Curriculum Vitæ et Studiorum

Valentina Tozzini

Personal Data

Name	Valentina Tozzini
Current position	Senior Scientist, Istituto Nanoscienze–CNR (National Research Council) NEST–Scuola Normale Superiore
Work Address	NEST–Lab, piazza San Silvestro, 12, 56127 Pisa, Italy Tel: +39–050–509433 Fax: +39–050–509417 e-mail: valentina.tozzini@nano.cnr.it

Education

July 1988	High School Diploma (*Maturità Scientifica*) at Liceo Ulisse Dini, Pisa, Italy. Top marks
1988 – 1992	Undergraduate fellow in Physics at SNS (Scuola Normale Superiore), Pisa
1988 – 1992	Undergraduate student in Physics, University of Pisa
March 12th 1993	MS Degree (*Laurea*) in Physics, University of Pisa. Cum laude
1993	Degree in Physics (*Diploma*), SNS - Pisa
May – Oct 1993	Post-graduate fellowship at INFM (National Institute of Condensed Matter Physics - Genova, Italy) and SNS
1993 – 1997	PhD fellow, SNS Pisa
Oct 16th 1997	PhD in Physics. Cum Laude
1997 – 1999	School of Medical Physics, University of Pisa
Nov 11th 1999	Medical Physics Specialization. Cum Laude

Career

Nov 1997–Nov 1999	Post-Doc fellowship at INFM-SNS, Pisa
Dec 1999–Jan 2000	Visiting Researcher at the Institute of Theoretical Physics, University of Nijmegen (NL)
Feb 2000–Jun 2003	Temporary Research Scientist at NEST (National Enterprise for nanoScience and nanoTechnology) – INFM, Scuola Normale Superiore, Pisa
Sep 2003–Mar 2004	Visiting Scholar at UCSD (University of California, San Diego, US), Dept of Chemistry and Biochemistry
Jun 2003–Apr 2008	Tenure Track Research Scientist at INFM – CNR, NEST-SNS Lab, Pisa
Apr 2008–Jan 2010	Staff Research Scientist at INFM – CNR (NEST Lab)
Jan 2010–	Senior Research Scientist at Istituto Nanoscienze – CNR, NEST-SNS, Pisa

Notes

Aug 2007–Jan 2008 Maternity leave
Jun 2010–Nov 2010 Maternity leave
Jan 2008–Sep 2008 Part–time
Nov 2010–Jun 2011 Part–time

Research

Current research

VT's research currently focuses on multi–scale modeling of complex systems, based on the synergistic use and development of *ab initio* methods (mainly Density Functional Theory (DFT)), atomistic Force Field (FF) based simulations and coarse grained-mesoscale models. These methods are applied to the study and design of new materials for clean energy and advanced electronics and of bio-systems for applications in bio-molecular medicine.

Multi-scale modeling of graphene and other 2D materials

DFT and (newly developed) atomistic empirical FF are used separately or in multi-scale combination to study 2D materials and the relationship between their morphology and their properties. Recent applications include

- **The curvature induced enhancement of reactivity** of graphene is studied as a possible mechanism to control adhesion of hydrogen for storage, or of other chemicals for functionalization
- **The substrate– or environment–induced morphology** of graphene is studied: natural rippling of supported graphene, curvature changes induced by electric fields or substrate coupling (piezo-and flexo-electricity), creation and distribution of substitutional defects, chemical decoration/functionalization, and localized electronic states induced by the substrate defects
- **The structure and properties of nano-porous graphene** are studied, focusing on its use for H-storage, supercaps and batteries. A protocol for computer design of 3D structures with tailored porosity has been optimized
- **The properties of WS_2 flakes supported by graphene** are studied, focusing on electronics and superlubric behavior
- **The dynamical control of local curvature induced by coherent phonons** is studied as a mean to transport and pump gases (e.g. H_2) through graphene multi-layers or 3D frameworks

Multi-scale approaches for macro-bio-molecules

- **Coarse Grained (CG) models development**. Minimalist models at the single residue resolution for proteins and nucleic acids and Meso-Scale (MS) at the single bead per molecule resolution are developed, combining bottom-up and top down parameterization procedures, with the aim of including both accuracy and transferability into the models. The different resolutions (CG, MS and also atomistic) are eventually coupled in a full multi-scale approach.
- **Applications**: the aggregating protein β-2 microglobulin, the unstructured α -syn-nuclein, viral capsids, aggregation between proteins and functionalized metal particles.

Specific software tools are implemented for these tasks, designed to be interfaced with commonly used simulation softwares, and freely distributed (see www.muscade-lab.it).

Previous research

2004–2013 Multi-Scale modeling of DNA replication and expression: DNA unwrapping of nucleosomes, supercoiling and replication of plasmids and translocation in the ribosome.

2006–2010 Multi-Scale modeling of HIV-1 replication: dynamics of HIV-1 protease and integrase, including the effects of mutations and of crowder agents within the cytoplasm.

2001–2014 Multi-scale modeling of photactive proteins: Combined *ab initio* and FF-based study of the relationship between structural, optical and vibrational properties of (G)FPs. Coarse Grained-mesoscale dynamics of diffusion and aggregation of FPs within the cytoplasm. Photo-cycle of rhodopsins.

1999–2000 Study of the structural, electronic and vibrational properties of III-V semiconductor clusters with fullerene topology with DFT based approaches.

