Curriculum Vitæ et Studiorum

Valentina Tozzini

Personal Data

Name	Valentina Tozzini
Current position	Researcher, Istituto Nanoscienze – CNR, NEST–Scuola Normale Superiore
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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 Researcher 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 Researcher at NEST – INFM – CNR (the National Research Council, Italy)
Apr 2008–Jan 2010	Researcher at NEST – INFM – CNR
Feb 2010–	Researcher at Istituto Nanoscienze – CNR, NEST-SNS Pisa

Notes

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

Research

Current research

VT's research currently focuses on multi–scale modeling of complex systems (biologic/organic molecules and materials), based on the synergistic use of *ab initio* methods (mainly Density Functional Theory (DFT)), atomistic Force Field (FF) based simulations and Coarse Grained-mesoscale models, with the aim of addressing the macroscopic scales in simulations without loosing the molecular scale accuracy. Applications are in bio-medical fields and in new technologies for energy and advanced electronics.

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. The parameterization strategy combines bottom-up with top down 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**
  - **HIV-1 replication cycle**: simulation of the action mechanisms of HIV-1 protease and HIV-1 integrase, including effect of mutation and of crowder agents within the cytoplasm.
  - **DNA replication and expression**: study of the first steps of DNA unwrapping in the nucleosomes and the supercoiling and denaturation bubble formation in plasmids were studied. Dynamics and translocation step in the Ribosome.
  - **Diffusion and aggregation of Green Fluorescent Proteins** within the citoplasm; Photo cycle of **Rhodopsins**.
  - **Currently in progress** the aggregating protein β-2 microglobulin, the unstructured α -syn-nuclein, viral capsids and particles.

Multi-scale modeling of Graphene-based materials

Graphene-based systems are studied with combining DFT with empirical force field based simulations with specific focus on controlling and exploiting the sheet rippling for applications

- **The curvature induced enhancement of reactivity** is evaluated as a possible mechanism to control hydrogen (or other chemicals) adhesion/detachment, for storage, functionalization or tailoring of electronic properties
- **The dynamical curvature control 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
- **Strategies to control local curvature** are evaluated, including flexo-electricity, functionalization with optically controllable spacers/pillars or coupling to piezo-electric substrates

Specific software tools are implemented for these tasks, designed to be interfaced with commonly used simulation softwares, and freely distributed.

Previous research

2001–2010	Photo-physics of the (Green) Fluorescent Proteins: combined *ab initio* and FF-based study of the relationship between structural, optical and vibrational properties
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, 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

2016–	**GrapheneCore1**:*Graphene-based disruptive technologies* Work Package 12 "Energy Storage" **Local coordinator**
2015–2017	**Marie Skłodowska-Curie Individual Fellowships**: *GRAFLEX: Graphene curvature, flexibility and reactivity control by means of external fields: theory and computer simulations*. **Principal Investigator** 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 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. **Local coordinator**
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 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 antiviral drugs*. National project **FISR**, in collaboration with Univ Padova, SISSA – Trieste, Univ Palermo, Univ Roma, Univ Modena, CNR Pisa. **Local 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. **Principal Investigator**

Projects for accessing High Performance Computing resources

	Project	Resource		Role
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

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

2015– *Computer Simulation Methods in Physicis of Matter*, course for MS degree in Physics, University of Pisa

2009– *Biophysics*, course for MS degree in Physics, University of Pisa

2009, 2012 Lessons within the course of *Molecular Biophysics* for PhD students at SNS

2008 Lessons at the CTBP Summer School *Coarse Grained Physical Modeling of Biological Systems: Advanced Theory and Methods* at UCSD

2007–2008 Lessons within the course *Computational structural biology* for PhD students at SNS

2007 Lessons within the course *Introduction to the Structure of Matter* for undergraduate students 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
– **2014**	Tommaso Cavallucci	PhD Physics (Cond Mat)		Supervisor
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

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)
March 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 .
2008 –	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

2015–	Editorial Board of *Frontiers in Molecular Biosciences*, speciality section "Mathematics of Biomolecules" (Reviewer Editor)
2015–	Adjoint professor of *Computer Simulation Methods in Physicis 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–	Adjoint professor of *Biophysics* at the University of Pisa, Dept of Physics
2014–2017	National Habilitation as Associate Professor of Theory of Condensed Matter Physics
2014–2017	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
Jun 2005	Coordinator of the Topical Session *Simulation biomolecular systems* at MMD Meeting (Genova)
Jul 2003	Director of the conference *New Frontiers in NanoBiotechonolgy* (SISSA, Trieste)
2000–	Regularly member of committees for PhD and Degrees, Post–Doc assignment and for students examinations
2000–	Regular activity as reviewer for international journals (Phys Rev Lett, J Phys Chem, J Chem Phys, Phys Rev, Biophys J, Biochemistry etc) Occasional activity as reviewer for national and international projects
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 researcher 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, Biophysics, Biochemistry
Other technical skills	Programming in Fortran, C, Basic; 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