CURRICULUM VITAE

Rosa Di Felice

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BRIEF CURRICULUM VITAE

Rosa Di Felice

Visiting Associate Professor University of Southern California, Dept. Physics&Astronomy
Senior research staff member of the Italian National Research Council (CNR), Institute of Nanoscience
CITIZENSHIP: Italy – LANGUAGES: Italian (mother tongue), English (fluent)
DATE OF BIRTH: 13th April 1967
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PROFESSIONAL HISTORY

- Associate Professor (tenure track) of Physics and Astronomy, University of Southern California, Los Angeles, CA, USA (1/1/2018-).
- Visiting Associate Professor of Physics and Astronomy, University of Southern California, Los Angeles, CA, USA (8/16/2017-12/31/2017).
- Associate Professor (Research) of Physics and Astronomy, University of Southern California, Los Angeles, CA, USA (10/1/2016-5/31/2017).
- Adjunct Associate Professor (Research) of Physics and Astronomy, University of Southern California, Los Angeles, CA, USA (9/1/2015-9/30/2016)
- Associate Professor (Research) of Physics and Astronomy, University of Southern California, Los Angeles, CA, USA (9/1/2013-8/31/2015).
- Senior CNR research staff member at the Center S3, CNR-NANO Institute, Modena, Italy (04/2009-).
- Member of the research staff of INFM-CNR at the National Center S3 in Modena, Italy (06/2006-04/2009).
- Tenure Track INFM Researcher, INFM National Center S3, Modena, Italy (01/2003-05/2006).
- Fixed-term INFM Researcher, Unit of Modena, Italy (12/1999-12/2002).
- INFM Postdoctoral Research Assistant, Department of Physics, University of Modena and Reggio Emilia, Modena, Italy (12/1997-11/1999).
- DARPA Postdoctoral Research Assistant, Xerox Palo Alto Research Laboratory, Palo Alto, CA, USA (01/1996-01/1998).

EDUCATION HISTORY

- 1992-1995: PhD in Physics, University of Rome “Tor Vergata”, Rome, Italy. Defense 17/10/1996, University of Bologna, Bologna, Italy.
- 1986-1992: BSc & MSc in Physics, University of Rome “Tor Vergata”, Summa cum Laude. Defense 10/04/1992, University of Rome “Tor Vergata”, Rome, Italy.

VISITING STAYS

- 1 year 2012: Dept. Biological Sciences, Molecular and Computational Biology section, University of Southern California, Los Angeles, CA, USA.
- 3 months October-December 2011: Dept. Physics, University of Southern California, Los Angeles, CA, USA.
- 3 weeks May 2010: Dept. Physics, University of Southern California, Los Angeles, CA, USA.
- 3 weeks September 2008: CNMS at Oak Ridge National Laboratory, TN, USA.
- 1 week July 2008: Institute of Physical Chemistry at the Hebrew University of Jerusalem (HUJI), Israel.
- 1 week August 2007: Institute of Physical Chemistry, HUJI, Jerusalem, Israel.
- 3 weeks December 2004 – January 2005: Department of Physics, University of São Paulo, Brazil.
- 1 week November 2004: Tel Aviv University and Hebrew University of Jerusalem, Israel.
- 3 weeks December 2003: Department of Physics, University of São Paulo, Brazil.
- 2 weeks August-September 2003: Department of Chemistry, Princeton University, NJ, USA.
- 1 month December 2002: Department of Physics, University of São Paulo, Brazil.

- 1 month March-April 2002: Department of Chemistry, Princeton University, NJ, USA.
- 1 month October 2001: Department of Chemistry, Princeton University, NJ, USA.
- 2 months April-May 2001: Department of Physics, University of São Paulo, Brazil.

RESEARCH INTERESTS (APPENDIX I).

Keywords. Theoretical biophysics, structure and electronic properties of DNA and proteins, conformational flexibility and thermodynamics, charge transfer in biological systems, molecule/surface interactions, biomolecular nanostructures, protein-DNA binding, hybrid materials and bio-nano-systems, Density Functional Theory, Molecular Dynamics, Quantum Computation applied to problems in nanosciences and biology.

RESEARCH SUPPORT (APPENDIX II)

- "Distributed Bridge Collaboration via Multiple Videowalls". USC Bridge Catalyst award – 100 k$ for three faculty, with Richard Weinberg (Cinematic Arts) and Art Toga (Neuroscience).
- "Classical and Quantum Computation in Nanoscience". USC WiSE major support – 25 k$. 06/2014-05/2015.
- MOPROSURF – "Modeling protein-surface interactions", co-PI. 590 k€ by the Italian Institute of Technology (IIT). 04/2010-09/2013.
- "Multi-scale modeling of chemically modified DNA sequences for nanotechnology and molecular biology", PI. 70 k€ by the Foundation CRMO, Modena, Italy. 09/2010-08/2012. International partner: CNMS at Oak Ridge National Laboratory, TN, USA.
- "Controlling the structure and function of metal supported organometallic nanostructures", co-PI. 40 k€ by the Italian Ministry for Research, 09/10-08/12.
- EC NANOSCI-ERA "Single Nano-Hybrid", PI. 04/2007-12/2010. 160 k€.
- EU IST-FET Open Project "DNA-based Nanodevices" (FP6, contract FP6-029192), PI. 05/2006-09/2010. 150 k€.
- EU IST-FET Open Project "DNA-based nanowires" (FP5, contract IST-2001-38951), PI. 01/2003-07/2006. 200 k€
- CNR-CNPq bilateral agreement (Italy-Brazil) "Electronic Properties of Biomolecules with Potential Applications in Electronic Devices" (2003-2004). Funding for visiting stays, 10 k€.
- Several supercomputing projects on a yearly basis from 2000 on.

PROFESSIONAL SERVICES

- Committees at USC: CBB Faculty evaluation 2017 (Dept. of Biological Sciences); CBB Faculty promotion 2016 (Dept. of Biological Sciences).
- Graduate committees at USC: Van Ngo (PhD defense, Physics, 10/2013); Atanu Acharya (qualifying, Chemistry, 01/2014; PhD defense, Chemistry, 10/18/2016); Roelof Groenewald (qualifying, Physics, 11/2015); Gaurav Kumar (qualifying, Chemistry, 01/2016); Jared Sagendorf (qualifying, Physics, 01/2018).
- CNR: Member of the Executive Board at S3 Modena (03/2004-12/2012); Member of the CNR editorial board (03/2010-12/2012); Member of search committees (Appendix IX).
- Associate Editor: European Physical Journal B, Springer (06/2008-); Scientific Reports, Nature (04/2013-).
- European Science Foundation: Member of the Steering Committee of the Psi-K network.
- Referee for international journals (Nature Nanotech., Nature Comm., Phys. Rev. Lett., Nano Lett., Phys. Rev. B, Appl. Phys. Lett., J. Appl. Phys., J. Am. Chem. Soc., J. Phys. Chem., Solid State Comm., Surf. Sci., J. Comput. Electronics, Nanotechnology, Eur. Phys. J. B, Biochimie).
- Referee for international funding bodies: National Science Foundation (NSF, USA), Austrian Science Fund (FWF, Austria), European Commission FP6 and FP7.
- Referee of Habilitation Thesis: Robert Stadler, University of Vienna, January 2011.
- Referee of external PhD thesis: Audrius Alkauskas (Basel, Switzerland, January 2006); Daniele Varsano (San Sebastian, Spain, March 2006).
- Conference organization: (1) Co-organizer of CECAM Workshop "Synergies between quantum computing and high-performance computing". Venue: ETH Zürich, Switzerland. August 22-24,

2017. (2) Co-Chair of the workshop "Hybrid excitations in nano-materials". Venue: Center S3 CNR-NANO, Modena, Italy. December 18-20, 2011. (3) Chair of the ESF (European Science Foundation) Conference on "Charge Transfer in Biosystems". Venue: Universitätszentrum Obergurgl, Obergurgl, Austria. July 17-22, 2011. (4) Chair of the EC-IST-FET-38951 Workshop "DNA-based Nanowires: on the Way from Biomolecules to Nanodevices". Venue: National Center S3 of INFM-CNR, Modena, Italy. October 7-8, 2005. More events in Appendix III.

TEACHING (APPENDIX IV).

- Undergraduate. Exercise classes on General Physics I (mechanics and thermodynamics) and II (electromagnetism and optics). University of Modena and Reggio Emilia. A total of 130 h 1998-2002. PHYS 162 (Honors class "Introduction to Electricity and Magnetism), Spring 2016, 4 units, USC [evaluation 5.00/5.00]. PHYS 408a (advanced electrostatics and magnetostatics), Fall 2016, 4 units, USC [evaluation 4.56/5.00].
- Topical lectures. Tips to write successful proposals within the FP7-ICT-FET initiative of the European Commission (CNR course on research management for staff members – Genova, Palermo, Roma 2009 & 2010).
- Guest lecturer in BISC 481 at USC (taught by Remo Rohs, Biology Department). Lecture on "The basics of Molecular Dynamics" (30 min in October 2012, 80 min in October 2013).

SUPERVISION & HOSTING (APPENDIX V).

- 7 PhD students
- 12 post-doctoral scientists
- 5 undergraduate students
- 9 undergraduate students for short training (~2-3 months)
- 1 collaborator for 3 weeks, plus several short visits by collaborators.

PUBLICATIONS AND TALKS (APPENDICES VI & VII).