1997–1999 Study of a hybrid QM/MM approach for the simulation of macromolecular systems. Applications to metal and semiconductor clusters embedded in Zeolites.

1998–1999 Medical Physics Specialization: Molecular modeling techniques and applications to biological macromolecules and complex systems.

1997 Phase transitions and defects in quantum crystals study based on DFT.

1993–1996 PhD project: Vibrational properties of condensed systems near the solid-liquid transition. Applications to: ^{3}He and ^{4}He, (2D and 3D) Wigner crystals, metal intercalates in graphite, "fast sound" in water near freezing.

1993 Mechanical properties of high temperature solids (alkali halides) with DFT.

1992–1993 MS Thesis: Dispersion relations of phonons in solids near fusion within the Density Functional Theory.

Projects and Collaborations

Projects

2018–2020 **Graphene flagship core project 2**: Work Package 12 "Energy Storage" **Local unit coordinator**

2018–2020 **Cnr-SRNSF (Shota Rustaveli National Science Foundation) Bilateral project** within the agreement of Scientific Cooperation between Italy and Georgia: *Morphing graphene chemical properties: a Density Functional Approach* **Italian PI**

2016–2018 **GrapheneCore1**:*Graphene-based disruptive technologies* Work Package 12 "Energy Storage" **Local unit coordinator**

2017–2018 **SEED project, Cnr**: *LOPE- DeveLopment of a Coarse Grained MOdel for Nanoparticle-Protein IntEractions* **co-PI**

2016–2018 **SCIADRO project, Regione Toscana**: *Utilizzo di flotte e sciame di droni dotati di sensori e tecnologie abilitanti innovative per la sicurezza del territorio e degli aeroporti* **Participant**

2015–2017 **Marie Skłodowska-Curie Individual Fellowships**: *GRAFLEX: Graphene curvature, flexibility and reactivity control by means of external fields: theory and computer simulations.* **PI** and supervisor of K Kakhiani, georgian researcher

2013–2016 **Graphene Flagship**: *Graphene-Based Revolutions in ICT and Beyond-Graphene*, Work Package 9 "Energy applications". Since September 2015: **Local unit coordinator**

2013–2015 *Computer modeling and simulation of nucleic acids structure and dynamics.* **"Canaletto" project** (Ministry of Foreign Affairs) within the executive programme for scientific and technological collaboration between Italy and Poland, in collaboration with University of Warsaw. **Italian PI**

2008–2012 *Development of fluorescent proteins for optical nanoscopy oriented to the study of cellular dynamics.* National Project **PRIN 2008** in collaboration with: Univ Genova, Univ di Milano-Bicocca, Univ Parma and Univ Milano. **Local unit coordinator**

2006–2011 *Connecting Biology with Chemistry through Multiscale Theory and Computer Simulation.* **NSF-CRC grant** in collaboration with Univ of Utah, Center of Biophysical Modeling and Simulation. **International collaborator**

2004–2011 *Coarse Grained models for Proteins*, collaboration with McCammon Group, UCSD, within **NIH grant**. **International collaborator**

2006 *Design of inhibitors for the hepatitis C virus protease: A theoretical, computational and experimental approach.* Trans-national initiative **Galileo** in collaboration with Politecnico di Torino and Ecole Polytechnique (Paris). **Local coordinator**

2002–2004 *A new approach to drug design: from statistical mechanics to the screening of anti-viral drugs.* National project **FISR**, in collaboration with Univ Padova, SISSA – Trieste, Univ Palermo, Univ Roma, Univ Modena, CNR Pisa. **Local unit coordinator**

2002–2003 *Molecular dynamics of the green fluorescent proteins: An insight into the nature of the dark states.* **Progetto Avanzato (PA)**, funded by INFM. **PI**

Projects for accessing High Performance Computing resources

	Project	**Resource**	**Role**
2018–2019	**ISCRA-C**:*Morphing graphene chemical properties: a Density Functional Approach* (MGchpDFA)	Tier0 Intel-Lenovo 400K Marconi@CINECA	coll
2016–2017	**PRACE**: *Simulation driven Morphing of supported Graphene* (SMoG)	15Mh	PI
2016–2017	**ISCRA-C**: *Quasi Free Standing Graphene Monolayer on SiC with H coverage vacancies: A Density Functional Theory study* (QFSGvac)	200K	PI
2016–2017	**ISCRA-C**: *Reactivity and interactions manipulation of curved graphene* (ReIMCGr)	200K	coll
2015–2016	**ISCRA-C**: *Electro-mechanical manipulation of graphene reactivity* (ElMaGRe)	Tier0 IBM-BG/Q Fermi@CINECA 1Mh	PI
2015	**ISCRA-B**: *Flexoelectricity in naturally corrugated graphene: a DFT study* (FlexoGra)	7Mh	PI
2013–2014	**PRACE**: *Controlling Hydrogen Binding to Corrugated Graphene*	38Mh	PI
2013	**ISCRA-C**: *Hydrogen on buckled graphene* (HBG)	5Mh	PI
2010–2012	**iit grants** *Multi-scale simulations of biological and organic systems*, *Hydrogen storage on corrugated graphene*	∼5Mh	PI, coll
2008–2009	**INFM grant**: *Coarse Grained modeling of IFP-based FRET systems*	IBM-SP6@CINECA	PI
2006	**INFM grant**: *One-bead coarse grained models for structural transitions in nucleic acids*	IBM-SP5@CINECA	PI

