student), Matteo Bragagnolo (BSc student) Università di Ferrara; F. Talpo (MSc student), D. Ballardini (BSc student), A. Piantavigna (BSc student), N. Circosta (BSc student), R. Bhatia (PhD student), N. Verziaggi (MSc student) , Università di Ferrara;

From 2021 – S. Merchiori (PhD student), J. D. Littlefair (Postdoc), A. Le Donne (Postdoc), Università di Ferrara; Daniele Ceneda (MSc student), Meysam Shahrooz (MSc student), Università di Roma "La Sapienza";

2020 - M. Tortora (PhD student), Università di Roma "La Sapienza";

2019 - M. Tortora (MSc student), Università di Roma "La Sapienza";

2018-2019 – E. Lisi (Postdoc), A. Battisti (Postdoc), University of Rome "La Sapienza";

2015-2019 – S. Marchio (PhD Student), University of Rome "La Sapienza";

2013-2016 – M. Amabili (Postdoc, PhD student, MSc student), University of Rome "La Sapienza";

2012 - M. Pourali (visiting PhD student), University of Rome "La Sapienza";

2012 – A. Choudhary (visiting MSc student, supervisioned MSc thesis), University College Dublin.

2011 – 2013 – A. Giacomello (PhD student), University of Rome "La Sapienza"; Dominika Lesniki (visiting BSc student from ENS Paris, supervisioned BSc thesis), University College Dublin.

2010 – P.-A. Geslin (visiting MSc master thesis from École Nationale de Mines St-Etienne, supervisioned MSc thesis), University College Dublin.

2010-2013 – M. Lauricella, J. Lucid, A. M. Elena (PhD students), University College Dublin.
2007-2013 – M. Ippolito (Postdoc e and permanent staff), CASPUR Supercomputing Centre;
2006-2009 – F. Sterpone (postdoc), CASPUR Supercomputing Centre;
2004-2011 – L. Ferraro (permanent), CASPUR Supercomputing Centre;
2003-2004 – C. Zazza (postdoc), CASPUR Supercomputing Centre;

Part XVI– Complete Publication List
Under Review

R1. "Functionalised MOFs for controlling in-situ Pd speciation for the selective hydrogenation of butadiene." Donato Decarolis, James King, Alin-Marin Elena, Linda Zhang, Jeff Armstrong, Ines Lezcano-Gonzalez, Michael Hirscher, Simone Meloni, Andrew M. Beale, Petra Ágota Szilágyi, Submitted to the Journal Mat Chem A. (IF: 9.3).

R2. "Triboelectrification during non-wetting liquids intrusion–extrusion into-from hydrophobic nanoporous silicon monoliths", L. Bartolomé, N. Verziaggi, M. Brinker, E. Amayuelas, S. Merchori, M. Z. Arkan, R. Eglītis, A. Šutka, M. Chorążewski, P. Huber, S. Meloni,* Yaroslav Grosu, Nano Energy (IF: 17), revision requested.

R3. Contribution to the roadmap "Lead-Free Perovskites and derivatives for Photogeneration: a roadmap to Sustainable Approaches for Photovoltaics and Photo(electro)catalysis", J. Phys: Ener (IF: 6.3).

Articles

116. "Exogenic and endogenic tuning of intrusion pressure in zinc imidazolate frameworks", A. Le Donne, J. D. Littlefair, E. Amayuelas, M. Tortora, S. K. Sharma, J. Mor, S. Merchiori, P. Zajdel, A. Piantavigna, G. Sigolo, Y. Grosu, S. Meloni, accepted for publication on J. Mat. Chem. A (IF: 9:30) DOI (pre-print version): 10.26434/chemrxiv-2025-qsvbn.

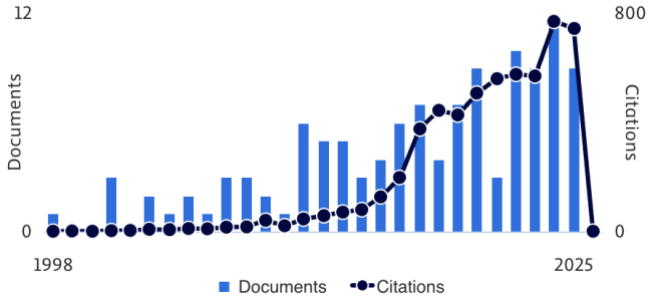


Figure 1: articles and citations vs year (SCOPUS, 5th August 2025)

115. "Size effects in Methane Splitting Catalyzed on Nickel Nanocrystals", Atashi N.; Palomares A.; Verziaggi N.; Martins L.; Mendes A.; Meloni S.; Prieto G., Accepted for publication on Applied Catalysis B (IF: 22.03); DOI: 10.1016/j.apcatb.2025.125817.

114. "Giovanni Ciccotti: a Renaissance physicist", Editorial to the special issue in honor of the 80's birthday of Giovanni Ciccotti, Sara Bonella, Daan Frenkel, George Jackson, S. Meloni, Rodolphe Vuilleumier, Mol. Phys. (IF: 1.8) DOI: 10.1080/00268976.2025.2483061.

113. "Impact of Porous Host Hydrophobicity on Hydration-Dehydration Cycles in Thermochemical Energy Storage Composites" E. Amayuelas; J. Chen; T. Zhang; S. Meloni*; Y. Ding; Y. Grosu, J. Colloid Interf. Sci. 693, 137605 (2025), DOI: 10.1016/j.jcis.2025.137605 (IF: 9.4)

112. "Water intrusion in hydrophobic MOFs with complex topology: A glimpse of the intrusion mechanism of Cu2(tebpz)", Sebastiano Merchiori, Daria Ballardini1, Andrea Le Donne, Ribhu Bhatia, Nicola Verziaggi, Cléophée Gourmand, Yaroslav Grosu, S. Meloni, J. Chem. Phys. 162, 064502 (2025) (IF: 4.4)

