EDUCATION
1999-2002: PhD in Chemistry, Univ. of Modena and R.E. (Register N. 158)
Oct 2000-Aug 2001: Marie-Curie PhD Fellow at Univ. of Ulm. (N. HPMT-CT-2000-00202)
1998: "Laurea" (MSc) in Chemistry, Univ. of Modena and R. E. (Register N.: 200855516/D2).
110/110 *cum Laude.*

EMPLOYMENT
From 26/12/18: Permanent Researcher at S3 CNR-NANO, Modena. Nr. 11985.
02/11/10-25/12/18: Fixed Term Researcher at S3 CNR-NANO, Modena (Prot. n. 26449 of
20/4/16 and Prot. n. 0002791 del 07/10/2010).
2007-2010: Post-doc at S3 CNR-NANO, Modena (INFM AR 11/2009, AR 37/2007)
2004-2007: Post-doc at CNR-ISOF, Bologna (Prot. 040317)
2002-2004: Post-doc at Politecnico di Milano

TEACHING
2021-2017: Adjunct Professor, *Chemical Physics of Biomolecules* on *Master Degree in Physics*,
Unimore. (*Rep. Nr. 102-2021, 27-2020, 25-2019, 183-2018, 100-2017) [36CFU]*
Nov 2020*: Lecturer for PhD course on "Intermolecular and Surface Forces", Unimore [3CFU]*
Member of the PhD evaluation committee *of the "PhD Defense" of F. Fontana (2020, Univ.
Milano Bicocca, IT), M. K. Bieniek (2019, KCL, UK), M. Slyngborg (2016, Univ. Aalborg, DK).*
2016-2015, 2009-2008: Teaching Assistant, *Exercise classes on General Physics A (mechanics
and thermodynamics), Univ. SMR* (Prot. DESD/CLIC-CLICG/2035/2016/PC/sg, Prot.
DESD/CLIC/1154/2015/PC/g, Prot. 722/2009, Prot. 630/2008)
Nov 2008: Guest lecturer *for PhD course at Unimore*
2000: Teaching Assistant, *Exercise classes on General and Inorganic Chemistry,* Unimore.

INTEREST AREA
*Keywords: Biomolecules, Proteins, DNA, Coarse Grained, Docking, MD, DFT, Optical, Electronic,
Plasmonic Properties*. A decade experience on multi-scale modeling of biological
macromolecules, protein-nanomaterials interfaces and protein folding/unfolding dynamics,
including atomistic calculations, docking *via* Brownian dynamics and CG models.

RESPONSABILITY OF SUPERCOMPUTING PROJECTS:
2020: PI of Supercomputing project "Molecular strategies to inhibit the COVID-19-cell
interaction" at ORNL, USA. CNMS2020-B-00433. Granted 1.000.000 CPU hours (2 years).
[Developing an in silico strategy to design biological inhibitors of SARS-CoV-2]
2020: PI of Supercomputing project "Molecular chimeras to inhibit the Covid-19-cell
interaction" at CINECA, IT. HP10C7TOOY (60.000 core-hours). [MD design of novel biologics]
2019: PI of Supercomputing HPC-Europa3 project "Building a Minimalist Model for the
interaction of Functionalized Metal Nanoparticles with supercharged GFP Proteins" at ICP,
Stuttgart, DE. HPC177BQ0O. Granted 40.000 node/hours. [Develompment of atomistic
potentials of biological macromolecules and NP to be included in Coarse Grained codes]
2018: PI of Supercomputing project *"Coarse Grained and Multi-scale modeling of bio-
functionalized nanoparticles "* at ORNL, USA. CNMS2018-338. Granted 1.000.000 CPU hours (2
years). [Developing CG models for biological macromolecules and nanomaterials]
2013: PI of Supercomputing project "Modeling the Interactions of Gold Nanoparticles with
DNA" at ORNL, USA. CNMS2013-064. Granted 1.000.000 CPU hours (2 years). [Providing
computational tools for DNA/Nanoparticle interactions.]
2010: PI of Supercomputing project "Multi-scale modelling of chemically modified DNA".
CNMS2010-034. Granted 1.000.000 CPU hours. [Multi-scale simulations to investigate the

effects induced by chemical modifications into the structural, electronic and conductivity properties of DNA]