2005	**INFM grant**: *A Coarse Grained Model for Molecular Dynamics Simulations of Biomolecular Aggregates*		PI
2003	**INFM grant**: *Photophysics of red and blue fluorescent proteins: tailoring fluorophores at the ends of the visible spectrum*	IBM-SP4@CINECA	PI
2002	**INFM grant**: *Modeling the dark states of the Green Fluorescent Proteins*	IBM-SP3@CINECA	PI
2001	**INFM grant**: *Modelling the Structure and Photodynamics of the Green Fluorescent Proteins*		PI

Other Collaborations

2018 –	*Development of Coarse Grained Models for biopolymers: fundamentals of reductionist approaches* with St.Petersburg Branch of the Steklov Research Institute of Mathematics and ITMO University, St Petersburg
2016 –	*Graphene modeling and functionalization* NTT Basic Research Laboratories, Japan; Kwansei Gakuin University, Japan
2004–2013	*Coarse Grained models for Nucleic Acids*, with Joanna Trylska's Group, Interdisciplinary Centre for Mathematical and Computational Modelling, Warsaw University
2005–2007	*Multi-scale model for the Nucleosome*, with Karine Voltz, Computational Biophysics Group at the University of Heidelberg
2006	*Chromophores of red homologues of GFPs* with Maurizio Persico's group, Dept of Chemistry, University of Pisa
2003	*Low frequency vibrational modes of GFPs*, with Salvatore Cannistraro's group, Biophysics and NanoScience Centre, Università della Tuscia (Italy)
1999–2006	*Ab initio simulations of chromophores* with Francesco Buda's group Gorlaeus Laboratories, Leiden University (NL)
1999–2000	*Ab initio simulations of semiconductor clusters* Annalisa Fasolino's group, Institute of Theoretical Physics, Univ of Nijmegen (NL)

Teaching

Curses and Lessons

2018– now	Module of *Numerical Methods for Physics* for MS degree in Physics, Univ of Pisa
2017– now	Module of *Condensed Matter Structure* course for BS degree in Physics, Univ of Pisa
2016– now	*Biophysics* course for MS degree in Materials and Nanotechnology, Univ of Pisa
2015–2018	*Computer Simulation Methods in Physics of Matter* course for MS degree in Physics, University of Pisa
2009– now	*Biophysics* course for MS degree in Physics, Univ of Pisa (a module since 2016-2017)
2009, 2012	Module of the the course of *Molecular Biophysics* for PhD in Biophysics at SNS
2008	Lessons at the CTBP Summer School *Coarse Grained Physical Modeling of Biological Systems: Advanced Theory and Methods* at UCSD
2007–2008	Module of the course *Computational structural biology* for PhD in Biophysics at SNS
2007	Module of the course *Introduction to the Structure of Matter* for MS Degree in Biology at SNS
2007	*A bottom-up approach to the biological matter: Experimental and modeling techniques from the (sub-)molecular to the macroscopic level*, course for PhD students in Applied Physics, University of Pisa
2002	*Computational Physics and Biology*, within the stage for MS students at SNS
1997	Practice lessons of *Thermodynamics and statistics* course for MS students at SNS

Students Tutorship

	Student	Degree	Thesis Title	Role
2018 **2014**	Tommaso Cavallucci	PhD Physics (Cond Mat)	Atomic and electronic properties of graphene based systems grown on silicon carbide: a Density Functional Theory study	Supervisor
2018	Antonella Meninno	MS Physics (Cond Mat)	JAGP and JLGVB: two *ansatzes* for the study of the electronic wave funciton of strongly correlated systems	Referee
	Matteo Becchi	MS Physics (Cond Mat)	Molecular Dynamics simulations of polymeric systems confined in thin films	Referee
	Andrea Cafforio	MS Physics (Cond Mat)	CO_2 adsorption on graphene/SiO_2 and on phosphorene substrates: the effect of surface corrugation	Referee
2017	Marcello Turtulici	MS Physics (Cond Mat)	Optical Properties of $SrNbO_3$	Referee
	Sara Fiori	MS Physics (Cond Mat)	Li-functionalized Graphene on Silicon Carbide	Referee
2015	Luca Pesce	MS Physics (Medical)	A minimalist model for the simulation of the structure and dynamics of disordered proteins	Supervisor
2014	Andrea Giuntoli	MS Physics (Theoretical)	A theoretical investigation of the fundamental properties of the minimalist models for proteins	Supervisor