111. "Crystallite Size Effects on the Heat of Water Intrusion/Extrusion into/from Metal-organic Frameworks", L. Johnson; A. Lowe; A. Le Donne, E. Arkan; S. Merchiori; L. Bartolome; E. Amayuelas, D. Mirani; G. Lopez; G. Grancini; M. Chorążewski, S. Meloni,* Y. Grosu, J. Phys. Chem. Lett. 16, 2089 (2025) (IF: 6.88)

- The article was assigned the cover of the issue

110. "Intrusion-extrusion of water into-from hydrophobic nanopores at high temperature: unexpected dependence of dewetting pressure above 200°C", Cléophée Gourmand, Luis Bartolomé; Eder Amayuelas; Elena Palomo del Barrio; S. Meloni; Yaroslav Grosu, Microporous and Mesoporous Materials, 384, 113461 (2025) (IF: 4.8)

107. “Effect of linker hybridization on the wetting of hydrophobic metal-organic frameworks”, E. Amayuelas, S. K. Sharma, J. Mor, L. Bartolomé, L. Johnson, A. Le Donne, G. Sigolo, P. Zajdel, S. Meloni,* Y. Grosu, accepted for publication on Microporous and Mesoporous Materials, 383 113423, (2025) (IF: 4.4)

105. “Effect of macro-structure of Ni-based catalysts on methane splitting systems”, Luís Alves, Vítor Pereira, Paula Dias, Tiago Lagarteira, S. Meloni, Gonzalo Prieto, Adélio Mendes, Fuel 379, 133115 (2025) (IF: 6.7)

109. “Foundations of molecular dynamics simulations: how and What”, G. Ciccotti, S. Decherchi and S. Meloni,* Rivista del Nuovo Cimento 48, 1-94, (2025) (IF: 5.9)

108. “Triboelectrification during water intrusion–extrusion into-from hydrophobic nanopores”, Luis Bartolomé, Josh Littlefair, Eder Amayuelas, Liam Johnson, Andrea Le Donne, Andris Šutka, Simone Meloni,* Yaroslav Grosu, Adv. Mater. Technol. 2024, 2401744 (IF: 6.4)

106. “Nucleation of multispecies crystals: methane clathrate hydrates, a playground for classical force models.”, Marvo Lauricella, Giovanni Ciccotti, S. Meloni*, Molecular Physics 122, e2410484 (2024) (IF: 1.9)

104. “Controlling Nanocluster Growth through Nanoconfinement: The Effect of the Number and Nature of Metal-Organic Framework Functionalities.”, James King, Zhipeng Lin, Federica Zanca, Hui Luo, Linda Zhang, Patrick Cullen, Mohsen Danaie, Michael Hirscher, S. Meloni, Alin M. Elena, and Petra Á. Szilágyi, Phys. Chem. Chem. Phys. 26, 25021 (2024) (IF: 4.6).

103. “Counterintuitive trend of intrusion pressure with temperature in hydrophobic MOF”.Sebastiano Merchiori, Andrea Le Donne, Mirosław Chorążewski, Mian Li, Dan Li, Alexander Lowe, Monika Geppert-Rybczynska, Lukasz Scheller, Paweł Zajdel, Yaroslav Grosu, Simone Meloni*, Small 20, 2402173 (2024) (IF:13.3)

- The article was assigned the cover of the issue

102. “Partial intrusion and extrusion in hydrophobic nanopores for mechanical energy dissipation”, G. Paulo, L. Bartolomé, O. Bondarchuk, S. Meloni*, Y. Grosu, A. Giacomello, J. Phys. Chem. C 128, 12036 (2024) (IF: 4.4), DOI: 10.1021/acs.jpcc.4c02900.

- The article was assigned the cover of the issue

101. “MiMiC: A High-Performance Framework for Multiscale Molecular Dynamics Simulations”, A. Antalík, A. Levy, S. Kvedaravičiūtė, S. Johnson, D. Carrasco-Busturia, B. Raghavan, F. Mouvet, A. Acocella, S. Das, V. Gavini, D. Mandelli, E. Ippoliti, S. Meloni,* P. Carloni, U. Rothlisberger, and J. M. Olsen, J. Chem. Phys. 161, 022501 (2024) (IF: 4.4), DOI: 10.1063/5.0211053

100. “Mild-temperature supercritical water confined in hydrophobic metal-organic frameworks”, Sebastiano Merchiori, Andrea Le Donne, Josh David Littlefair, Mirosław Chorążewski, Mian Li, Dan Li, Alexander Lowe, Monika Geppert-Rybczynska, Paweł Zajdel, Yaroslav Grosu, Simone Meloni, J. Am. Chem. Soc. 2024, 146, 19, 13236–13246 (IF: 15.0), DOI: 10.1021/jacs.4c01226

99. “Negative compressibility in metastable elastocapillary systems”, D. Caprini, F. Battista, P. Zejdel, G. Di Muccio, C. Guardiani, B. Trump, A. Andreevich Yakovenko, E. Amayuelas, L. Bartolome, S. Meloni,* Y. Grosu, C. Massimo Casciola and A. Giacomello, Nature Communications 15, 5076 (2024) (IF: 16.6)

98. “Multiscale Biomolecular Simulations in the Exascale Era”, D. Carrasco-Busturia, E. Ippoliti, S. Meloni, U. Rothlisbergerd, Jógvan Magnus Haugaard Olsen, Accepted for publication in Current Opinions in Structural Biology 86, 102821 (2024) (IF: 2.8), https://doi.org/10.1016/j.sbi.2024.102821

97. “Highly efficient and stable perovskite solar cells via a multifunctional hole transporting material”, J. Zhou, L. Tan, Y. Liu, H. Li, X. Liu, M. Li, S. Wang, Y. Zhang, C. Jiang, R. Hua, W. Tress, S. Meloni,* C. Yi, Joule 8, 1691 (2024) (IF: 46.048), DOI: 10.1016/j.joule.2024.02.019