- 119 papers in international peer-reviewed journals: 1 Nature Mater., 2 Nature Nanotech., 1 Nano Lett., 4 Phys. Rev. Lett., 2 J. Am. Chem. Soc., 4 ACS Nano, 3 Adv. Mater., 30 J. Phys. Chem. B&C&Lett, 15 Phys. Rev. B, 5 Appl. Phys. Lett. Full list of publications in Appendix VI. H-index = 32 (ISI); 39 (GS). Citations = 3372 (ISI); 4679 (GS).
- 6 book chapters and 12 proceedings/newsletters.
- 57 invited lectures at various conferences, annual meetings of physical societies, tutorial and technical lectures at the leading universities and research centers in Europe, North America and Asia. Details in Appendix VII.

5 RELEVANT SELECTED PUBLICATIONS IN THE LAST 10 YEARS.

- G. I. Livshits, A. Stern, D. Rotem, N. Borovok, G. Eidelshtein, A. Migliore, E. Penzo, S. J. Wind, R. Di Felice, S. Skourtis, J. C. Cuevas, L. Gurevich, A. B. Kotlyar, D. Porath, "Long-range charge transport in single G-quadruplex DNA molecules", *Nature Nanotech.* **9**, 1040 (2014).
- S. P. Hancock, T. Ghane, D. Cascio, R. Rohs, R. Di Felice, R. C. Johnson, "Control of DNA Minor Groove Width and Fis Protein Binding by the Purine 2-amino Group", *Nucl. Acids Res.* **41**, 6750-6760 (2013).
- A. Migliore, S. Corni, D. Varsano, M. L. Klein, R. Di Felice, "First-principles effective electronic couplings for hole transfer in natural and size-expanded DNA", *J. Phys. Chem. B* **113**, 9402 (2009).
- D. Varsano, L. A. Espinosa-Leal, X. Andrade, M. A. L. Marques, R. Di Felice, A. Rubio, "A gauge invariant method for molecular chiroptical properties in TDDFT", *Phys. Chem. Chem. Phys.* **11**, 4481 (2009).
- E. Shapir, A. Calzolari, C. Cavazzoni, D. Ryndyk, G. Cuniberti, A. B. Kotlyar R. Di Felice, and D. Porath, "Electronic structure of single DNA molecules resolved by scanning tunneling spectroscopy", *Nature Materials* **7**, 68 (2008).

OUTREACH

- http://www.rai.tv/dl/RaiTV/programmi/media/ContentItem-7ffb5dbe-6f13-4bbc-bc82-c74ac64ae9e0.html. Superquark, RAI1 TV, Italy; August 20, 2015.

APPENDIX I – RESEARCH INTERESTS AND EXPERIENCE.

Research Interests.

Keywords. Theoretical biophysics, structure and electronic properties of DNA and proteins, conformational flexibility and thermodynamics, charge transfer in biological systems, molecule/surface interactions, biomolecular nanostructures, protein-DNA binding, hybrid materials and bio-nano-systems, Density Functional Theory (DFT), Molecular Dynamics (MD), Quantum Computation applied to high-performance computational problems.

Theoretical and computational physics of matter, with emphasis on ab-initio studies of biological molecules and molecules interacting with surfaces. Specific topics include:

1 Capabilities, limits and extensions of solid-state computational tools (DFT and tight-binding) to study biomolecules appealing for electronic applications. The investigated biomolecules are: (i) natural and modified nucleic acids; (ii) copper metalloproteins; (iii) model β-sheet peptides on solid surfaces in a wet environment.

2 Theory of charge mobility in biomolecules: links between the solid-state-like charge transport through extended orbitals and the charge transfer between localized molecular sites (Marcus-Hush-Jortner Theory).

3 Methodological development to compute electron transfer rates in biomolecular systems within density functional theory. Application to: (i) electron exchange between two electron transfer proteins in an azurin dimer; (ii) hole exchange between two adjacent planes in stacked dimers of duplex and quadruplex DNA, as well as chemically modified DNA, with different sequences.

4 Use of molecular dynamics simulations to sample the conformational effects on the electronic and optical properties of biological molecules. Application to DNA duplexes, triplexes, tetraplexes and duplexes with non-natural bases.

5 Role of the solvent in the electronic structure and charge properties of DNAs and proteins. Investigation of a continuum solvent and discrete coordination water molecules.

6 Optical absorption and circular dichroism of chiral molecules including natural and modified DNAs.

7 DFT-based parametrization of classical force fields for modified nucleobases and for protein-surface and DNA-surface interaction.

8 DFT studies of the adsorption of organic molecules and biomolecules on metal surfaces, with aromatic and alkylic molecules, in the diluted coverage range and in the range of self-assembled-monolayers: nucleobases/Au(111), amino-acids/Au(111), methanethiol/Au(111), pentacene/Cu(100), DPDI/Cu(111), mercaptobenzoxazole/Cu(100), and others. Different regimes of molecule-metal hybridization from chemisorption to weak interaction.

9 Molecular dynamics simulations of protein-binding DNA oligomers and of protein-DNA bound complexes.

10 Electronic structure of organic and inorganic polymers that can serve as new nanowires for electronic applications. Free-standing polymers, interfaces with metal surfaces, and junctions with two metal electrodes. Current investigations are devoted to specific polymers MMX (metal-metal-halogen chains that coordinate various lateral organic groups) and MoSI compounds.

11 Methodological development to address excited-state transport mechanisms, as well as dispersion interactions for a suitable description of molecule-molecule and molecule-inorganic coupling.

12 Ab-initio theory and empirical modeling of the structure, electronic properties and optical excitations of hybrid metal/semiconductor interfaces and nanoparticles (nano-dumbbells).

13 Impact of quantum computation on nanosciences spanning chemistry, materials science, physics and biology.

Many of these activities include direct collaboration with experimental groups for guidance and interpretation.

Research Experience.

- Mechanisms of protein-DNA binding and genome-wide detection. Molecular dynamics simulations of protein-DNA complexes and of protein-binding DNA oligomers. Machine learning approach to the binding specificity. Exploring solutions by quantum machine learning.
- Interaction of proteins and DNA with solid surfaces by DFT electronic structure calculations and classical MD simulations. Available force fields do not contain parameters to account for the interaction between a metal surface and a biological molecule. Hence, they are not suitable to simulate a protein or a DNA molecule on a metal surface. Such parameter can be obtained from extensive DFT calculations of amino acids and DNA bases on a target metal surface and then used in classical MD runs. Several viable configurations should be considered by DFT, to ensure a wide coverage of possible dynamical conformations.
- Hybrid biomolecular electronics: conduction in biomolecules. The approach by first-principle calculations. The case of guanine stacks and hydrogen-bonded structures. Extension to the calculation of transport properties, dipolar interactions, and electronic structure of aggregates of other DNA bases. Search for possible conductive structures through DNA derivatization: metal inclusion inside the helical motif, unconventional quadruple helices made of only the guanine base (G4-DNA), aromatic expansion of nucleotides, other exotic conformations and base alterations. Conductive polymers that can be hybridized with DNA. Structure-dependent electronic properties and optical properties.
- Electron transfer in proteins. Development of an original method to compute transfer integrals within DFT and application to an azurin dimer. Conformational sampling of the whole dimer in a water box by classical MD, to select geometries for quatum calculations. Electronic structure of the selected geometries by DFT, after pruning the system to only the electron transfer active centers, plus two bridging water molecules. Good methodological performance. Role of water molecules in electron transfer reactions.
- Protein-based transistors: calculation of the electronic properties of active centers, and of the structural characteristics that control adhesion to the electrodes; simulation of device geometry (transistor, scanning tunneling microscope) to calculate the reorganization energy for the electron transfer process; simulation of transistor operation through modeling.
- Adsorption of aromatic molecules on metals by DFT: the case of pentacene on Cu(100). Determination of the adsorption configuration and electronic properties. Interpretation of the adsorption mechanism and metal-molecule electronic hybridization. Ab initio DOS compared to photoemission experimental studies.
- Thiol-metal chemisorption: explicit study for the case of cysteine ad cystine molecules on the Au(111) surface, mercaptobenzoxazole on Cu(100), methanethiol on Au(111). For the latter system, the interest is both in the evaluation of AFM detachment barriers and in the interpretation of structural measurements. Visiting stay at Princeton Univ.

- Silicon Carbide. Clean and hydrogen-covered reconstructions and electronic properties by DFT. Role of stacking at the surface. Adatom mobility and growth kinetics by kinetic Monte Carlo simulations. Postdoc at INFM-Italy.
- Surface reconstruction in the very early deposition stages. Nitride quantum dots. Postdoc at Xerox PARC and INFM-Italy.
- Catalytic materials: the case of aluminum oxide. Clean and hydrogenated basal surface. Reaction to water and epitaxy of the material. Postdoc at Xerox PARC.
- Group-III nitrides, zincblende and wurtzite GaN and AlN. Polar and non-polar surfaces and thin films. Link between lattice mismatch and two-dimensional film stability. Postdoc at Xerox PARC.
- First-principle calculations of surface reconstructions. Thermodynamic stability and dynamical evolution. Car-Parrinello Molecular Dynamics. Phonon spectra from the dynamical trajectories. Applications to clean and hydrogenated Si(111) and GaAs(110) surfaces. MSc and PhD.

Technical skills.