	Tommaso Cavallucci	MS Physics (Cond Mat)	Density Functional Theory simulations of the electromechanical properties of naturally corrugated epitaxial graphene	Supervisor
	Antonio Rossi	MS Physics (Cond Mat)	Corrugated graphene hydrogenation with Density Functional Theory based simulations	Supervisor
2013	Marco Galimberti	MS Physics (Medical)	*Simulazioni di dinamica molecolare classica con modelli a bassa risoluzione della proteasi di HIV-1* – Classical Molecular Dynamics Simulations of HIV-1 protease with Coarse Grained Models	Supervisor
	Paolo Dell'Osso	MS Physics (Cond Mat)	*Impurezze Coulombiane in un foglio di grafene: soluzione analitica del problema di Dirac–Kepler* – Coulomb defects in a graphene sheet: analytical solution of the Dirac–Kepler problem	Referee
	Giulia LB Spampinato	MS Physics (Cond Mat)	A Minimalist Model for Simulation of Structure and Dynamics of Helical Polypeptides	Supervisor
	Anna Bochicchio	MS Physics (Cond Mat)	Multi–Scale simulations of β-2microglobulin	Supervisor
	Francesco Tavanti	MS Physics (Medical)	*Dinamica molecolare delle rodopsine con modelli multi-scala* – Molecular Dynamics of Rhodopsins with multi-scale models	Supervisor
2013 2008	Fabio Trovato	PhD Molecular Biophysics	Molecular Dynamics Simulations of biopolymers within the cell environment: Minimalist models for the Nucleic Acids and Green Fluorescent Proteins in the cytoplasm	Supervisor
2009	Paolo Elvati	PhD Chemistry	Modeling and application of a coarse grained force field for surfactants and polymeric membranes	Referee
2007	Fabio Trovato	MS Physics (Cond Mat)	*Modello Minimalista per Acidi Nucleici: studio delle proprietà e delle transizioni strutturali del DNA tramite dinamica molecolare* – Minimalist model for Nucleic Acids: a molecular dynamics study of properties and structural transitions of DNA	Supervisor
2004	Pietro Amat	MS Chemistry	*Proprietà elettroniche e strutturali del cromoforo di AsCP* – Structural and Electronic Properties of the asCP chromophore	Co-supervisor
2004 1998	Riccardo Nifosí	PhD Physics	Molecular mechanisms of Green Fluorescent Protein Photophysics	Co-supervisor
2010 1998			Occasional activity as tutor for undergraduate students at SNS	Tutor

Science popularization, dissemination and journalism

Sep 29 2018 Participation to the Science Picnic organized by the IliaUni Tbilisi State University, Tbilisi, Georgia. Installation, poster and practical demonstration about Graphene: the plastic of XXI century

Jul 2016 Article The future of graphene (Le prospettive del grafene) in the magazine "Platinum – Aziende e Protagonisti", special issue on Reserch and Innovation, July 2018, distributed with economy-oriented Newspapers (IlSole24Ore, in Italy)

Nov 20th 2017 Participation as Team teacher to the Mission Zero Astro-Pi challenge – a science and coding competition for students organized by ESA – in the primary school "Damiano Chiesa" (Istituto Comprensivo "Leonardo Fibonacci", Pisa, Italy). Introductory lesson for the class: Why does the International Space Station "flight"? Why do the astronauts float? (Perché la stazione spaziale "vola"? Perché gli astronauti fluttuano?)

Mar 6-10 2017 Series of lessons in the primary school "Damiano Chiesa" (Istituto Comprensivo "Leonardo Fibonacci", Pisa, Italy) organized within the framework of the Biophysics Week, on behalf of the SIBPA (Societ Italiana di Biofisica Pura e Applicata). Lessons title Matter and life: what happens when biologists and phyisicists work together? (Materia e vita: cosa succede quando biologi e fisici lavorano insieme?)

Nov 2016 Article Morphing graphene (La manipolazione del grafene) in the magazine "Platinum – Aziende e Protagonisti", special issue on Reserch and Innovation, November 2016, distributed with economy-oriented Newspapers (IlSole24Ore, in Italy)

Feb 16 2016 Conference Perché il grafene sta diventando il materiale del futuro? (Why is graphene the future material?), serie "Caffè-scienza Firenze & Prato", Prato, Palazzo Banci Buonamici

2014 – 2015 Member of the Scientific Committee of the Science Festival of Genoa.

Oct 2015 Interview for a contribution to PRACE Digest 2015, celebrating the achievements of women in HPC, page 30, (2015)

Mar 6 2014 Conference "Il grafene: dalla ricerca in laboratorio... ai grandi magazzini " (Graphene from laboratory reasearch to commercial centers), serie "iit si racconta... Caffè scientifici", Genova, Caffè Marescotti-Cavo.

Nov 18 2013 Conference La semplice complessità del grafene (The simple complexity of graphene), Auditorium della Regione FVG, Pordenone. Satellite conference for the annual Science Festival "Imparare Sperimentando"

Oct 2013 Contributions to the Internet Festival, Pisa : conference and talk show "Grafene Superstar"(Oct 11th); participation to the radiophonic program "Caterpillar" (Oct 10th), Radio2 ; interview for RaiNews24 .

Sep 2013 Co-funder of the no-profit cultural association "Hypatiæ – Arte e Scienza" aimed at organizing multicultural events connecting arts with science.

2008–2014 Contributor to "Fisica in Medicina" (the Bulletin of the Italian Medical Physics Society, see publication list)

2012–2013 Contributor to the section "ScienzaViva" to the on-line newspaper "Lo Schermo":

Due parole sul Premio Nobel per la Chimica 2013 (Oct 2013)

Speciale San Valentino: I segreti del cuore (Feb 2013)

Il Lego a DNA (Dic 2012)

Il Supercalcolatore di Kobe: Arriva dal Giappone il più potente computer mai creato (Oct 2012)

Feb 2012 Contribution with a didactic movie on graphene and hydrogen to the science exhibition "Imparare Sperimentando, 7th edition" (Pordenone, `http://www.impararesperimentando.it/`)

2011 Contribution to the press release and divulgation articles on national and local newspapers about Graphene

Interview for a radiophonic science news program on SBS radio (Melbourne – Italian section), about Graphene and Hydrogen

2009–2010 Co-author of scientific divulgation papers for italian on-line journals:

V. Pellegrini e V. Tozzini *La Nanotecnologia: un passaggio verso un mondo di opportunità* `http://www.capannoricreativa.org/ita/le_nanotecnologie.html`

V. Pellegrini e V. Tozzini *E l'uomo inventò il grafene artificiale* in *Villaggio Globale* Sett 2009 `http://www.vglobale.it/`

2008 Author of papers of non-technical papers about molecular modeling on the journal *Fisica in Medicina*

2008 Participation to a radiophonic science divulgation program (*Piacere Scienza*) on the italian station Radio Bruno

Assignments – Commissions of trust

2018–2024 National Habilitation as Full Professor of Applied Physics

2017–2023 National Habilitation as Full Professor of Condensed Matter Physics (Theory)

2017– Member of the Marie Curie Alumni Association (MCAA)

2016– Remote referee for ERC, StG, panel PE4 (Physical and analytical Chemical Sciences)

2015– Editorial Board of *Frontiers in Molecular Biosciences*, section "Bioiological Modeling and Simulations" (Reviewer Editor)

2015– Adjunct professor of *Computer Simulation Methods in Physics of Matter* at the University of Pisa, Dept of Physics

2011– Reviewer of projects for assignment of computer resources of class Tier within PRACE (Partnership for Advanced Computing in Europe), ISCRA (Italian SuperComputing Resource Allocation), and LISA (Interdisciplinary Laboratory for Advanced Simulation, Regione Lombardia) at CINECA

2009– Adjunct professor of *Biophysics* at the University of Pisa, Dept of Physics

2010–2016 Reviewer of international projects or national projects for other countries: Unit Through Knowledge Fund (Ministry of Science, Croatia, 2010), topic: properties of artificial amino-acids; NFS (USA, 2011), Topic: modeling of proteins; PISCOPIA program (co-fund of Marie Curie program, 2015), topic: dynamics of biomolecules; NWO (Netherlands, 2015), topic: magnesium doped graphene; SONATA BIS (National Polish Science Center, 2015), topic: design of proteins; HARMONIA (National Polish Science Center, 2016), topic: UNRES development; NWO (Netherlands, 2016), topic: modeling of photosystems

2013–2019 National Habilitation as Associate Professor of Condensed Matter Physics (Theory)

2013–2019 National Habilitation as Associate Professor of Applied Physics

2007–2008 Member of the CNR–INFM committee for the assignment of computational resources of the CINECA national supercomputing facility

2000– Regularly member of committees for PhD and Degrees, Post–Doc assignment and for students examinations

2000– Regular activity as reviewer for international journals including Nature Comm, JPC, JCTC, PRB, PRL and many others (see publons)

2000–2001 National habilitation as Professor of Mathematics and Physics in High Schools. In 2001, obtained a permanent position as Mathematics and Physics Professor in the High School Liceo Scientifico Statale "C Livi", (Prato, Italy), declined for incompatibility with the research scientist position

Languages

	spoken – comprehension	**written – reading**
Italian	Mother Language	
English	fluent	very good
Spanish	good	working knowledge
French	fair	fair
German	basic	basic

Basic knowledge and other skills

Professional expertise	Condensed Matter Physics, Computational Physics, Computer Modeling and Simulations, Materials Science, Biophysics, Biochemistry
Other technical skills	Programming in Fortran, C, Basic, Python; editing in html Long experience as user of software for molecular modeling and simulation Experience as system manager of workstations and clusters with Unix or Unix-like operating systems