96. “Improved hole extraction and band alignment via interface modification in HTM-free Ag/Bi double perovskite solar cells”, Fabian Schmitz, Ribhu Bhatia, Julian Burkhart, Pascal Schweitzer, Marco Allione, Jaime Gallego, Piotr Piotrowski, Jakub Cajzl, Piotr Paszke, Gour Mohan Das, Dorota A. Pawlak, Federico Bella, Derck Schlettwein, Francesco Lamberti, Simone Meloni,* Teresa Gatti, Solar RRL 8, 2300965 (2024) DOI: 10.1002/solr.202300965; (IF: 9.173)

95. "Tuning Wetting-Dewetting Thermomechanical Energy for Hydrophobic Nanopores via Preferential Intrusion", Bartolome, L.; Anagnostopoulos, A.; Lowe, A.; Ślęczkowski, P.; Amayuelas, E.; Le Donne, A.;

Wasiak, M.; Chorążewski, M.; Meloni, S.*; Grosu, Y., J. Phys. Chem. Lett. 2024, 15, 880, DOI: 10.1021/acs.jpclett.3c03330; (IF: 6.888)

94. “Exploring the Heat of Water Intrusion into a Metal Organic Framework by Experiment and Simulation”, A. R. Lowe, P. Ślęczkowski, E. Arkan, A. Le Donne, L. Bartolomé, E. Amayuelas, P. Zajdel, M. Chorążewski, S. Meloni,* Y. Grosu, ACS Appl. Mater. Interfaces 2024, 16, 4, 5286, DOI: 10.1021/acsami.3c15447, IF: 9:229

93. "The effect of crystallite size on the flexibility and negative compressibility of hydrophobic metal-organic frameworks", Johnson, Liam; Mirani, Diego; Bartolome, Luis; Amayuelas, Eder; Alejandro Lopez, Gabriel; Grancini, Giulia; Trump, Benjamin; Carter, Marcus; Yakovenko, Andrey; Meloni, Simone;* Zajdel, Pawel; Grosu, Yaroslav, Nano Lett. 2023, 23, 23, 10682, DOI: 10.1021/acs.nanolett.3c02431; (IF: 12.262)

92. “Hydrophobicity and Hydrophilicity of Molecular Scale Textured Surfaces: the Case of Zeolitic Imidazolate Frameworks, an Atomistic Perspective”, A. Le Donne, J. Littlefair, M. Tortora, S. Merchiori, L. Bartolomé, Y. Grosu, S. Meloni, J. Chem. Phys. 2023, 159, 184709, DOI: 10.1063/5.0173110 (IF: 4.4)

91 – “Fabrication of superhydrophobic metallic porous surfaces via CO2 and water processing”, Anagnostopoulos, A. Nikulin, S. Knauer, O. Bondarchuk, M. E. Navarro Rivero, L. Tiejun, T. Karkantonis, E. Palomo del Barrio, M. A. Chorążewski, Y. Li, Y. Ding, S. Meloni,* Y. Grosu, Appl. Surf. Sci. 2023, 632, 157546, DOI: 10.1016/j.apsusc.2023.157546 (IF: 6.2)

90. “Optimization of the Wetting-Drying Characteristics of Hydrophobic Metal Organic Frameworks via Crystallite Size: The Role of Hydrogen Bonding between Intruded and Bulk Liquid”, L. J. W. Johnson, G. Paulo, L. Bartolomé, E. Amayuelas, A. Gubbiotti, D. Mirani, A. Le Donne, G. A. López, G. Grancini, P. Zajdel, S. Meloni,* A. Giacomello, Yaroslav Grosu, J. Colloids Interf. Sci. 645, 775-783 (2023); (IF: 9.071)

89. “Effect of Coarse Graining in Water Models for the Study of the Kinetics and Mechanism of Clathrate Hydrates Nucleation and Growth”, M. Lauricella, S. Meloni,* G. Ciccotti, J. Chem. Phys, Special Issue for 150th anniversary of nucleation theory, DOI: 10.1063/5.0140951 (IF: 3.488)

88. “Mechanism of water intrusion into flexible ZIF-8: liquid is not vapor“, E. Amayuelas, M. Tortora, L. Bartolomé, J. D. Littlefair, G. P., A. Le Donne, B. Trump, A. A. Yakovenko, M. Chorążewski, A. Giacomello, P. Zajdel, S. Meloni,* Y. Grosu, Nano Lett. 23, 5430–5436, (2023); (IF: 12.262)

87. “Classical nucleation of vapor between hydrophobic plates”, A. Tinti, A. Giacomello, S. Meloni,* and C. M. Casciola, J. Chem. Phys. 158, 134708 (2023); (IF: 3.488)

86 “Impact of Donor Halogenation on Reorganization Energies and Voltage Losses in Bulk-heterojunction Solar Cells”, H. Wu, Z. Ma, M. Li, H. Lu, A. Tang, E. Zhou, J. Wen, Y. Sun, W. Tress, J. Magnus Haugaard Olsen, S. Meloni,* Z. Bo Z. Tang, Energy Environ. Sci. 2023, 16, 1277-1290, DOI: 10.1039/D3EE00174A, (Impact factor: 39.17)

85. "The impact of secondary channels on the wetting properties of interconnected hydrophobic nanopores”, G. Paulo, A. Gubbiotti, Y. Grosu, S. Meloni,* and A. Giacomello, Comm. Phys. 6, 21 (2023), (Impact factor: 6.497)

D2 – “Research Briefing” article: “Kavitation an Flüssig-Flüssig-Grenzflächen: Strömungsmechanik”, P. Pfeiffer, C.-D. Ohl, S. Meloni, Physik in Unserer Zeit 2023, 51, 8-9, DOI: 10.1002/piuz.202370105

D1 – “Research Briefing” article: “The formation of gas bubbles at liquid–liquid interfaces”, P. Pfeiffer, S. Meloni, Nature Physics 2022, 18, 1410-1411

84. “Heterogeneous cavitation from atomically smooth liquid–liquid interfaces”, P. Pfeiffer, M. Shahrooz, M. Tortora, C. M. Casciola, R. Holman, R. Salomir, S. Meloni,* Claus-Dieter Ohl, Nature Physics 2022, 18, 1431–1435, DOI: 10.1038/s41567-022-01764-z, (Impact factor: 19.864)