- Plane-wave periodic density functional theory electronic structure calculations: quantum-espresso (www.quantum-espresso.org).
- Density functional theory electronic structure calculations in localized basis sets: NWChem (http://www.emsl.pnl.gov/capabilities/computing/nwchem/).
- Optical properties by real-time real-space time-dependent density functional theory: `octopus` (http://www.tddft.org/programs/octopus/).
- Generation and testing of numerical pseudopotentials for electronic structure calculations.
- Molecular dynamics simulations (NAMD, GROMACS) and force fields (AMBER, CHARMM, OPLS).
- Protein and nucleic acid databank: www.pdb.org.
- Visualization of structures and dynamical trajectories of crystals and biomolecules: gOpenMol, XCRYSDEN, VMD, pyMOL and others.
- Plotting: grace, Origin.
- Basics of nucleic acid builders.
- Programming languages: Fortran.
- Operating systems: MAC OS, Windows, Linux.
- Use of parallel supercomputers and PC clusters.
- Proposal writing. Scientific and administrative project management, budgeting. Web submission.

APPENDIX II – PROJECT COORDINATION AND PARTICIPATION.

1. Future

- I have submitted a grant proposal on "Binding mechanisms in class 2 CRISPR systems by a combined computational-experimental approach". NSF CHEM CLP, 10/31/2017.
- I am a collaborator in a NIH proposal by Peter Qin (Chemistry) on CRISPR-Cas9 genome editing system (submitted 11/6/2017).

2. Submitted in 2014-2016, not funded

- "Mechanisms of replication fork stability through heterochromatic G4-structures", pre-proposal submitted to HFSP on 3/28/2016. Co-I.
- "QuBBD: Quantum machine learning as a new tool in computational biology", submitted to NSF-QuBBD on 7/30/2015. Requested funding 100 k$. PIs: Daniel Lidar (USC Engineering, Chemistry and Physics) and Remo Rohs (USC Biology, Chemistry, Physics and Computer Science). Co-I.
- "Quantum machine learning as a new tool in computational biology". Submitted to NIH as R21 proposal on 2/19/2015. Requested funding 275 k$ (after overheads). PIs: Daniel Lidar (USC Engineering, Chemistry and Physics) and Remo Rohs (USC Biology, Chemistry, Physics and Computer Science). Co-I.
- "Multi-unit G-quadruplex: higher-order structure and interactions with small molecules". Submitted to NSF-CHEM on 10/31/2014. Total budget 703,571 k$. PIs: Peter Qin (USC Chemistry) and Rosa Di Felice.
- "Modeling binding mechanisms of nucleic acids on inorganic surfaces (DNA@SURF)". Submitted to NSF-ENG-CBET-IPT on 11/05/2014. Total budget 327,347 k$. Single PI.
- "Multi-scale computation of electron transfer through G-quadruplex DNA". Submitted to NSF-MPS-DMR-CMMT on 10/31/2014. Total budget 606,800 k$. Single PI.

3. Principal Investigator in National and International Projects.

- "All-atom simulation of the Amyloid-beta-42 peptide interacting with gold nanoparticles (AmyGoNP)". 13th PRACE Call. 25,000,000 supercomputing hours.
- "Distributed Bridge Collaboration via Multiple Videowalls". USC Bridge Catalyst award – 100 k$ for three faculty, with Richard Weinberg (Cinematic Arts) and Art Toga (Neuroscience).
- "Classical and quantum computation in nanosciences". University of Southern California WiSE Major Support for Faculty. 06/2014-05/2015. Funding 25 k$.
- Co-PI in project "MOPROSURF – Modeling protein/surface interactions". 3 years 04/2010-03/2013. In collaboration with Stefano Corni at CNR-NANO-S3, Modena, Italy. Funding 590 k€ by the Italian Institute of Technology (IIT).
- "Multi-scale modeling of chemically modified DNA sequences for nanotechnology and molecular biology". 2 years 09/2010-08/2012. International partner: Miguel Fuentes-Cabrera and Bobby G. Sumpter, Center for Nanophase Materials Science (CNMS), Oak Ridge National Laboratory, TN, USA. Funding: 70 k€ by the Foundation CRMO, Modena, Italy.
- "Controlling the structure and function of metal supported organometallic nanostructures", co-PI. 09/10-08/12. National PRIN project. National coordinator: Maria Grazia Betti (University of Rome "La Sapienza", Rome, Italy). CNR co-PI: Stafano Fabris (CNR-IOM-DEMOCRITOS, Trieste, Italy). Funding 40 k€ by the Italian Ministry for Research.
- Coordinator of the Italian partner in the Project EC NANOSCI-ERA "Single Nano-Hybrid". Project coordinator: Fabrice Vallee, CNRS Universite Lyon 1. 04/2007-12/2010. Other partners: Uri Banin (Hebrew University of Jerusalem, Israel), Carsten

Soennichsen (University of Mainz, Germany). Funding 160 k€ (total project funding 760 k€).

- Coordinator of the theoretical activity in the EU IST-FET Open Project "DNA-based Nanodevices" (FP6, contract FP6-029192), administrative coordinator Dr. A. B. Kotlyar, Tel Aviv University, and scientific coordinator Dr. D. Porath, Hebrew University of Jerusalem. 05/2006-09/2010. Funding 150 k€ (total project cost 2250k€).
- Coordinator of the theoretical activity in the EU IST-FET Open Project "DNA-based nanowires" (FP5, contract IST-2001-38951), administrative coordinator Dr. A. B. Kotlyar, Tel Aviv University, and scientific coordinator Dr. D. Porath, Hebrew University of Jerusalem. 01/2003-07/2006. Funding 200 k€ (total project cost 1150 k€).
- Coordinator for the Italian partner in the CNR-CNPq bilateral agreement to perform research in the field of "Electronic Properties of Biomolecules with Potential Applications in Electronic Devices" (2003-2004). Rosa Di Felice (INFM-S3 Modena, Italy), Helena M. Petrilli (Instituto de Fisica, Universidade de São Paulo, Brazil). Funding for visiting stays, ~10 k€.
- Coordinator of several National Projects published by the INFM "Parallel Computation Initiative" for the allocation of computing time on the supercomputers at CINECA, Bologna, from January 2000 to June 2010. The Projects run on a yearly basis. The initiative has been transformed in the ISCRA regular call [Italian SuperComputing Resource Allocation, http://hpc-iscra.cineca.it/], first deadline June 2010. See section 5 in this document.
- Coordinator of international supercomputing projects. See section 6 in this document.

4. Participation in National and EU Projects.

- Participation in the Regional Laboratory of Emilia Romagna NANOFABER, coordinator Prof. C. Taliani (CNR Bologna).
- Participation in the MIUR FIRB-NOMADE (2003-2006), national coordinator Prof. R. Cingolani (NNL Lecce), local coordinator Prof. E. Molinari.
- Participant in the PRA 1MESS 2000-2003, coordinator Prof. C.M. Bertoni, Modena.
- Participant in the PRA SINPROT 2000-2003, coordinator Dr. P. Facci, Modena.
- Participant in the EU IST-FET Open Project SAMBA, coordinator Prof. R. Cingolani, INFM NNL Lecce. September 2001-August 2004.
- Participant in three PRINS, dedicated to molecule/metal coupling of different kinds. Coordinatori: A. Morgante (INFM-Trieste), M.G. Betti (INFM-Roma1).

5. List of National Supercomputing Projects for computing time at CINECA.

- 2000/2001 (refereed, completed): *Electronic Properties of Nucleoside-based Solids*.
- 2001 (refereed, completed): *Ab-initio study of SiC surfaces and surface defects in the frame of SiC growth*.
- 2001-2002 (granted, completed): *First-principle study of the Cu site of the electron-transfer-protein Azurin*.
- 2001-2002 (granted, completed): *Electronic properties of model oligonucleotides: G4 and poly(C)-poly(G)*.
- 2002 (refereed, completed): *First-principle study of the Cu site of the electron-transfer-protein Azurin*.
- 2002 (refereed, completed): *Electronic properties of model oligonucleotides: G4 and poly(C)-poly(G)*.

- 2002 (refereed, completed): *A DFT study of Self-Assembled organic monolayers on metal surfaces*.
- 2002 (refereed, visiting grant, completed): *A DFT study of Self-Assembled organic monolayers on metal surfaces*.
- 2002 (refereed, completed): *Ab-initio study of SiC surfaces and the implication for epitaxial growth*.
- 2003 (refereed, completed): *Ab initio Simulation of Electron-Transfer (Bio)Molecules with Potential Applications in Electronic Devices.*
- 2003 (refereed, completed): *Simulation of DNA-based Molecular Nanowires.*
- 2003 (refereed, completed): *A DFT study of thiol-terminated (bio)molecules on metal surfaces.*
- 2003 (refereed, completed): *Theoretical Simulations of the Early Stages of SiC growth at the Atomic Level over a Broad Range of Time Scales.*
- 2004 (refereed, completed): *Redox active centers in (bio)molecules: the electron transfer mechanisms*.
- 2004 (refereed, completed): *Ab initio description of molecular transport: Towards the inclusion of electron correlation effects*.
- 2004 (refereed, complete): *Ab-initio investigation of DNA-based nanowires obtained via metal incorporation and nucleotide modifications*.
- 2004 (refereed, completed): *Ab-initio investigation of the hybrid interface between thiolates, dithiolates, and disulfides with metal surfaces*.
- 2004 (refereed, completed): *Theoretical Simulations of the Early Stages of SiC growth at the Atomic Level over a Broad Range of Time Scales*.
- 2005 (refereed, completed): *Ab initio electronic transport in molecular nanostructures.*
- 2005 (refereed, completed): *Electronic properties of DNA-structured synthetic polymers.*
- 2005 (refereed, completed): *Ab-initio investigation of hybrid molecule/metal interfaces: chemisorption and physisorption.*
- 2005 (refereed, completed): *Theoretical Simulations of the surface doping in semiconductors.*
- 2006 (refereed, completed): *Electronic properties and conformation of DNA derivatives for envisaged nano-electronics applications.*
- 2006 (refereed, completed): *Ab initio electronic transport in molecular nanostructures.*
- 2008 (refereed, completed): *Adsorption and self-assembly of molecules and polymers on metal surfaces.*
- 2010 (refereed, completed): *Simulating protein unfolding under pulling force.* ISCRA class A. [http://hpc-iscra.cineca.it/]

6. List of International Supercomputing Projects.

- 2016-2017 (refereed, running): *All-atom simulation of the Amyloid-beta-42 peptide interacting with gold nanoparticles (AmyGoNP)*. PRACE European supercomputing initiative (25000000 core-hours on Marconi-KNL, CINECA, Italy).
- 2008-2009 (refereed, completed): *Electronic structure of synthetic DNA with aromatic insertions*. CNMS-ORNL, Oak Ridge National Laboratory, TN, USA. Includes supercomputing time allocation at NERSC, Berkely.
- 2010-2011 (refereed, completed): *Multi-scale modeling of chemically modified DNA sequences for nanotechnology and molecular biology*. CNMS-ORNL, Oak Ridge National Laboratory, TN, USA. Includes supercomputing time allocation at NERSC, Berkely.