Conferences

Invited Talks to Conferences

Sep 27–28 2018	Effects of supported graphene defects Symposium in honor of prof Giuseppe Grosso *A fresco of contemporary condensed matter physics* (Pisa Italy)
Sep 10–12 2018	Graphene imperfections: defects or effects? Italy/Canada Bilateral Workshop *Nanomaterials for Devices* (Montreal, Quebec, Canada)
Dec 12–16 2016	Morphing graphene for energy applications. Conference *Materials.it 2016* (Catania, Italy)
Feb 3–6 2016	Multi-scale simulations from graphene to macro-biomolecules. Workshop *Biophysics of Molecules: structure, dynamics and function* (Bressanone, Italy)
Sep 14–18 2015	Manipulating graphene properties at the nano-scale. Conference *GraphIta* (Bologna, Italy)
June 9 2015	Graphene manipulation at the nano-scale Workshop *Graphene Retreat 2015* (Lucca, Italy)
Dec 10 2014	Multi-scale simulations of Biomolecular systems. Workshop of The Science Europe Committee for Life, Environmental and Geo Sciences *Computational modelling of complex spatial structures and processes in Natural and Life Sciences* (Bruxelles)
Nov 20–21 2014	Minimalist Models for proteins: The past and the future. Workshop CECAM *Advanced modeling to investigate biomolecules* (Genoa)
Oct 20–21 2014	Hydrogen Storage in Graphene. Workshop Graphene Connect – *Energy Application* (Dresden)
Jun 17–20 2014	Multi-Scale Simulations of Rippled Hydrogenated Graphene. Workshop *New Frontiers in Multiscale Modelling of Advanced Materials* (Trento, Italy)
June 12 2014	Multi-Scale modeling and simulation Devices development: MuScaDe. Meeting of Compunet, the computational platform of Italian Institute of Technology
Sep 11–13 2013	Multi-Scale molecular dynamics in soft matter. Industrial Forum for Multiscale Materials Modelling and Training (Bologna)
Sep 19–20 2012	Controlled (de-)hydrogenation of corrugated graphene. XCVIII Congresso Nazionale della Società Italiana di Fisica (Napoli)
Sep 2–6 2012	Minimalist models of Biopolymers: Latest advances and applications. Conference TACC 2012, *Theory and Applications of Computational Chemistry* (Pavia, Italy)
Jul 9 2012	Reversible Hydrogen Storage by Controlled Buckling of Graphene Layers. Workshop *Graphene Day* (Pisa, Italy)
Jun 20–21 2012	Hydrogen on corrugated graphene. SINFO Workshop (Parma, Italy)
Mar 25–29 2012	Minimalist model for Biopolymers: recent applications open problems and perspectives 243rd American Chemical Society Meeting, Symposium in Honor of Andy McCammon (San Diego, CA).
Sep 7–10 2009	One-Bead Models for Biopolymers: State of the art, open problems, perspectives. CECAM Workshop *Coarse-Graining Biological Systems: Towards Large-Scale Interactions and Assembly* (Lausanne).
Jul 11–15 2009	Bridging atomistic– and meso–scale with minimalist models for biomolecules. European Biophysics Congress (Genoa 2009).
Dec 19 2008	Minimalist models for large-scale modeling of bio-systems. Conference *Winter Modeling 2008* (Cnr Pisa, Italy).
Aug 11–15 2008	One Bead Coarse Grained Models: the Balance between Accuracy and Predictive Power. CTBP Summer School *Coarse Grained Physical Modeling of Biological Systems: Advanced Theory and Methods* (UCSD)
Jun 23–27 2008	A multi-scale approach to the photophysics of the intrinsically fluorescent proteins. CPMD 2008 *Modeling and computation of structure and dynamics of condensed phase systems* (ICTP, Trieste, Italy)
Jul 3–7 2006	Variation of Color and Photodynamics within the family of Intrinsically fluorescent Proteins. Meeting of the Psi-k Network *Progress in ab initio modeling of biomolecules: methods and applications* (Lorentz Center – Leiden)
Oct 4–7 2005	Extremely Coarse Grained Models for Large Time-scale Molecular Dynamics Simulations. Workshop *Multiscale Modeling in Biological Systems* (Snowbird, Salt Lake City, Utah).
Sept 10–11 2004	Modeling Intrinsically Fluorescent Proteins. *Highlights in the quantum theory of condensed matter* - A symposium to honor Mario Tosi on his 72nd birthday (Pisa SNS, Italy).
May 15–16 2004	Modeling the Intrinsically Fluoresecent Proteins. Workshop INFM-Democritos-Psi-K *Ab Initio Modeling in Biological Systems* (SISSA, Trieste).

Oct 28–Nov 8 2002	Modeling Photophysics and Optical Switching in Green Fluorescent Proteins. Workshop ICTP-INFM *Entanglement at the Nanoscale* (Trieste, Italy)
Sep 21–22 2001	Modeling the Photophysics of the Green Fluorescent Proteins. Workshop: *Single particle methodologies in biophysics and biotechnology* (LENS, Firenze, Italy).
Mar 25–28 2001	Formazione e Stabilità di Fullereni di semiconduttori III-V *XX Convegno di Fisica Teorica e Struttura della Materia* Fai della Paganella (Trento, Italy)
Nov 25–28 1998	Dinamica Molecolare Ibrida Classica–Ab initio per simulazione di macromolecole. Annual Meeting of section GNSM "Collective Properties" of Cnr (Perugia, Italy).
Jun 10–12 1998	Simulazioni di dinamica molecolare: uno strumento di indagine microscopica in campo biomedico. Conference *Procedure operative di misura e valutazioni dosimetriche nelle attività sanitarie* (San Miniato, Pisa, Italy)

Invited seminars

Feb 23 2016	Multi-scale simulations from bio-molecules to graphene. *Colloquia* of the dept of Physicis of University of Pisa. Host: Prof Alejandro Kievsky
Sep 16th 2014	Multi-scale modeling of complex systems: Theory, implementation and application. Jülich Forschungzentrum – IAS – GRS. Host: Prof Paolo Carloni
Jan 15 2014	Hydrogenated-rippled graphene: a multi-scale approach. University of Trento, Lab of bio-inspired & graphene nano-mechanics. Host: Prof Nicola Pugno
Dec 7 2011	Minimalist models for bio-molecules: open problems and perspectives. University of Modena and Reggio Emilia. Host: Prof Elisa Molinari
Oct 24 2005	Coarse Grained Models for Large Time-scale Molecular Dynamics Simulations. ICM (Interdisciplinary Center for Mathematical and Computational Modeling) - Warsaw University. Host: Prof Joanna Trylska
Jan 9 2004	Modeling the optical switching in green fluorescent proteins. CTBP (Center for Theoretical BioPhysics) UCSD (University of California San Diego). Host Prof J.A. McCammon
Nov 20 2002	Molecular Modeling at NEST: methods and applications. SienaBiotech (siena Italy)
Nov 23 2001	Tecniche di simulazione QM/MM applicate a sistemi biologici. Università della Tuscia – Viterbo. Host: Prof Salvatore Cannistraro
Feb 14 2001	Modelling the Photophysics of Green Fluorescent Protein. SISSA (Trieste, Italy). Host: prof Paolo Carloni
Feb 8 2001	A Molecular Dynamics approach to the study of III-V semiconductor Fullerenes and Green Fluorescent Proteins. ESRF (Grenoble, France). Host Dr Fabio Pistolesi
Feb 3 2000	An Hybrid Quantum–Classical Approach to Molecular Dynamics Simulations of Complex Systems. Institute of Theoretical Physics, University of Nijmegen. Host Prof Annalisa Fasolino
Apr 12 1999	Meccanismi di Fluorescenza delle Green Fluorescent Proteins: Fenomenologia e Modelli. Institute of biophysics – Cnr (Pisa)
Dec 18 1998	Dinamica Molecolare Ibrida Classica–Ab initio per simulazioni di Macromolecole. Applicazioni a zeoliti e cromofori naturali .University of Rome III Host. Prof Mauro Rovere
Apr 9th 1997	Applicazione della Teoria del Funzionale di Densità allo studio di proprietà vibrazionali di sistemi condensati vicino alla transizione liquido-solido. University of Modena. Host: prof Elisa Molinari
Nov 1995	DFT: applicazione al calcolo delle curve di dispersione dei fononi in cristalli fortemente anarmonici. Università dell'Aquila. Host: Prof Giancarlo Ruocco