- Press release Unife: https://www.unife.it/it/notizie/2023/scienza-cultura-e-ricerca/cavitazione-ridurre-masse-tumorali-studio-nature-physics
- https://www.ansa.it/emiliaromagna/notizie/2023/01/16/tumori-studio-nuova-chance-per-ridurre-le-masse_fa734760-25f2-4d8a-bbd7-7c7a0d6a823e.html
- https://www.telestense.it/tumori-studio-unife-nuova-chance-per-ridurre-le-masse-20230116.html
- https://www.ilrestodelcarlino.it/ferrara/cronaca/tumori-ricerca-da-unife-una-nuova-strada-per-ridurre-la-massa-del-cancro-b4mw5pt0

- https://www.insalutenews.it/in-salute/masse-tumorali-ridotte-in-modo-non-invasivo-bolle-di-cavitazione-per-rimuovere-il-tessuto-malato/
- Nuova ferrara (guardare pezzo nella cartella dell'articolo – richiamo in prima pagina)

83. "Photoprotection in metal halide perovskites by ionic defect formation", N. Phung, A. Mattoni, J. A. Smith, D. Skroblin, H. Köbler, L. Choubrac, J. Breternitz, J. Li, T. Unold, S. Schorr, C. Gollwitzer, I. G. Scheblykin, E. L. Unger, M. Saliba, S. Meloni,* A. Abate; A. Merdasa, Joule 2022, 6, 2152–2174, DOI: 10.1016/j.joule.2022.06.029 (Impact factor: 46.048)

- Press release Unife: https://www.unife.it/it/notizie/2022/scienza-cultura-e-ricerca/perovskiti-fotovoltaico
- https://greenreport.it/news/energia/energia-solare-con-le-perovskiti-un-meccanismo-di-auto-protezione-per-il-materiale-fotovoltaico-del-futuro/
- https://emiliaromagnaeconomy.it/energia-solare-perovskiti-un-meccanismo-di-auto-protezione-per-il-materiale-fotovoltaico-del-futuro/
- https://www.emiliaromagnanews24.it/energia-solare-perovskiti-un-meccanismo-di-auto-protezione-per-il-materiale-fotovoltaico-del-futuro-248300.html

82. "Turning molecular spring into nano-shock absorber: the effect of macroscopic morphology and crystal size on the dynamic hysteresis of water intrusion-extrusion into-from hydrophobic nanopores", P. Zajdel D. Madden, R. Babu, M. Tortora, D. Mirani, N. Tsyrin, L. Bartolomé, E. Amayuelas, D. Fairen-Jimenez, A. R Lowe, M. Chorążewski, J. B. Leao, C. M. Brown, M. Bleuel, V. Stoudenets, C. M. Casciola, M. Echeverría, F. Bonilla, G. Grancini, S. Meloni, Y. Grosu, ACS applied materials & interfaces 14, 26699 (2022) DOI: 10.1021/acsami.2c04314, IF: 9:229

81 - "Intrusion and extrusion of liquids in highly confining media: bridging fundamental research to applications", A. Le Donne,a, A. Tinti, E. Amayuelas, H. Kumar Kashyap, G. Camisasca, R. C. Remsing, R. Roth, Y. Grosu, S. Meloni,* Advances in Physics: X 2022, 7, 2052353, DOI: 10.1080/23746149.2022.2052353, IF: 8.7

80 - "The Double Life of Methanol: Experimental Studies and Non-Equilibrium Molecular-Dynamics Simulation of Methanol Effects on Methane-Hydrate Nucleation", M. Lauricella, Reza Ghaani, P. K. Nandi, S. Meloni,* B. Kvamme, Niall J. English, J. Phys. Chem. C 2022, 126, 6075−6081, DOI: 10.1021/acs.jpcc.2c00329, IF: 4.126

79 - "Kinetics of Metal Halide Perovskite Conversion Reactions at the Nanoscale", N. Arora, A. Greco, S. Meloni,* A. Hinderhofer, A. Mattoni, U. Rothlisberger, J. Hagenlocher, C. Caddeo, S. M. Zakeeruddin, F. Schreiber, M. Graetzel, R. H. Friend, M. I. Dar, Communication Materials 2022, 3, 22, DOI: 10.1038/s43246-022-00239-1, IF: to be assigned in 2023.

78 – "Subnanometer Topological Tuning of the Liquid Intrusion/Extrusion Characteristics of Hydrophobic Micropores", Bushuev Yuriy, Grosu Yaroslav, Chorążewski Mirosław, Simone Meloni*, Nano Lett. 2022, 22, 6, 2164–2169, DOI: 10.1021/acs.nanolett.1c02140, IF: 11.238

77. "Wavefunction-based electrostatic-embedding QM/MM using CFOUR through MiMiC", T. Kirsch,, J. M. Olsen, V. Bolnykh, S. Meloni, E. Ippoliti,U. Rothlisberger, M. Cascella, Michele; J.Gauss J. Chem. Theory Comput. 2022, 18, 13–24, DOI: 10.1021/acs.jctc.1c00878, IF: 6.006

76. "Crystal-size-induced band gap tuning in perovskite films", A. Ummadisingu, S. Meloni,* A. Mattoni, W. Tress, M. Grätzel, Angew. Chem. Int. Ed. 2021, 60, 21368–21376, DOI: 10.1002/anie.202106394, IF: 15.336

75. "Liquids intrusion-extrusion in-from non-wettable nanopores for technological applications", A. Giacomello, C. M. Casciola, Y. Grosu, S. Meloni* Eur. Phys. J. B 2021, 94, 163, IF: 1.440

74 – "Giant Negative Compressibility by Liquid Intrusion into Superhydrophobic Flexible Nanoporous Frameworks", Marco Tortora, Paweł Zajdel, Alexander Rowland Lowe, Mirosław Chorążewski, Juscelino B. Leão, Grethe V. Jensen, Markus Bleuel, Alberto Giacomello, Carlo Massimo Casciola, Simone Meloni,* and Yaroslav Grosu, Nano Lett. 2021, 21, 2838-2853, DOI: 10.1021/acs.nanolett.0c04941 IF: 11.238