- 2013 (refereed, completed): *Molecular Dynamics simulations of p53-DNA complexes*. Anton computer at Pittsburgh supercomputing center, PA, USA. In collaboration with Remo Rohs (USC Los Angeles).
- 2013-2014 (refereed, running): *Electronic structure of G4-DNA by ab initio calculations*. CNMS-ORNL, Oak Ridge National Laboratory, TN, USA. Renewed by 1 year until February 2015.

APPENDIX III – CONFERENCE/MEETING ORGANIZATION

Occurred.

- CECAM Workshop "Synergies between quantum computing and high-performance computing". Chair: Rosa Di Felice (USC, CNR-NANO). Co-organizers: Elisa Molinari (CNR-NANO), Sara Bonella (EPFL), Ivano Tavernelli (IBM Zurich), Matthias Troyer (ETH Zurich), Daniel Lidar (USC), Seth Lloyd (MIT). 13000 CHF from CECAM. ETH Zurich, August 22-24, 2017. https://www.cecam.org/workshop-1464.html
- Workshop "Hybrid excitations in nano-materials". Chair: Rosa Di Felice. Co-chairs: Guido Goldoni, Fabrice Vallee, Danny Porath. 15 k€ Fondazione Cassa di Risparmio di Modena (CRMO). December 18-20 2011.
- Psi-K workshop "Hybrid excitations in nano-materials". Co-funding of the workshop just above. 3.5 k€. December 18-20 2011.
- Chair of the ESF (European Science Foundation) Conference on "Charge Transfer in Biosystems". Venue: Universitätszentrum Obergurgl, Obergurgl, Austria. July 17-22, 2011. Conference plan at http://www.esf.org/activities/esf-conferences/details/2011/confdetail354.html?conf=354&year=2011. ESF grant 40 k€.
- Psi-K workshop proposal "Charge Transfer in Biosystems". Co-funding of the above ESF Conference. Request 9 k€. Granted 8 k€.
- Project meeting "DNA-NANODEVICES" (FP6-029192). Venue: Dept. of Physics Univ. "La Sapienza" and Hotel Artdeco, Roma, Italy. July 3-4, 2009.
- Project meeting "DNA-NANODEVICES" (FP6-029192). Venue: Hotel Cetarium, Castellammare del Golfo (TP), Italy. May 3-4, 2008.
- Project meeting "DNA-based Nanowires" (IST-2001-38951). Venue: National Center S3 of INFM-CNR, Modena, Italy. October 9-10, 2005.
- IST-FET-38951 Workshop "DNA-based Nanowires: on the Way from Biomolecules to Nanodevices". Venue: National Center S3 of INFM-CNR, Modena, Italy. October 7-8, 2005.

APPENDIX IV – TEACHING

- Fall 2016, Lecturer of PHYS 408a: “Electricity and Magnetism”, 4 units. University of Southern California, Los Angeles, USA. Evaluation mean score 4.56.
- Spring 2016, Lecturer of PHYS 162: “Introduction to Electricity and Magnetism”, Honors. 4 units. University of Southern California, Los Angeles, USA. Evaluation mean score 5.
- October 10, 2013, Los Angeles (USA): Lecture on “The basics of Molecular dynamics”, 80 min. Within the undergraduate course BISC 481. Host Remo Rohs, Department of Biology, University of Southern California.
- October 2, 2012, Los Angeles (USA): Lecture on “The basics of Molecular dynamics”, 30 min. Within the undergraduate course BISC 481. Host Remo Rohs, Department of Biology, University of Southern California.
- November 19, 2010, Genova (Italy): Lecture on “Practical hints to write successful proposals within the EC-ICT-FET”, 30 min, within a full-day training initiative for CNR staff.
- June 17, 2010, Genova (Italy): Lecture on “Preparing a competitive proposal. Self-evaluation, resource planning and budgeting”, 2h. The lecture was part of a 1-week course on Research Management organized for its personnel by the Italian National Research Council (CNR).
- May 7, May 28 and June 18, 2009: Lecture on “Preparing a competitive proposal. Self-evaluation, resource planning and budgeting”, 2h each lessons in Palermo, Roma and Genova (Italy), respectively. The lecture was part of a 1-week course on Research Management organized for its personnel by the Italian National Research Council (CNR).
- April-June 2002: Teaching Assistant, Department of Electrical and Telecommunication Engineering, Università di Modena e Reggio Emilia, Modena, Italy. Excercise classes on General Physics II: Electromagnetism and Optics (20 h).
- October-December 2000: Teaching Assistant, Department of Industrial and Management Engineering, Università di Modena e Reggio Emilia, Reggio Emilia, Italy. Excercise classes on General Physics II: Electromagnetism and Optics (20 h).
- October-December 1999: Teaching Assistant, Department of Industrial and Management Engineering, Università di Modena e Reggio Emilia, Reggio Emilia, Italy. Excercise classes on General Physics II: Electromagnetism and Optics (20 h).
- September 1998: Lecturer, Department of Industrial and Management Engineering, Università di Modena e Reggio Emilia, Reggio Emilia, Italy. Introductory classes: Basic principles of General Physics (20 h).
- September-October 1998: Lecturer, Department of Mathematics, Università di Modena e Reggio Emilia, Modena, Italy. Introductory classes on mathematics (analysis) for first-year students of Mathematics and of Physics (20 h).
- October-November 1998: Teaching Assistant, Department of Chemistry, Università di Modena e Reggio Emilia, Modena, Italy. Exercise classes on General Physics I: Mechanics and Thermodynamics (30 h).

APPENDIX V – SUPERVISION & TRAINING, HOSTING OF COLLABORATORS

Undergraduate students

- Marta Rosa & Roberto Covino (pre-doc 3-month fellowships CNR-NANO-S3, October-December 2010 3 months).
- Tahereh Ghane (pre-doc 1 year fellowship at S3 INFM-CNR, 2008).
- Giovanni Borghi (MSc thesis, University of Modena, 2000).
- Arrigo Calzolari (MSc thesis, University of Modena, 1999).

Graduate students

- Marta Rosa (Physics & Nanoscience, University of Modena – 2013). Now postdoc at SISSA, Trieste, Italy.
- Tahereh Ghane (Nanoscience, University of Modena – 2011). Postdoc at TU Dresden, Germany, and now postdoc at TU Berlin, Germany.
- Agostino Migliore (Physics, University of Modena – 2006). Now research assistant professor at Duke University, USA, after postdocs at UPENN, USA, Tel Aviv University, Israel and Duke.
- Andrea Ferretti (Physics, University of Modena – 2004). Now tenured researcher at CNR-NANO-S3 Modena, Italy.
- Maria Clelia Righi (Physics, University of Modena – 2004). Now tenure track researcher at University of Modena and Reggio Emilia, Italy, after several years of fixed-term appointment.
- Arrigo Calzolari (Physics, University of Modena – 2002). Tenured researcher at CNR-NANO-S3 Modena, Italy.
- Carlo Antonio Pignedoli (Physics, University of Modena – 1998). Now member of the permanent research staff at EMPA Zürich, Switzerland.

PostDocs

- Wenming Sun (CNR-NANO-S3 Modena, from November 2011 to December 2014). Now research associate at the National Green building material lab, Beijing, China.
- Marcelo Alves dos Santos (INFM-S3 Modena, March 2008 to February 2010). Now left research, after a posdoc at the Federal University of São Paulo, Brazil.
- Giorgia Brancolini (INFM-S3 Modena, October 2007 to August 2010). Now non-permanent research staff member at CNR-NANO-S3, Modena, Italy.
- Rosangela de Paiva (INFM-S3 Modena, April 2007 to January 2010). Now assistant professor at the Federal University of São João del Rei, Brazil.
- Daniele Varsano (INFM-S3 Modena, April 2006 to March 2010). Now tenured researcher at CNR-NANO-S3 Modena, Italy, after a fixed-term faculty position at the University of Roma “La Sapienza”, Rome, Italy.
- Manuela Cavallari (INFM-S3 Modena, 2005). Now employed at a private company in Modena, Italy, after few years at a technology transfer business in the same city.
- Andrea Ferretti (INFM-S3 Modena, January 2005 to December 2008). Now tenured researcher at CNR-NANO-S3, Modena, Italy, after postdocs at MIT Boston and University of Oxford.
- Stefano Corni (INFM-S3 Modena, January 2003 to December 2004). Now Full Professor at University of Padova, Italy, after tenure-track and tenured research appointments at CNR-NANO-S3, Modena, Italy.