Contribution to Conferences (only those as presenting author)

Oct 29–30 2018	Substrate induced defects in graphene as opportunities for advanced applications. NANO-meeting 2018 (Pisa). **Poster**
Apr 19–22 2016	Morphing graphene at the nano-scale: from simulations to applications. Conference *Graphene 2016* (Genoa). **Poster**
Jun 24 2015	Hydrogen interaction with statically and dynamically rippled graphene. Conference *Graphene Week 2015* (Manchester). **Poster**
Apr 23 2015	Simulazioni multi-scala in materia condensata: un progetto che dura da mezzo secolo. Congressino del Dipartimento di Fisica, (Pisa, Italy). **Poster**
Jun 23–27 2014	Designing graphene for energy applications. Conference *Graphene Week 2014* (Gothemburg). **Talk**

May 8 2014	Multi-Scale Simulations of Graphene for Energy Applications. Conference *Graphene 2014* Toulouse (France). **Talk**
Sep 2–5 2013	A quantum-atomistic-continuum 3-scale modelling of graphene hydrogenation. International Conference on Diamond and Carbon Materials, Riva del Garda (TN). **Talk**
Feb 21–22 2011	Multi-Scale modeling NEST. I Workshop on Condensed Matter Physics and Computational Material Science DMD-Cnr 2011 (Roma). **Talk**
Apr 30– May 4 2005	A Coarse Grained Model for slow and anharmonic motions in proteins and macromolecular aggregates: Applications to HIV-1 protease and the 70S Bacterial Ribosome. VI European Symposium of the American Protein Society (Barcellona, Spagna). **Poster**
Oct 13–18 2003	Modeling the molecular mechanism of optical switching in Green fluorescent Proteins. First International Meeting on Applied Physics (Badajoz, Spain). **Poster**
Jun 23–25 2003	Photophysics of red and blue fluorescent proteins: tailoring fluorophores at the ends of the visible spectrum. INFMeeting 2003, (Genova, Magazzini del Cotone). **Poster**
Jun 24–28 2002	Engineered GFP dynamics for biomolecular electronics and protein monitoring. INFMeeting 2002, (Bari). **Talk**
Apr 18–19 2002	Proteine Verdi Fluorescenti per la Bioelettronica. *Workshop dei Ricercatori INFM* (Genoa). **Talk**
Jun 18–22 2001	Spontaneous Formation and Stability of III-V Semiconductor Hollow Clusters: an *Ab Initio* Study of a new Class of Fullerenes. INFMeeting 2001 (Roma–EUR). **Talk**
Jun 14–18 1999	An Hybrid Quantum–Classical Molecular Dynamics Simulation for Semiconductor Clusters in Zeolites. INFMeeting 1999 (Catania, Italy). **Talk**
Jun 25–30 1998	A Combined Quantum-Classical Method for Molecular Dynamics Simulations of Large Systems. INFMeeting 1998, Rimini **Poster**
Apr 22–25 1996	Dispersion curves of highly anharmonic phonons in 2-d Wigner crystal via density functional theory. Conference of the Condensed Matter Division of European Physical Society (Baveno-Stresa, Italy). **Poster**
Mar 30– Apr 2 1996	Curve di dispersione di fononi fortemente anarmonici nel cristallo di Wigner bidimensionale. XV Convegno Nazionale di Fisica Teorica e Struttura della Materia (Fai della Paganella, Trento). **Poster**
Jul–Aug 1995	^{4}He: links between spectrum of liquid near crystallization and vibrational properties of solid near melting. Workshop *Classical and Quantum Liquids* (ICTP, Trieste, Italy). **Talk**
May 29– Jun 11 1995	^{4}He: links between spectrum of liquid near crystallization and vibrational properties of solid near melting. National Condensed Matter Physics Conference (Napoli, Italy). **Poster**
Apr 8–11 1995	^{4}He: legami tra lo spettro del liquido vicino alla cristallizzazione e le proprietà vibrazionali del solido vicino alla fusione. XIV Convegno Nazionale di Fisica Teorica e Struttura della Materia (Fai della Paganella, Trento). **Poster**
Jul 1994	DFT applied to vibrational properties of solids near melting. Workshop *Strongly Correlated electron Systems* (ICTP, Trieste). **Talk**
Jul 1994	Phonons in quantum Solids near Melting. Workshop *Classical and Quantum Liquids* (ICTP, Trieste). **Talk**
Apr 6–9 1994	Proprietà vibrazionali ed elastiche del cristallo di Wigner di elettroni prossimo alla fusione. XIII Convegno di Fisica Teorica e Struttura della Materia (Fai della Paganella, Trento). **Poster**