73 – "On the accuracy of molecular simulation-based predictions of koff values: a Metadynamics study", Riccardo Capelli, Wenping Lyu, Viacheslav Bolnykh, Simone Meloni, Jógvan Magnus H Olsen, Ursula Rothlisberger, Michele Parrinello, Paolo Carloni, J. Phys. Chem. Lett. 2020, 11, 6373 (2020), DOI: 10.1021/acs.jpclett.0c00999, IF: 6.71

72 – “Defect Dynamics in MAPbI3 Polycrystalline Films: The Trapping Effect of Grain Boundaries”, Alessandro Mattoni, Simone Meloni,* Helvetica Chimica Acta 103, e2000110 (2020), DOI: 10.1002/hlca.202000110, IF: 2.309

71 – “The interplay among gas, liquid and solid interactions determines the stability of surface nanobubbles”, Marco Tortora, Simone Meloni,* Beng Hau Tan, Alberto Giacomello, Claus-Dieter Ohl, Carlo Massimo Casciola, Nanoscale 12, 22698 (2020), DOI: 10.1039/d0nr05859a (2020), IF: 6.895.

70 – “Hierarchical macro-nanoporous metals for leakage-free high-thermal conductivity shape-stabilized phase change materials”, Y. Grosu, Y. Zhao, A. Giacomello, S. Meloni, J.-L. Dauvergne, A. Nikulin, E. Palomo, Y. Ding, A. Faik, Applied Energy, 269, 115088 (2020), DOI: 10.1016/j.apenergy.2020.115088, IF: 9.27

69 – Opinion article: “MiMiC: Multiscale Modeling in Computational Chemistry”, V. Bolnykh, J. M. H. Olsen, S. Meloni, M. P. Bircher, E. Ippoliti, P. Carloni, and U. Rothlisberger, Frontiers in Molecular Biosciences, 7, 45 (2020), DOI: 10.3389/fmolb.2020.00045, IF: 3.565

68 – “Molecular Basis of CLC Antiporter Inhibition by Fluoride”, Chiariello M.G., Bolnykh V., Ippoliti E., Meloni S., Olsen J.M.H., Beck T., Rothlisberger U., Fahlke C., Carloni P., Journal of the American Chemical Society, 142, 7254-7258 (2020). DOI: 10.1021/jacs.9b13588, IF: 14.695.

67 – “The Role of Grain Boundaries on Ionic Defect Migration in Metal Halide Perovskites”, N. Phung, A. Al-Ashouri, S. Meloni, A. Mattoni, S. Albrecht, E. L. Unger, A. Merdasa, A. Abate, Advanced Energy Materials 1903735 (2020), DOI: doi.org/10.1002/aenm.201903735, IF: 24.884

66 – “Atomistic origins of the limited phase stability of Cs-rich FACsPbI mixtures”, A. Boziki, D. J. Kubicki, A. Mishra, S. Meloni, L. Emsley, M. Grätzel, and U. Rothlisberger, Chemistry of Materials 32, 2605-2614 (2020), DOI: 10.1021/acs.chemmater.0c00120, IF: 10.159

65 - “Wetting and recovery of nano-patterned surfaces beyond the classical picture”, S. Marchio, S. Meloni,* A. Giacomello, C. M. Casciola, Nanoscale 11, 21458-21470 (2019), IF: 6.970

64 – “Extreme Scalability of DFT-Based QM/MM MD Simulations Using MiMiC.” Bolnykh V., Olsen J.M.H., Meloni S., Bircher M.P., Ippoliti E., Carloni P., Rothlisberger U., Journal of Chemical Theory and Computation 15, 5601-5613 (2019), DOI: 10.1021/acs.jctc.9b00424, IF: 5.399

- Authors contribution reported in the article

63 - “Halide Versus Nonhalide Salts: The Effects of Guanidinium Salts on the Structural, Morphological, and Photovoltaic Performances of Perovskite Solar Cells”, M. Hayal Alotaibi, Y. A. Alzahrani, N. Arora, A. Alyamani, A. Albadri, Hamad Albrithen, I. H. Al-Lehyani, S. M. Alenzi, A. Z. Alanzi, F. S. Alghamdi, S. M. Zakeeruddin, S. Meloni,* M. I. Dar, and M. Graetzel, Solar RRS 1900234 (2019), DOI: 10.1002/solr.201900234. IF: 8.582

62 – “MiMiC: A Novel Framework for Multiscale Modeling in Computational Chemistry”, J. M. H. Olsen, V. Bolnykh, S. Meloni, E. Ippoliti, M. P. Bircher, P. Carloni, and U. Rothlisberger, J. Chem. Theory Comput. 15, 3810 (2019); DOI:10.1021/acs.jctc.9b00093, IF: 5.399

- Authors contribution reported in the article

61 – “Dual Effect of Humidity on Cesium Lead Bromide: Enhancement and Degradation of Perovskite Films”, D. Di Girolamo, M. I. Dar, D. Dini, L. Gontrani, R. Caminiti, A, Mattoni, M. Grätzel and S. Meloni,* Journal of Materials Chemistry A 7, 12292-12302 (2019), IF: 9.931

- Press release Sapienza https://www.uniroma1.it/it/notizia/pannelli-solari-perovskite-come-migliorarne-lefficienza 7 May 2019
- Interview on the national radio broadcast Radio24, 30 May 2019: http://www.radio24.ilsole24ore.com/programma/smart-city/trasmissione-maggio-2019-210431-ACUiRkK

60 – “How far does the defect tolerance of lead-halide perovskites range? The example of Bi impurities introducing efficient recombination centers.”, M. Yavari, F. Ebadi, S. Meloni, Z. S. Wang, T. Chien-Jen Yang, S. Sun, H. Schwartz, Z. Wang, B. Niesen, J. Durantini, P. Rieder, K. Tvingstedt, T. Buonassisi, W. C. H. Choy, A. Filippetti, T. Dittrich, S. Olthof, J.-P. Correa-Baena and W. Tress, Journal of Materials Chemistry A 7, 23838-23853 (2019), DOI: 10.1039/C9TA01744E, IF: 9.931