- HouYu Zhang (INFM-S3 Modena, November 2002 to December 2004). Now faculty at State Key Laboratory of Supramolecular Structure and Materials, Jilin University, China.
- Arrigo Calzolari (INFM-S3 Modena, March 2003 to December 2006). Now tenured researcher at CNR-NANO-S3, Modena, Italy.
- Carlo A. Pignedoli (INFM Unit of Modena, 2000/2002). Now member of the permanent research staff at EMPA Zürich, Switzerland.
- Francesca De Rienzo (INFM Unit of Modena, 2001/2002). Now technical staff member at Dept. Chemistry, University of Modena and Reggio Emilia, Modena, Italy.

Visitors

- Karsten Leding Jensen (Master student at Aalborg University, Denmark, for training on DFT calculations of metal surfaces; 3 weeks October 2011).
- Marcos Brown Gonçalves (postdoc Universidade de São Paulo, Brasil; 1 week July 2011).
- Leonardo Andres Espinosa Leal (PhD student at UPV/EHU San Sebastian, Spain, under the supervision of Prof. Angel Rubio to perform collaborative activity within the EC Project "DNA-based Nanowires"; 4 weeks October 2009, 4 months March-June 2010).
- Emerson Rengifo Carpintero (PhD student from Universidad del Valle, Colombia, March-August 2009).
- Gaurav Jaithliya (3rd–year student at IIT Delhi, internship May-July 2010).
- Garima Jaithliya (2nd–year student at IIT Bombay, internship May-July 2007).
- Setty-Venkat Anurag (3rd-year student at IIT Bombay, internship May-July 2006). PhD University of Maryland, USA, 2014. Now employed at EXL USA, http://www.exlservice.com.
- Daniele Varsano (PhD student at UPV/EHU San Sebastian, Spain, under the supervision of Prof. Angel Rubio to perform collaborative activity within the EC Project "DNA-based Nanowires"; 4 weeks in October 2003, 2 weeks in December 2004).
- Helena M. Petrilli (Professor at Universidade de São Paulo – Brazil, for a CNR-CNPq bilateral agreement; 3 weeks in November 2003; 3 weeks in October-November 2004).

APPENDIX VI – PUBLICATION LIST

Published Papers in International Journals (Reverse Chronological Order)

1. W. Sun, D. Varsano, R. Di Felice, "Electronic structure of G-quadruplexes over 10 μs trajectories", manuscript in preparation.
2. R. D. Teo, B. J. G. Rousseau, E. R. Smithwick, R. Di Felice, D. N. Beratan, A. Migliore, "Delineating the mechanisms of DNA-mediated signaling between [4Fe4S] proteins", manuscript submitted.
3. M. Rosa, R. Di Felice, S. Corni, "Adsorption mechanisms of nucleobases on the hydrated Au(111) surface", manuscript under review.
4. R. Li, R. Di Felice, R. Rohs, D. Lidar, "Quantum versus classical machine learning applied to a simplified computational biology problem", NPJ QI **4**, 14 (2018). DOI: 10.1038/s41534-018-0060-8.
5. N. Tangprasertchai, X. Zhang, R. Di Felice, I. Slaymaker, C. Vazquez Reyes, W. Jiang, R. Rohs, P. Qin, "CRISPR-Cas9 mediated DNA unwinding detected using site-directed spin labeling", *ACS Chem. Biol.* **12***,* 1489 (2017). DOI: 10.1021/acschembio.6b01137.
6. L. Bellucci, G. Bussi, R. Di Felice, S. Corni, "Fibrillation-prone conformations of the amyloid-β-42 peptide at the gold/water interface", *Nanoscale* **9**, 2279 (2017). DOI: 10.1039/C6NR06010B.
7. W. Sun, D. Varsano, R. Di Felice, "Effect of G-quadruplex topology on Electronic Transfer Integrals", *Nanomaterials* **6**, 184 (2016).
8. S. Mohn, N. Stolyarchuk, T. Markurt, R. Kirste, M. P. Hoffmann, R. Collazo, A. Courville, R. Di Felice, Z. Sitar, P. Vennéguès, M. Albrecht, "Polarity control in Group-III-Nitrides beyond Pragmatism", *Phys. Rev. Applied* **5**, 054004 (2016).
9. X. Zhang, C. Xu, R. Di Felice, J. Sponer, B. Islam, P. Stadlbauer, Y. Ding, L. Mao, Z. Mao, P. Qin, "Conformations of Human Telomeric G-Quadruplex Studied Using a Nucleotide-Independent Nitroxide Label", *Biochem.* **55**, 360-372 (2016). DOI: 10.1021/acs.biochem.5b01189.
10. M. Rosa, D. Koch, S. Corni, R. Wade, R. Di Felice, "Docking of DNA duplexes on a gold surface", *J. Self-Assembly and Molec. Electr.* **3**, 1-18 (2015).
11. M. Rosa, S. Corni, R. Di Felice, "van der Waals effects at molecule-metal interfaces", *Phys. Rev. B* **90**, 125448 (2014). DOI 10.1103/PhysRevB.00.005400.
12. Gideon I. Livshits, Avigail Stern, Dvir Rotem, Natalia Borovok, Gennady Eidelshtein, Agostino Migliore, Erika Penzo, Shalom J. Wind, Rosa Di Felice, Spiros Skourtis, Juan Carlos Cuevas, Leonid Gurevich, Alexander B. Kotlyar, Danny Porath, "Long-range charge transport in single G-quadruplex DNA molecules", *Nature Nanotech.* **9**, 1040 (2014). DOI: 10.1038/NNANO.2014.246
13. M. Rosa, S. Corni, R. Di Felice, "Correction to 'A Density Functional Theory Study of Cytosine on Au(111)'", *J. Phys. Chem. C* **118**, 16301 (2014). DOI: 10.1021/jp5058176.
14. W. Sun, A. Ferretti, D. Varsano, G. Brancolini, S. Corni, R. Di Felice, "Electron Transfer Rates at a Bio-Inorganic Interface", *J. Phys. Chem. C* **118**, 18820 (2014). DOI: 10.1021/jp507346a.
15. M. Rosa, S. Corni, R. Di Felice, "Enthalpy-Entropy Tuning in the Aggregation of Nucleobases at the Au(111) Surface", *J. Chem. Theory Comput.* **10**, 1707 (2014). **DOI:** 10.1021/ct401117g.
16. V. Ngo, R. Di Felice, S. Haas, "Ion Selectivity and Conduction of a synthetic tetramolecular G-quadruplex", *J. Phys. Chem. B* **118**, 864 (2014). DOI: 10.1021/jp408071h.

17. R. Dong, A. Calzolari, R. Di Felice, A. El-Shafei, M. Hussain, M. Buongiorno Nardelli, "Optical enhancement in heteroleptic Ru(II) isomeric dyes with extended carbazole antennas", *J. Phys. Chem. C* **118**, 8747 (2014). **DOI:** 10.1021/jp409733a.
18. S. Casalini, M. Berto, F. Leonardi, A. Operamolla, C. A. Bortolotti, M. Borsari, W. Sun, R. Di Felice, S. Corni, C. Albonetti, O. Hassan Omar, G. M. Farinola, F. Biscarini, "Self-Assembly of mono-/bi-dentate oligoarylene thiols onto polycrystalline Au", *Langmuir* **29**, 13198 (2013). DOI: 10.1021/la402217c.
19. G. Brancolini, A. Migliore, S. Corni, M. Fuentes-Cabrera, F. J. Luque, R. Di Felice, "Dynamical treatment of charge transfer through duplex nucleic acids containing modified adenines", *ACS Nano* **7**, 9396 (2013). DOI: 10.1021/nn404165y.
20. W. Sun, S. Corni, R. Di Felice, "Reactivity of the ZnS($10\bar{1}0$) surface to small organic ligands by density functional theory", *J. Phys. Chem. C* **117**, 16034 (2013). DOI: 10.1021/jp801542s.
21. P. O. Heidarsson, M. R. Otazo, L. Bellucci, A. Mossa, A. Imparato, E. Paci, S. Corni, R. Di Felice, B. B. Kragelund, C. Cecconi, "Single-molecule folding mechanism of an EF-hand neuronal calcium sensor", *Structure* **21**, 1812 (2013). DOI: 10.1016/j.str.2013.07.022.
22. L. Bellucci, S. Corni, R. Di Felice, E. Paci, "The Structure of Neuronal Calcium Sensor-1 in Solution Revealed by Molecular Dynamics Simulations", PloS ONE **8**, e74383 (2013). DOI: 10.1371/journal.pone.0074383.
23. M. Rosa, S. Corni, R. Di Felice, "The interaction of DNA bases with the Au(111) surface", *J. Chem. Theory Comput.* ***9,*** 4552 (2013). DOI: 10.1021/ct4002416.
24. T. Zhou, L. Yang, Y. Lu, I. Dror, A. C. Dantas Machado, T. Ghane, R. Di Felice, R. Rohs, "DNAshape: high-throughput prediction of DNA shape on a genomic scale", *Nucl. Acids Res.* **41**, W56-W62 (2013). doi:10.1093/nar/gkt437.
25. S. P. Hancock, T. Ghane, D. Cascio, R. Rohs, R. Di Felice, R. C. Johnson, "Control of DNA Minor Groove Width and Fis Protein Binding by the Purine 2-amino Group", *Nucl. Acids Res.* **41**, 6750-6760 (2013). doi:10.1093/nar/gkt357.
26. Marta Rosa, Wenming Sun, Rosa Di Felice, "Interaction of DNA Bases with Gold Substrates", *J. Self-Assembly and Molec. Electronics* **1**, 41 (2013).
27. L. Bellucci, G. Brancolini, A. Calzolari, O. Carrillo Parramon, S. Corni, R. Di Felice, "Proteins and Peptides at Gold Surfaces: Insights from Atomistic Simulations", *ACS Symposium Series* **1120**, 229 (2012).
28. Wenming Sun and Rosa Di Felice, "The nature of the interaction of natural and size expanded guanine and gold clusters: a DFT study", *J. Phys. Chem. C* **116**, 24954-24961 (2012). DOI: 10.1021/jp3079277.
29. M. Rosa, S. Corni, R. Di Felice, "A Density Functional Theory Study of Cytosine on Au(111)", *J. Phys. Chem. C* **116**, 21366 (2012). DOI: 10.1021/jp305833c.
30. T. Ghane, G. Brancolini, D. Varsano, R. Di Felice, "The optical properties of triplex DNA from Time-Dependent Density Functional Theory", *J. Phys. Chem. B* **116**, 10693 (2012). DOI: 10.1021/jp304818s.
31. M. H. Lee, G. Brancolini, R. Gutiérrez, R. Di Felice, and G. Cuniberti, "Probing charge transport in oxidatively damaged DNA-sequences under the influence of structural fluctuations", *J. Phys. Chem. B* **116**, 10977 (2012). DOI: 10.1021/jp2091544.
32. Gonzalo Givaja, Oscar Castillo, Eva Mateo, Almudena Gallego, Carlos J. Gómez-García, Arrigo Calzolari, Rosa Di Felice, Félix Zamora, "Electrical Behaviour of Heterobimetallic MM´X-Chain Polymers $PtM(EtCS_2)_4I$ (M = Ni, Pd)", *Chem.: A Eur. J.* **18**, 15476 (2012). DOI: 10.1002/chem.201200995.