2010: PI of supercomputing HPC-Europa++ project "Multi-scale modelling of artificial DNA derivatives" at BSC. Granted 30.000 CPU hours. [Development of classical force fields to study chemically modified DNA duplex]

2008-2016: PI and Co-PI of 8 annual supercomputing projects at CINECA (es. IscraB HP10BWX7N3 in 2014 and HP10BUR6WI in 2012)

PARTICIPATION TO EU PROJECTS:

10.2016-present: ERC TAME-PLASMONS *A theoretical chemistry approach to time-resolved molecular plasmonics*. PI S. Corni [Development of multi-scale computational tools (from coarse grained to atomistic simulations) for the study of the interaction between proteins and inorganic surfaces, with applications in nanomedicine]

2008-2009: NEST-STREP Prosurf. *Computational Toolbox for Protein-Surface docking.* Coord. E. Molinari, PI S. Corni [Development of new multi-scale computational methods]

2009-2012: "MaECENAS-Nanoscale Optical-to-Mechanical Energy Conversion: Coupling Nano-Object with Light Powered Molecular Lifters", PI. S. Corni [Development of techniques for the control of nano-movements of photoisomerizable molecules fed by light absorption]

2007-2010: *DNA-based nanoelectronic devices (DNAnanoDEVICES).* PI R. Di Felice [Developing DNA-based nanodevices]

2004-2006: *ESF-SONS BIONICS.* PI P. Samorì [Design and synthesis of hybrid supramolecular systems for the control of optical and electrical response]

PARTICIPATION TO NATIONAL PROJECTS:

2016-2018: PI of SEED CNR national project (GAE PUSEED04), *LOPE-DeveLopment of a Coarse Grained Model for Nanoparticle-Protein IntEractions.* Granted Budget: 15.000 Euro. PI G. Brancolini [Development of a CG methodology to study the Nanoparticle-Protein interactions]

2014-2017: PRIN project. *Assessing protein system dynamics and thermodynamics: a novel NMR approach at single-residue resolution.* PI S. Corni [Experimental study at the atomic level of protein in the presence of nanoparticles]

2010-2013: IIT-Seed project *MOPROSURF-MOdeling PROtein SURFace interactions.* PI S. Corni [Development of computational tools for the study of the interaction between proteins and inorganic surfaces]

2010-2012: CRMO project *Multi-scale modeling of chemically modified DNA sequences.* PI R. Di Felice [Development of computational methods and tools for extended biological systems]

EDITORIAL SERVICES

10.2020-02.2021: Guest Editor of the Thematic Issue "Molecular Simulations of Functionalized Nanoscale Materials", IJMS, ISSN 1661-6596

08.2016-today: Member of the Royal Society of Chemistry, London, UK

09.2014-today: Member of the Journal of SAME, Aalborg, DK

01.2016-01.2017: Associate Editor for *RSC Advances*, UK [98 referred papers, reported on Publons, Web of Science (ResearcherID AAY-3318-2020)]

2015: Guest Editor of the Thematic Issue "Molecular Self-Assembly: Synergy of Modelling and Experiment", Vol.3, Journal of SAME (2015), ISSN 2245-4551

Reviewer for scientific journals: Langmuir, RSC Advances, J Phys Chem B, Int. J. Quantum. Chem., J. Chem. Phys., et al.