- Press release Sapienza https://www.uniroma1.it/it/notizia/pannelli-solari-perovskite-come-migliorarne-lefficienza

- Interview on the national radio broadcast Radio24, 30 May 2019: http://www.radio24.ilsole24ore.com/programma/smart-city/trasmissione-maggio-2019-210431-ACUiRkK
- Authors contribution reported in the article

59 – "What determines spontaneous liquid extrusion from nanopores?", M. Amabili, Y. Grosu, A. Giacomello, S. Meloni*, A. Zaki, F. Bonilla, A. Faik , C.M. Casciola, ACS Nano 13, 1728–1738 (2019), IF: 13.942

58 - "Hydrophilicity and Water Contact Angle on Methylammonium Lead Iodide", C. Caddeo, D. Marongiu, S. Meloni, A. Filippetti, F. Quochi, M. Saba and A. Mattoni, Advanced Materials Interfaces 6, 1801173 (2019), IF: 4.834

57 – "Viscosity at the nanoscale: confined non-wetting liquid dynamics and thermal effects for self-recovering nano-bumpers", Grosu Y., Giacomello A., Meloni S., González-Fernández L., Chorazewski M., Geppert-Rybczynska M., Faik A., Nedelec J.-M., Grolier J.-P., J. Phys. Chem. C 122, 14248-14256 (2018), IF: 4.536

56 – "Pressure control in interfacial systems: atomistic simulations of vapor nucleation", Marchio S., Meloni S.*, Giacomello A., Valeriani C., Casciola C. M., J. Chem. Phys., 148, 064706 (2018), IF: 2.965

55 – "Self-Recovery Superhydrophobic Surfaces: Modular Design", Lisi E., Amabili M., Meloni S.*, Giacomello A., and Casciola C. M., ACS Nano 12, 359 (2018), IF: 13.942

- Press release "Sapienza" 22 February 2018, https://www.uniroma1.it/it/notizia/dai-vetri-autopulenti-alle-eco-imbarcazioni-basso-attrito-ecco-come-i-nuovi-materiali;
- News reported by national press agencies, Ask A News: i) http://www.askanews.it/scienza-e-innovazione/2018/02/22/ricerca-team-sapienza-progetta-nuovo-materiale-superidrofobico-pn_20180222_00154/, ii) Galileo: https://www.galileonet.it/2018/03/materiale-superidrofobico/, iii) LinkedIn: https://www.linkedin.com/pulse/arrivo-nuovi-materiali-nanostrutturati-super-umberto-pivatello;
- Interview on the national radio broadcast Radio24, 26 March 2018: http://www.radio24.ilsole24ore.com/programma/smart-city/effetto-loto-sanno-come-155552-gSLAYnz6cC

54 – "Activated Wetting of Nanostructured Surfaces: Reaction Coordinates, Finite Size Effects, and Simulation Pitfalls", M. Amabili, S. Meloni, A. Giacomello, and C.M. Casciola, J. Phys. Chem. B 122, 200 (2018), IF: 3.177

53 - "Intrusion and extrusion of a liquid on nanostructured surfaces", Amabili M., Giacomello A., Meloni S.,* Casciola C. M., J. Phys.: Condens. Matter 29, 014003 (2017), IF: 2.678

- Selected for the "Highlights 2017" of the Journal of Physics: Condensed Matter: http://iopscience.iop.org/journal/0953-8984/page/Highlights-2017

52 – "Collective Molecular Mechanisms in the CH3NH3PbI3 Dissolution by Liquid Water", Caddeo C., Saba M. I., Meloni S., Filippetti A., and Mattoni A., ACS Nano 11, 9183 (2017), IF: 13.942

51 – "Collapse of superhydrophobicity on nanopillared surfaces" Amabili M., Giacomello A., Meloni S., Casciola C.M., Phys. Rev. Fluids 2, 034202 (2017), IF: 2.021

50 – "Mechanisms and Nucleation Rate of Methane-Hydrate by Dynamical Nonequilibrium Molecular Dynamics.", Lauricella M., Ciccotti G., English N. J., Peters B., Meloni S., J. Phys. Chem. C 121, 24223 (2017), IF: 4.536

49 – "Computational Characterization of the Dependence of Halide Perovskite Effective Masses on Chemical Composition and Structure." Ashari-Astani N., Meloni S., Salavati A. H., Palermo G., M Grätzel M., and Rothlisberger U., J. Phys. Chem. C 121, 23886 (2017), IF: 4.536

48 - "Focus Article: Theoretical aspect of vapour nucleation at structured surfaces", Meloni S.*, Giacomello A., Casciola C. M., J. Chem. Phys. 145, 211802 (2016) special issue "Nucleation: New Concepts and Discoveries", Kenneth Kelton e Daan Frenkel Eds., IF: 2.965

47 - "Extended intermolecular Interactions Governing Photocurrent-Voltage Relations in Ternary Organic Solar Cells", Tress W., Beyer B., Ashari Astani N., Gao F., Meloni S., Rothlisberger S., J. Phys. Chem. Lett. 7, 3936 (2016), IF: 9.353

46 - “Origin of unusual bandgap shift and dual emission in organic-inorganic lead halide perovskites”, Dar M. I., Jacopin G., S. Meloni‡, Mattoni A., Arora N., Boziki A., Zakeeruddin S. M., Röthlisberger U., Graetzel M., Science Advances 2, e1601156 (2016), IF: 11.511,

- Authors contribution reported in the article
- Press release “Sapienza” 21 December 2016, https://www.uniroma1.it/it/node/26174
- ESI “Highly Cited Paper” of the Web of Knowledge: “top one percent in each of the 22 ESI subject areas per year”