33. Errez Shapir, Alexander B. Kotlyar, Giorgia Brancolini, Rosa Di Felice and Danny Porath, "Energy gap reduction in DNA by complexation with metal ions", *Adv. Mater.* **23**, 4290 (2011). DOI: 10.1002/adma.201101100.
34. Ehud Shaviv, Olaf Schubert, Marcelo Alves dos Santos, Guido Goldoni, Rosa Di Felice, Fabrice Vallee, Natalia Del Fatti, Uri Banin, Carsten Soennichsen, "The absorption properties of metal-semiconductor hybrid nanoparticles", *ACS Nano* **5**, 4712 (2011). DOI: 10.1021/nn200645h.
35. Giorgia Brancolini and Rosa Di Felice, "Combined effects of metal complexation and size expansion in the electronic structure of DNA base pairs", *J. Chem. Phys.* **134**, 205102 (2011).
36. Rosa Di Felice and Stefano Corni, "Simulation Of Peptide/Surface recognition", *J. Phys. Chem. Lett.* **2**, 1510 (2011).
37. Errez Shapir, Lior Sagiv, Tanya Molotsky, Alexander B. Kotlyar, Rosa Di Felice and Danny Porath, "Electronic Structure of G4-DNA by Scanning Tunneling Spectroscopy", *J. Phys. Chem. C* **114**, 22079 (2010).
38. Arrigo Calzolari, Giancarlo Cicero, Carlo Cavazzoni, Alessandra Catellani, Rosa Di Felice and Stefano Corni, "Hydroxyl-rich β-sheet adhesion to the gold surface in water by first-principle simulations", *J. Am. Chem. Soc.* **132**, 4790-4795 (2010). DOI: 10.1021/ja909823n.
39. Rosangela de Paiva and Rosa Di Felice, "Density Functional Theory Calculations of Ultra-thin Epitaxial Au Overlayers on CdS(0001) and CdS(000$\bar{1}$)", *J. Phys. Chem. C* **114**, 3998 (2010). DOI: 10.1021/jp910337b.
40. Marcelo Alves dos Santos, Rosa Di Felice and Guido Goldoni, "Dielectric functions of CdSe and CdS semiconductor nanoparticles from the optical absorption spectra", *J. Phys. Chem. C* **114**, 3776 (2010). DOI: 10.1021/jp910337b.
41. Alejandro Guijarro, Oscar Castillo, Lorena Welte, Arrigo Calzolari, Pablo J. Sanz Miguel, Carlos J. Gómez-Garcia, David Olea, Rosa di Felice, Julio Gómez-Herrero, Felix Zamora, "MMX as conductors: from single crystals to nanostructures", *Adv. Funct. Mater.* **20**, 1451 (2010).
42. Ori Cohavi, Stefano Corni, Francesca De Rienzo, Rosa Di Felice, Kay E. Gottschalk, Martin Höfling, Daria Kokh, Elisa Molinari, Gideon Schreiber, Alexander Vaskevich, Rebecca C. Wade, "Protein-surface interactions: challenging experiments and computations", *J. Molecular Recogn.* **23**, 259 (2010). DOI: 10.1002/jmr.993.
43. Lorena Welte, Arrigo Calzolari, Rosa Di Felice, Felix Zamora, Julio Gómez-Herrero, "Highly conductive nanoribbons of coordination polymers", *Nature Nanotech.* **5**, 110 (2010). DOI: 10.1038/NNANO.2009.354.
44. Álvaro Vazquez-Mayagoita, Oscar Huertas, Giorgia Brancolini, Agostino Migliore, Bobby G. Sumpter, Modesto Orozco, F. Javier Luque, Rosa Di Felice, Miguel Fuentes-Cabrera, "A*b initio* Study of the Structural, Tautomeric, Pairing and Electronic Properties of Seleno-Derivatives of Thymine", *J. Phys. Chem. B* **113**, 14465 (2009).
45. Manuela Cavallari, Anna Garbesi and Rosa Di Felice, "Porphyrin intercalation in G4-quadruplexes by molecular dynamics simulations", *J. Phys. Chem. B* **113**, 13152 (2009). DOI: 10.1021/jp9039226.
46. Rosa Di Felice, Stefano Corni, Elisa Molinari, "Computational challenges about nanosctructures and biosystems at surfaces", *Il Nuovo Cimento C* **32**, 57 (2009). DOI: 10.1393/ncc/i2009-10370-3.
47. Dmitry Ryndyk, Errez Shapir, Arrigo Calzolari, Danny Porath, Rosa Di Felice, and Giovanni Cuniberti, "STM spectroscopy of single DNA molecules", *ACS Nano* **3**, 1651 (2009). DOI: 10.1021/nn800238g.
48. Lisbeth Munksgaard Nielsen, Anne I.S. Holm, Daniele Varsano, Umesh Kadhane, Søren Vrønning Hoffmann, Rosa Di Felice, Angel Rubio, and Steen Brøndsted Nielsen,

"Fingerprints of bonding motifs in DNA duplexes of adenine and thymine revealed from circular dichroism: synchrotron radiation experiments and TDDFT calculations", *J. Phys. Chem. B* **113**, 9614 (2009). DOI: 10.1021/jp9032029.

49. Agostino Migliore, Stefano Corni, Daniele Varsano, Michael L. Klein and Rosa Di Felice, "First-principles effective electronic couplings for hole transfer in natural and size-expanded DNA", *J. Phys. Chem. B* **113**, 9402 (2009). DOI: 10.1021/jp904295q.
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51. Daniele Varsano, Leonardo A. Espinosa-Leal, Xavier Andrade, Miguel A. L. Marques, Rosa Di Felice, Angel Rubio, "A gauge invariant method for molecular chiroptical properties in TDDFT", *Phys. Chem. Chem. Phys.* **11**, 4481 (2009). DOI: 10.1039/b903200B.
52. Rosangela de Paiva and Rosa Di Felice, "Electronic structure of Au/CdSe interfaces", *ACS Nano* **2**, 2225 (2008).
53. Alejandro Guijarro, Oscar Castillo, Arrigo Calzolari, Pablo J. Sanz Miguel, Carlos J. Gómez-García, Rosa Di Felice, Félix Zamora, "Electrical conductivity in Platinum-dimer columns", *Inorganic Chemistry* **47**, 9736 (2008).
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57. Marcos Brown Gonçalves, R. Di Felice, Oleg Hh. Poleshuk, H.M. Petrilli "Ab initio study of the EFGs at the N sites in Imidazole", *Hyperfine Interactions* **181**, 53 (2008).
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75. Rosa Di Felice and Stefano Corni, “Computational approach to study electron-transfer proteins: Azurin for bio-molecular devices”, *Comput. Phys. Comm.* **169**, 9 (2005).
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Book Chapters (Reverse Chronological Order)

1. R. Di Felice, A. Migliore, D. Varsano, "DNA from first principles", in "Encyclopedia of Nanotechnology", 6th edition, B. Bhushan Ed., Springer (2015). ISBN 978-94-017-9780-1. DOI 10.1007/978-94-007-6178-0_100950-1.
2. Rosa Di Felice, "DNA-based Nanoelectronics", in "Nanobioelectronics: Electrons, Biology, and Medicine", A. Offenhauser and R. Rinaldi eds., Springer series "Nanostructure Science and Technology", Springer, New York, 2009, pp. 43-79. ISBN: 978-0-387-09458-8. E-ISBN: 978-0-387-09459-5. DOI: 10.1007/978-0-387-09459-5.
3. Rosa Di Felice and Danny Porath, "DNA-based Nanoelectronics", in "NanoBioTechnology: BioInspired devices and materials of the future", O. Shoseyov and I. Levy eds., Humana Press, Totowa (NJ, USA), July 2007. ISBN13: 978-1-58829-894-2. ISBN10: 1-58829-894-9.
4. Rosa Di Felice and Arrigo Calzolari, "Electronic structure of DNA derivatives and mimics by Density Functional Theory", in "'Modern methods for theoretical physical chemistry of biopolymers", pp. 485-507, ed. by Evgeni B. Starikov, James P. Lewis and Shigenori Tanaka, Elsevier (2006).
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7. Carlo Maria Bertoni, Guido Roma, Rosa Di Felice, "Electronic Structure of Adsorbates on Surfaces. Adsorption on Semiconductors.", in *Handbook of Surfaces II*, pp. 247-283, editors M. Scheffler and K. Horn, Elsevier (2000).