Organization of Scientific Meetings & Chairing

Feb 4–6 2019	CECAM Workshop Multiscale modelling from Macromolecules to Cell: Opportunities and Challenges of Biomolecular Simulations, (Lausanne, Switzerland). **Organizer and Scientific Committee Member**
Dec 12–16 2016	Conference Materials.it 2016 (Catania, Italy). **Chair person** of the Session: *Mechanical properties of 2D materials composites*
Sep 22–26 2014	100^o National congress of SIF (Società Italiana di Fisica), Pisa. **Chair person** of the *Condensed Matter Physics* session
Jun 22–25 2005	MMD-Meeting - Matter, Materials and Devices (Genova). **Coordinator of topical session** Simulating biomolecular systems
Jul 14–19 2003	Conference New Frontiers in NanoBiotechnology: monitoring protein function with single-protein resolution ICTP, Trieste (Italy). **Director**

Project meetings

Sep 28 – Oct 2 2018	Bilateral Italy–Georgia Meering. Tbilisi, Georgia.
May 24–25 2018	Graphene-Core2 WP12–SPH5 Meeting, Palaiseau, France. **Talk**
Oct 23–24 2017	WP12 Graphene-Core1 Progress Meeting, Cambridge, UK. **Talk**
Apr 6 2017	WP12 Graphene-Core1 Progress Meeting, Bologna, Italy. **Talk**
Nov 2–3 2016	WP11-WP12 Graphene-Core1 Progress Meeting, Grenoble, France. **Talk**
Aug18–19 2016	WP12 Graphene-Core1 Storage Task meeting, Umeå, Sweden. **Talk**
May 5-6 2015	WPE.4 Hydrogen Storage@Cnr-NANO. Graphene Flagship: WP9 Progress report meeting, Rome, Tor Vergata. **Talk**
Mar 9–14 2915	*Graphene 2015* and *CELENEC Workshop* (Standardization committee), (Bilbao, Spain)
Oct 21–22 2014	WPE.4 Hydrogen Storage@Cnr-NANO, Graphene Flagship: WP9 Progress report meeting, Dresden. **Talk**
May 12–13 2014	WPE.4 Hydrogen Storage@Cnr-NANO. Graphene Flagship: WP9 Progress meeting, CEA, Grenoble.**Talk**
Jan 15–2014	T 9.4 Hydrogen storage. WP9.4 Meeting, Flagship Graphene. (FBK Trento) **Talk**
Jan 14- 2014	Hydrogen interaction with graphene: modeling and simulations. TI-Itron meeting, (iit genova). **Talk**
Nov 4–5 2013	Hydrogen Storage in Graphene Kick-off meeting, WP9 Flagship Graphene (iit, Morego, Genova). **Talk**
Sep 14–16 2011	Reversible hydrogen storage by controlled buckling of graphene layers. Graphene Roadmap Consultation Workshop: First Principle Computational Methodologies for 2D Materials, Lancaster (UK). **Talk**
Oct 5–6 2010	Multiscale Molecular Modeling@NEST Kick-off meeting of the Institute of Nanoscience-CNR (Matraia, Lucca). **Poster**

Attended Workshop, Schools and Curses

Jun 27–30 2001	11^{th} Annual Meeting of the ICRS (International Cannabinoids Research Society), San Lorenzo de El Escorial (Madrid).
Mar 7–16 2000	"Life Science Regional Training Workshop", Università di Modena. Attended curses: (i) Advanced Hypothesis/3D Database Techniques; (ii) Structure-Based Drug Design with Insight II; (iii) Introduction to Life Science Modeling with Insight II; (iv) Homology-Based Protein Design
Apr 28 1999	Workshop "MSI Software for materials and life science" (CINECA Bologna)
Feb 17–19 1999	"Cardiovascular Radiation Therapy III" (Washington D.C.)
Jun 22– Jul 6 1997	research Workshop on condensed matter physics (ICTP, Trieste): Miniworkshop on "Quantum Monte Carlo simulation of Liquids and Solids"
Jul 1–17 1996	Research Workshop on condensed matter physics (ICTP, Trieste); Adriatico research conference "The electron quantum liquid in systems of reduced dimensions"; Miniworkshop "Strong electron correlations"
Sep 29– Oct 9 1996	3rd Balkan School of Physics, "Highlights in Condensed Matter Physics" (Kas-Antalia, Turkey)
Oct 1995	VI Scuola Nazionale di Fisica della Materia, (Villa Gualino, Torino, Italy)
Sep 1994	V Scuola Nazionale di Fisica della Materia, (Villa Gualino, Torino)
Oct 1993	IV Scuola Nazionale di Fisica della Materia, (Villa Gualino, Torino)
Jul 1993	Workshop "Strongly correlated Electron Systems" at ICTP
Aug 1992	Workshop "Correlated Electron Systems" and "Classical and Quantum liquids" at ICTP (International Centre of Theoretical Physics, Trieste