45 - “Ionic polarization-induced current-voltage hysteresis in CH3NH3PbX3 perovskite solar cells”, S. Meloni, T. Moehl, W. Tress, M. Franckevičius, M. Saliba, Y.H. Lee, P. Gao, M. K. Nazeeruddin, S. M. Zakeeruddin, U Rothlisberger, M. Graetzel, Nature Communications 7, 10334 (2016), IF: 12.124,

- Authors contribution reported in the article
- Press release EPFL 17 Febbraio 2016: https://actu.epfl.ch/news/solving-hysteresis-in-perovskite-solar-cells/
- ESI “Highly Cited Paper” of the Web of Knowledge: “top one percent in each of the 22 ESI subject areas per year”

44 - “Entropic Stabilization of Mixed A-Cation ABX3 Metal Halide Perovskites for High Performance Perovskite Solar Cells”, Yi C., Luo J., Meloni S.‡, Boziki A., Ashari-Astani N., Grätzel C, Zakeeruddin S. M., Röthlisberger U., and Grätzel M., Energy and Environmental Science 9, 656 (2016), IF: 29.518

- Mentioned in Science In Depth http://science.sciencemag.org/content/351/6269/113.full
- ESI “Highly Cited Paper” of the Web of Knowledge: “top one percent in each of the 22 ESI subject areas per year”

43 - “Valence and conduction band tuning in halide perovskites for solar cells applications”, Meloni S., Palermo G., Ashari Astani N., Grätzel M., Roethlisberger U., J. Mat. Chem. A 4, 15997 (2016), IF: 8.867

42 - “Clathrate structure-type recognition: application to hydrate nucleation and crystallisation”, Lauricella M., Meloni S.*, Liang S., English N. J., Kusalik P. G., Ciccotti G., J. Chem. Phys. 142, 244503 (2015), IF: 2.894

41 - “Free Energies for Rare Events: Temperature Accelerated MD and MC”, Meloni S.* and Ciccotti G., The European Physical Journal Special Topics, 10.1140/epjst/e2015-02418-7 (2015), IF: 1.862

40 - “Unravelling the Salvinia paradox: design principles for submerged superhydrophobicity”, M. Amabili, A. Giacomello, S. Meloni, and C.M. Casciola, Advanced Materials Interfaces 2, 1500248 (2015), selected for the cover and Materials Views, IF: 4.834

- Backcover of the issue
- Appeared in Materials Views,

39 – “Mechanism of the Cassie-Wenzel transition via the atomistic and continuum string methods” Giacomello A., Meloni S.*, Mueller M., Casciola C. M., J. Chem. Phys. 142, 104701 (2015), IF: 2.894

38 – “Nucleation of silicon nanoparticles in amorphous silicon dioxide matrices”, Meloni S.*, AIP Conf. Proc. 1624, 95 (2014)

37 – “Relaxation of a steep density gradient in a simple fluid: comparison between atomistic and continuum modeling.” M. Pourali, S. Meloni*, F. Magaletti, A. Maghari, C.M. Casciola and G. Ciccotti, J. Chem. Phys., 141, 154107 (2014), IF: 2.952

36 - “Methane Clathrate Hydrate Nucleation Mechanism by Advanced Molecular Simulations”, Lauricella M., Meloni S.*, English N. J., Peters B., Ciccotti G., J. Phys. Chem. C, 118, 22847 (2014), IF: 4.772

35 – “Massively parallel molecular dynamics simulation of formation of clathrate-hydrate precursors at planar water-methane interfaces: insights into heterogeneous nucleation”, English N., Lauricella M., Meloni S., J. Chem. Phys. 140, 204714 (2014), IF: 2.952

34 – “Equilibrium and Rate Constants, and Reaction Mechanism of the HF Dissociation in the HF(H2O)7 Cluster by ab Initio Rare Event Simulations”, Elena A., Meloni S.*, and Ciccotti G., J. Phys. Chem. A, 117, 13039 (2013), IF: 2.775

33 – “Geometry as a catalyst: how vapor cavities nucleate from defects” Giacomello A., Chinappi M., Meloni S., Casciola C. M., Langmuir 29, 14873 (2013), IF: 4.384

32 - “An observable for vacancy characterization and diffusion in crystal”, Geslin P.-A., Ciccotti G., and Meloni S.*, J. Chem. Phys. 138, 144103 (2013), IF: 3.122

31 - “Probing the Structures of Hydrated Nafion in Different Morphologies Using Temperature-Accelerated Molecular Dynamics Simulations”, Lucid J., Meloni S.*, McKernan D., Spohr E., Ciccotti G., J. Phys. Chem. C, 117, 774 (2013), IF: 4.835

30 – Editorial, Hansen J.-P., Meloni S., Vuilleumier R., Molecular Physics 111, 3335 (2013)

29 - "Metastable wetting on superhydrophobic surfaces: continuum and atomistic views of the Cassie–Baxter/Wenzel transition", Giacomello A., Chinappi M., Meloni S., Casciola C. M., Phys. Rev. Lett., 109, 226102 (2012), IF: 7.943

28 - “Early Stage of the Dehydrogenation of NaAlH4 by Ab Initio Rare Event Simulations”, Sterpone F., Bonella S., Meloni S.*, J. Phys. Chem. C, 116,19636 (2012), IF: 4.814

27 - “Cassie-Baxter and Wenzel States on a Nanostructured Surface: Phase Diagram, Metastabilities, and Transition Mechanism by Atomistic Free Energy Calculations”, Giacomello A., Meloni S.*, Chinappi M., Casciola C. M., Langmuir, 28, 10764 (2012), IF: 4.187

26 - “The influence of silicon nanoclusters on the optical properties of a-SiNx samples: A theoretical study”, Guerra R., Ippolito M., Meloni S., Ossicini S., Appl. Phys. Lett., 100, 181905 (2012), IF: 3.794

25 - "Theory and methods for rare events", Bonella S., Meloni S.*, G. Ciccotti, Eur. Phys. J. B, 85, 97 (2012) – invited review article, IF: 1.282

24 - "Combining rare events techniques: phase change in Si nanoparticles.", Orlandini S., Meloni S.*, Ciccotti G., J. Stat. Phys. 145, 812 (2011), IF: 1.397