Other Publications (Reverse Chronological Order)

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11. Rosa Di Felice and Danny Porath, “Visions in Bio-Molecular Nano-Electronics in FP7”, *E-nano Newsletter* **3**, 9 (2006). http://www.phantomsnet.net
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16. Rosa Di Felice, John E. Northrup, Jörg Neugebauer, “Energetics of AlN epitaxial wetting layers on SiC(0001)”, published in: *III-V Nitrides*, *MRS Symposia Proceedings* **449**, edited by T. Moustakas, B. Monemar, I. Akasaki, and F. Ponce (MRS, Pittsburgh, Pennsylvania, 1996).
17. Rosa Di Felice, Maria Laura Mantovani, Carlo Maria Bertoni, “Ab-initio Molecular Dynamics calculations: a parallel implementation of the Car-Parrinello method”, *Proceedings of the 4th Euromicro Workshop on Parallel and Distributed Processing*, Braga, Portugal (1996).
18. Anatoli I. Shkrebtii, Carlo Maria Bertoni, Rosa Di Felice, Rodolfo Del Sole, “Atomic and Electronic Structure, Phonons and Optical Properties of Si(100) at 300 K and 900 K”, *Proceedings of the 22nd International Conference on the Physics of Semiconductors*, Vancouver, Canada (1994).
19. Rosa Di Felice, Anatoli I. Shkrebtii, Fabio Finocchi, Carlo Maria Bertoni, “Structural, Dynamical and Electronic Properties of Clean and Hydrogenated GaAs(110) Surfaces from ab-initio Molecular Dynamics", *Proceedings of the 21st International Conference on the Physics of Semiconductors*, Beijing, China (1992).

APPENDIX VII – INVITED TALKS & SEMINARS

Invited Talks (Reverse chronological order).

1 April 2, 2013. First Italy-Israel Nano-Workshop, Hebrew University of Jerusalem, Israel. Title: “The interaction of biomolecules with gold substrates”.

2 November 28, 2012. CECAM Workshop on “Functional Dynamics of Biomolecules”, Lugano, Switzerland. Title: “Multi-step simulation of DNAs and proteins in different environments”.

3 October 11, 2012. Workshop on “Self-Assembly and Molecular Electronics (SAME)”, Aalborg, Denmark. Title: “The interaction of DNA bases with gold substrates”.

4 August 21, 2012. Workshop on “Open many body systems, quantum computing and correlations, classical and quantum”, Cuernavaca, Mexico. Title: “Theory of molecule/surface interactions”.

5 September 11-14, 2011. 2nd International Training School on G-Quadruplexes, “Self-assembled guanosine structures for molecular electronic devices”, Spa, Belgium. Title: “Structure and electronic properties of G-quadruplexes – modeling”.

6 June 28-30, 2011. Third International Meeting on G-quadruplex and G-assembly, Grand Hotel Vesuvio, Sorrento (NA), Italy. Title: “Dynamics and optics of G4-porphyrin stacks”.

7 September 13-14, 2010. Annual user meeting of the Center for Nanophase Materials Science, Oak Ridge National Laboratory, TN, USA. Title: “Computational investigation of modified DNA”.

8 April 19-27, 2010. School and Conference on “Emergent Properties and Novel Behavior at the Nanoscale”, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India. Title School Lecture: “Computational investigation of DNA derivatives for nanoelectronics”. Title Conference talk: “Theoretical investigation of nanostructures and biosystems at surfaces”.

9 June 20-25 2009. European Science Foundation Research Conference “Self-assembly of guanosine derivatives: from biological systems to nanotechnological applications”, Universitätszentrum Obergurgl Ötz Valley, Innsbruck, Austria. Title: “Simulation of G4-DNA *Nanowires*”.

10 May 11-15 2009. International Workshop on “DNA-Based Nanotechnology: Construction, Mechanics, and Electronics (DNATEC)”, Dresden Max Planck Institute for Physics of Complex Systems, Dresden, Germany. Title: “Density functional theory and molecular dynamics of DNA-derivatives for nano-electronics”.

11 January 8-10 2009. “Total Energy” workshop, ICTP, Trieste. Title: “Electronic structure properties of DNA”.

12 May 29 2008. Conferenza “Calcolo Scientifico nella Fisica Italiana” (CSFI08), Centro Congressi SGR, Rimini, Italy. Title: “Computational challenges about nanostructures and biosystems at surfaces”.

13 May 23-30 2008. Workshop on “Transition Metal Chalco/Halide Nanostructures” (TMCN 2008), Bernardin Congress Center, Portoroz, Slovenia. Title: “Electronic hybridization at the MoSI/Au interface”.

14 April 20 2007. Vielberth Symposium on “Modeling DNA charge migration”, Regensburg, Germany. Title: “Quantum and classical simulations of DNA derivatives”.

15 September 2006. Annual National Conference of the Italian Physical Society (SIF), Torino, Italy. Title: “First-principle calculation of transport through nano-junctions”.

16 September 2006: ESF Exploratory Workshop “Self-assembly of guanosine derivatives: from quadruplex DNA to biomolecular devices”, Bled, Slovenia. Title: “Classical and quantum atomistic simulations of G4-wires”.

17 June 2006: I SCUOLA SUI MATERIALI MOLECOLARI PER FOTONICA ED ELETTRONICA, Villaggio Telis Arbatax (Tortolí), Italy. Title: “DNA-based molecular electronics”.

18 June 2006: Winnipeg Symposium on “Charge Migration in DNA: Physics, Chemistry & Biology Perspectives”, University of Manitoba, Winnipeg, Canada. Title: “DFT electronic structure calculations of DNA-derivatives”.

19 March 2006: Workshop on “First-principle approaches to optical and photoemission spectra”, Munich, Germany. Title: “Electronic structure of DNA-based derivatives and mimics by DFT”.

20 September 2004: “Conference on Computational Physics 2004”, Genova, Italy. Title: “Self-standing and metal-supported molecular nanostructures: metal-biomolecule coupling”.

21 May 2004: INFM-DEMOCRITOS & Psi-K Workshop on “Ab Initio Modelling in Biological Systems”, Trieste, Italy. Title: “Assembly of transition metal ions in DNA-like quadruple and double helices”.

22 February 2004: International Workshop on “Advances in Molecular Electronics: From Molecular Materials to Single-Molecule Devices”, Max-Planck-Institut Dresden, Germany. Title: “Metal modifications in DNA-based Nanowires”.

23 July 2003. ICTP-INFM Conference “New Frontiers in Noano-biotechnology: Monitoring Protein Function with Single Molecule Resolution”, Trieste, Italy. Title: “Theoretical Studies of Metals in DNA”.

24 May 2003. NANOMEETING 2003, Minsk, Belarus. Title: “Computer simulation of Biomolecular Nanostructures”.

25 July 2002. ISASST5: 5th International School on the Application of Surface Science Techniques and 23rd Course of the School of Solid State Physics. Ettore Majorana Center, Erice, Italy. Title: “Computational Physics of Organic- and Bio-Objects at surfaces”.

26 November 2001: International Meeting on the Theory of Metalloproteins, Department of Chemistry, Leiden University, The Netherlands. Title: “The Adsorption of Cysteine Radicals on Au(111) surfaces”.

27 January 2001: First National Meeting on Silicon Carbide, CNR-MASPEC, Parma, Italy. Title: “SiC(0001) surfaces: stacking defects and the implications for growth of silicon carbide”.

28 January 1998: International Conference on the Physics and Chemistry of Semiconductor Interfaces (PCSI 25), Salt Lake City, Utah, USA. Title: “First Principles Study of AlN Epitaxy on SiC and Al_2O_3”.

Seminars (Reverse chronological order).

29 October 6 2017. Biophysics seminar series at the University of Southern California, Keck School of Medicine and Dornsife School of Letters, Arts and Sciences, Los Angeles, CA, USA. Title: “Multi-step simulation of natural and modified DNAs”. Host: Robert Farley.

30 May 2 2017. Department of Physics and Astronomy, University of Southern California, Los Angeles, CA, USA. Title: “Theory of proteins and nucleic acids on inorganic surfaces”. Host: Stephan Haas.

31 June 29 2016. CNR-NANO Modena, Italy. Title: “Simulation of the CRISPR-Cas9 genome-editing system”. Host: Elisa Molinari.

32 April 17 2013. Department of Physics, Nanyang Technical University, Singapore. Title: “Multi-step simulation of natural and modified DNAs”. Host: Anh Tuan Phan.

33 June 12 2012. Department of Physics, Sichuan University, Chengdu, China. Title: “Theory of molecule/surface interactions”. Host: Hong Zhang.

34 April 17 2012. Department of Biology, Molecular and Computational Biology sector, University of Southern California, Los Angeles, CA, USA. Title: “Computational approach to the electronic structure of DNAs and proteins”. Host: Fengzhu Sun.