23 - "Hydrodynamics from statistical mechanics: combined dynamical-NEMD and conditional sampling to relax an interface between two immiscible liquids.", Orlandini S., Meloni S.*, Ciccotti G., Phys. Chem. Chem. Phys. 13, 13177 (2011), IF: 3.573

22 - "Order-disorder phase change in embedded Si nanoparticles", Orlandini S., Meloni S.*, Colombo L., Phys. Rev. B 83, 235303 (2011), IF: 3.691

21 - "Hydrodynamics from dynamical non-equilibrium MD", Orlandini S., Meloni S.*, and Ciccotti G., AIP Conference Proceedings 1332, 77-95 (2011)

20 - "Atomistic structure of amorphous silicon nitride from classical molecular dynamics simulations.", Ippolito M. and Meloni S.*, Phys. Rev. B 83 165209 (2011), IF: 3.691

19 - "Temperature Accelerated Monte Carlo (TAMC): a method for sampling the free energy surface of non-analytical collective variables.", Ciccotti G. and Meloni S.*, Phys. Chem. Chem. Phys. 13, 5952 - 5959 (2011), IF: 3.573

18 – “Mechanisms of self-diffusion in stoichiometric and substoichiometric amorphous silicon dioxide”, Orlandini S., Meloni S.*, Ippolito M., Colombo L., Phys. Rev. B 81, 014203 (2010), IF: 3.774

17 – “Modified single sweep method for reconstructing free-energy landscapes”, Monteferrante M., Bonella S., Meloni S., Ciccotti G., Molecular Simulation 35, 1116 (2009), IF: 1.502

16 - “Calculations of free energy barriers for local mechanisms of hydrogen diffusion in alanates”, Monteferrante M, Bonella S., Meloni S., Vanden-Eijnden E, Ciccotti G, Sci. Model. Simul. 15, 187-206 (2008), IF: 0.883

15 – “Interface structure and defects of silicon nanocrystals embedded into a-SiO2”, Ippolito M., Meloni S.*, Colombo L., Appl. Phys. Lett., 93, 153109 (2008), IF: 3.726

14 - “Structural and electronic properties of metal doped organic semiconductors”, Zazza C., Meloni S., Palma A., Mod. Phys. Lett. B 22, 1609-1631 (2008) – invited review article, IF: 0.471

13 - “Dissociative vs. Molecular Adsorption of Phenol on Si(100)2x1: A First Principle Calculation”, Carbone M., Meloni S., Caminiti R., Phys. Rev. B, 76, 085332 (2007), IF: 3.172

12 – “Efficient particle labeling in atomistic simulations”, Meloni S*, Rosati M, Colombo L, J. Chem. Phys., 126, 121102 (2007), IF: 3.044

11 - “Quasi-One-Dimensional K-O Chain in PTCDA Thin Films: Evidence from First-Principles Calculations”, Zazza C, Meloni S, Palma A, Knupfer M, Fuentes GG, Car R, Phys. Rev. Lett. 98, 046401 (2007), IF: 6.944

10 - “Ab Initio Simulation of Carbon Clustering on an Ni(111) Surface: A Model of the Poisoning of Nickel-Based Catalysts”, Kalibaeva G, Vuilleumier R, Meloni S*, Alavi A, Ciccotti G, Rosei R, J. Phys. Chem. B, 110, 3638-3646 (2006), IF: 4.115

9 - “Molecular and Solid State (8-hydroxy-quinoline) aluminum Interaction with Magnesium: a First Principles Study”, Meloni S, Palma A, Kahn A, Schwartz J, Car R, J. Appl. Phys., 98, 023707 (2005), IF: 2.498

8 - “Computational Materials Science application programming interface (CMSapi): a tool for developing applications for atomistic simulations”, Meloni S.*, Rosati M., Federico A., Ferraro L., Mattoni A., Colombo L., Comp. Phys. Comm., 169, 462-466 (2005); IF: 1.644

7 - “Boron ripening in amorphous silicon by large scale molecular dynamics simulations”, Mattoni A, Colombo L, Meloni S, Federico A, Rosati M, Comp. Mater. Sci. 30, 43-149 (2004), IF: 1.424

6 - “Chemistry between magnesium and multiple molecules in tris(8-hydroxyquinoline) aluminum films”, Meloni S, Palma A, Schwartz J, Kahn A, Car R, J. Am Chem. Soc., 125, 7808-7809 (2003), IF: 6.516

5 - “Energy-dispersive X-ray diffraction on thin films and its application to superconducting samples”, Albertini VR, Paci B, Meloni S, Caminiti R, Bencivenni L, J. Appl. Crystallogr., 36, 43-47 (2003), IF: 2.324

4 - “SO2Cl2, SOCl2: energy dispersive X-ray diffraction, ab initio and molecular dynamics calculation”, Meloni S., Pieretti A., Bencivenni L., Albertini V.R., Sadun C., Caminiti R., Comput. Mater. Sci., 20, 407-415 (2001), IF: 0.67

3 - “A novel implicit Newton-Raphson geometry optimization method for density functional theory calculations”, Filippone F, Meloni S, Parrinello M, J. Chem. Phys., 115, 636-642 (2001), IF: 3.147

2 – “The monoclinic I2 structure of bassanite, calcium sulphate hemihydrate (CaSO4 – 0.5H2O)”, Ballirano P, Maras A, Meloni S, Caminiti R, Eur. J. Mineral., 13, 985-993 (2001), IF: 1.577

1 - “Low-energy electron scattering from the water molecule: Angular distributions and rotational excitation”, Gianturco FA, Meloni S, Paioletti P, Lucchese RR, Sanna N, J. Chem. Phys. 108, 4002-4012 (1998), IF: 3.147

Book chapters

1 - “Calculations of free energy barriers for local mechanisms of hydrogen diffusion in alanates”, Monteferrante M, Bonella S, Meloni S, Vanden Eijnden E, Ciccotti G in Lecture Notes in Computational Science and Engineering, 2009, Volume 68, 187-206

In Faith,

Simone Meloni