35 February 23 2012. Department of Chemistry, University of North Texas, Denton, TX, USA. Title: “Computational approach to DNAs and proteins for bio-nanotechnologies”. Host: Marco Buongiorno Nardelli.

36 February 14 2012. Information Sciences Institute (ISI), Marina Del Rey, CA, USA. Title: “Computational approach to DNAs and proteins for bio-nanotechnologies”. Host: Bob Lucas.

37 February 18 2011. Department of Physics, University of Southern California (USC), Los Angeles, CA, USA. Title: “Multi-step theoretical approach to DNAs and proteins”.

38 May 6 2010. Division of Chemistry and Chemical Engineering, California Institute of Technology (Caltech), Pasadena, USA. Title: “The structure and electronic properties of DNA derivatives by computational methods”. Host: Jacqueline Barton.

39 October 12 2009. Department of Physics, University of Southern California (USC), Los Angeles, CA, USC. Colloquium title: “Theoretical investigation of nanostructures and biosystems at surfaces”. Host: Moh El-Naggar.

40 November 24 2009. Department of Physics, University of Graz, Austria. Colloquium title: “Theoretical investigation of nanostructures and biosystems at surfaces”. Host: Ulrich Hohenester.

41 October 7 2008. Department of Physics, University of Southern California (USC), Los Angeles, CA, USA. Seminar title: “Computational investigation of DNA-derivatives for nano-electronics”. Host: Stephan Haas.

42 September 19 2008. Department of Physics, North Carolina State University (NCSU), Raleigh, NC, USA. Seminar title: “Computational investigation of DNA-derivatives for nano-electronics”. Host: Marco Buongiorno Nardelli.

43 May 14 2008. S3-seminar, National Center S3, Modena, Italy. Seminar title: “Computational investigation of DNA-derivatives for nano-electronics”. Host: Paolo Facci.

44 April 2008. Department of Physics, University of Southern California (USC), Los Angeles, USA. Title: “Theoretical methods for the investigation of nano-materials”. Host: Stephan Haas.

45 August 2007. Institute of Physical Chemistry, Hebrew University of Jerusalem, Israel. Title: “Theoretical methods for the various properties of matter”. Host: Danny Porath.

46 July 2006. Department of Physics, Paderborn University, Germany. Physics Colloquium. Title: “Computation of the electronic and transport properties of (bio)molecular nanostructures”. Host: Wolf Gero Schmidt.

47 March 2006. Department of Physical Chemistry, Institute of Chemistry, The Hebrew University of Jerusalem, Israel. Title: “Computation of the electronic and transport properties of biomolecular nanostructures”. Host: Danny Porath.

48 January 2006, Institut für Physik, Universität Basel, Switzerland. Title: “Coherent electronic transport in nanostructures and beyond”. Host: Christoph Brüder & Alexis Baratoff.

49 April 2005, PARC Palo Alto, CA, USA. Title: “First-principle computational approach to the investigation of biomolecules”. Host: Dr. John E. Northrup.

50 October 2004, MPI Mainz, Germany. Title: “Adsorption of thiols on metal surfaces by DFT calculations”. Hosts: Prof. Klaus Kremer, Dr. Markus Deserno.

51 May 2004, UAM Madrid, Spain. Title: “The interaction of metals with the biological world”. Host: Prof. Julio Gomez-Herrero.

52 February 2003, ENEA Casaccia, Roma, Italy. Title: “Computer Simulation of Biomolecular Nanostructures”. Host: Dr. Fabrizio Cleri.

53 April 2003, Scuola Normale Superiore and INFM-NEST, Pisa, Italy. Title: “Computer Approach to the Investigation of BioMolecules for Device Applications”. Host: Dr. Valentina Tozzini.

54 December 2001: Department of Physics, Technische Universität, Berlin. Title: “The Dissociative Chemisorption of NH_3 Molecules on GaN(0001) Surfaces”. Host: Prof. Wolfgang Richter.

55 May 2001: Department of Physics, Universidade Federal de Rio de Janeiro, Brazil. Title: “Electronic Properties of Model Guanosine Assemblies and their Role in DNA Conductivity”. Host: Prof. Rodrigo Capaz.

56 May 2001: Department of Physics, Universidade de São Paulo, Brazil. Title: “Nitride Surfaces and Thin Films from First Principles Calculations”. Host: Prof. Marilia J. Caldas.

57 November 1997: Lawrence Berkeley National Laboratory, Berkely, California, USA. Title: “First Principles Study of AlN Epitaxy on SiC and Al_2O_3”. Host: Prof. Eugene E. Haller.

APPENDIX VIII – PUBLIC MEDIA

- April 2015. Video shooting on "D-Wave quantum computing device", at USC. The video was realized by Italian documentary director Barbara Bernardini with two assistants, for inclusion in a 10-min documentary on quantum computation. The documentary was broadcast on the main Italian public TV RAI1 on August 20 2015, in the program Superquark, which was launched in 1981 to target scientific outreach in Italy. http://www.rai.tv/dl/RaiTV/programmi/media/ContentItem-7ffb5dbe-6f13-4bbc-bc82-c74ac64ae9e0.html (in Italian). The link reports the entire program, while the documentary on quantum computing starts at about 1h 43 m.
- August 2014. Brief interview with Sanden Totten, KPCC Los Angeles, for a Science Friday story. Whole audio piece: https://soundcloud.com/sanden-totten/science-friday-live-from-fiction-to-fact-by-sanden-totten.
- April 2009. EC ICT FET-Open movie. http://www.youtube.com/watch?v=_HwZcqcE0nw&feature=related
- January 13, 2009. "Il Corriere della Sera", "Corriere Magazine" insert (national newspaper, weekly insert).
- January 2, 2009. "Oxides and DNA: the time for substance" by Mauro Munafò, in Italian. Article on EC projects in Italy. Published in Nòva, weekly insert of "Il Sole 24 Ore" (national newspaper).
- January 21, 2008. "The other life of DNA: matter for nanotech", in Italian. Published online http://www.ricercaitaliana.it/primopiano/pp_dettaglio-128.htm [link no longer active]
- December 4, 2007. "Modena, Cnr has decoded the electronic structure of Dna", in Italian. Follow-up to the INFM press release about the paper on DNA published in Nature Materials 2008. Published in "Il Quotidiano della Calabria" (local newspaper, Calabria).
- November 27, 2007. "The electronic structure of Dna revealed by researchers from Modena", in Italian. Follow-up to the INFM press release about the paper on DNA published in Nature Materials 2008. Published in "Il Resto del Carlino" (local newspaper, Modena).
- November 27, 2007. "It will thus be possible to cure radiation damage: the study reveals for the first time the electronic structure of the Dna molecule", in Italian. Follow-up to the INFM press release about the paper on DNA published in Nature Materials 2008. Published in "L'informazione" (local newspaper, Modena).
- November 26, 2007. "Biochip market: the turning of Dna", by Paola Jadeluca, in Italian. Follow-up to the INFM press release about the paper on DNA published in Nature Materials 2008. Published in "Repubblica Affari & Finanza", weekly insert of "La Repubblica" (national newspaper).
- November 2007. "DNA without secrets: its electronic structure revealed by an Italian research team", in Italian. Published online http://www.galileonet.it/news/9163/dna-senza-segreti

APPENDIX IX – SEARCH COMMITTEES

- Postdoc position at the Italian Institute of Technology (IIT), December 2013.
- "CNR 364.96" 2009. National call for a permanent position in the CNR research staff. Selections done in 2011.
- "CNR NANO AR 013/2010 MO" (Head). 1 postodoc position (1-year fellowship, renewable). Selection completed October 25, 2010 in Modena, Italy.
- "CNR NANO 002/2010 MO" (Member). 1 position for a fixed-term researcher (2-year contract, renewable). Selection completed September 10, 2010 in Modena, Italy.
- "CNR IOM AR 007/2010 TS SISSA" (Head). 1 postodoc position (1-year fellowship, renewable). Selection completed September 9, 2010 in Trieste, Italy.
- "CNR-INFM AR 042/2009 MO" (Head). 1 postdoc position (1-year fellowship, renewable). Selection completed January 21, 2010 in Modena, Italy.
- "CNR-INFM AR 66/2008 MO" (Member). 1 postdoc position (1-year, renewable). Selection completed January 16, 2009.
- "CNR-INFM AR 56/2008" (Member). 1 postdoc position (1-year fellowship, renewable). Selection completed November 17, 2008 in Modena, Italy.
- "CNR-INFM BS 05/2008" (Member). 1 PhD position (3-year fellowship). Selection completed April 9, 2008 in Modena, Italy.
- "CNR-INFM AR 04/2007 MO" (Head). 1 postdoc position (1-year felowship, renewable). Selection completed March 13, 2007 in Modena, Italy.
- "CNR-INFM AR 19/2007 MO" (Member). 1 postdoc position (1-year felowship, renewable). Selection completed March 27, 2007 in Modena, Italy.
- "CNR-INFM 965/2005" (Member). 1 postdoc position (2-year fellowship). Selection completed March 14, 2005 in Modena, Italy.
- "CNR-INFM 1002/2005" (Member). 1 postdoc position (1-year fellowship, renewable). Selection completed December 27, 2005 in Modena, Italy.
- "CNR-INFM 1001/2005" (Head). 1 postdoc position (1-year fellowship, renewable). Selection completed January 10, 2006 in Modena, Italy.
- "INFM 584/2002" (Member). 1 postdoc position (2-year fellowship). Selection completed July 1, 2002 in Modena, Italy. No fellowship awarded.

Los Angeles, March 21st, 2018

Rosa Di Felice