OTHER SERVICES

2016-2024: Member of the CNR NANO Institute Council. [Representative of all Researchers and Technologists at the Institute, drafting the the Institute Annual Scientific Report]

STUDENTS/POST-DOC SUPERVISED
Supervisor of S. Dutta (post-doc at CNR-NANO), D. Montepietra (PhD at Unimore), I. Marrone (MSc at Unimore), A. Sarti (BSc at Unimore), F. Sonego (BSc at Unimore), D. Vignudelli (MSc at Unimore), M.C. Maschio (PhD at Unimore), T. Ghane (PhD now at Berlin Univ.) and M. Rosa (PhD now at Unipd). Undergraduate student E. Calzati (MSc at Unimore)

RESEARCH AWARDS AND HONOURS:
2016: Admitted as a Member of the Royal Society of Chemistry (date: 08/2016)
2010: CNR SHORT TERM MOBILITY Collab. w R. Wade, HITS, Heidelberg, Germany. [Promote IT-DE bilateral cooperation]
2009:CNR SHORT TERM MOBILITY: Collab. w M. Fuentes-Cabrera, CNMS, Oak Ridge Nat. Lab., TN, USA (duration 6 weeks). [Promote IT-USA bilateral cooperation]
2009: COST SHORT TERM SCIENTIFIC MISSION, COST-STSM-MP0802-04778. Collaboration with G. Cuniberti [Promote IT-DE bilateral cooperation]
2009: DFG Grant, Code CU 44 / 12-1. Collab. w G. Cuniberti, TU Dresden, DE. [Promote the IT-DE bilateral cooperation]

CONFERENCE ORGANIZATION
August 11-14, 2019: Organization Committee of the 27th AMC Conference, Stockholm, S
October 29-30, 2018: Organization Committee of NANOMEETING 2018, SNS, Pisa, IT.
November 16-18, 2016: Organization Committee of the 3rd SAME Conference, Aalborg, DK
March 13th-14th 2014: Organization Committee of the 7th "WINTER MODELLING" 2014: San Geminiano, Unimore, IT

CHAIRMAN IN INTERNATIONAL CONFERENCES
7th-visegrad-symposium. Promoting Body: Czech Academy of Sciences, Nove Hrady, CZ, 21-24/07/2017
5th-visegrad-symposium. Promoting Body: Department of Chemical Informatics, University of Szeged, H, 17-20 / 06/2015
WINTER MODELING" Workshop, San Geminiano, Unimore, IT. 13-14 / 03/2014

INVITED SPEAKER AT INTERNATIONAL CONFERENCES
International Symposium "Debugging NanoBio-Interfaces to Promote Clinical Translation" Mainz, DE. December 5-7,2019
IAAM European Advanced Material Congress, Stockolm, S. August 11-14, 2019
CECAM "Biomolecular mechanisms at functionalized solid surfaces", May 14-17, 2019 (https://www.cecam.org/workshop1709/)
CECAM "Multiscale Modelling from Macromolecules to Cell: Opportunities and Challenges of Biomolecular Simulations", February 4-6, 2019
7th Visegrad Symposium on Structural Systems Biology, Nove Hrady, CZ, 21-24/6/17 (http://nh.cas.cz/vsssb17/invited-speakers/)
3rd SAME Conference, Aalborg, DK, 16-18/11/16
6th Visegrad Symposium on Structural Systems Biology, Warsaw, PL, 19-21/6/16 (http://troll.cent.uw.edu.pl/vsssb2016/speakers.html)
TMS2016, 145th Annual Meeting, Nashville, TN, USA, 14-18/2/16 (http://www.programmaster.org/PM/PM.nsf/ ApprovedAbstracts)
Nano Italy, I Edition, Rome, IT, 21-24/9/15 (http://www.nanoitaly.it/nanoitaly/en/)

5th Visegrad Symposium on Structural Systems Biology, Szeged, H, 17-20/6/15 (http://www.drugcent.eu/programme-5th-visegrad)
CECAM Workshop, Toulouse, F, 24-26/3/14 (http://www.cecam.org/workshop-1-1061.html)
2nd SAME Conference, Aalborg, DK, 27-29/8/14 (http://www.same.riverpublishers.com/index14.php)
ET4HEALTH, Modena, IT, 28-29/10/13 (http://www.et4health.unimore.it/site/home/scientific-program.html)
CECAM-HQ-EPFL, "Grand Challenges in Understanding Interfaces Between Hard and Soft Matter", Lausanne, CH, 11-14/5/11 (http://www.cecam.org/workshop-1 -516.html)
CECAM-HQ-EPFL, "ProSurf, Modeling Protein Interactions with Solid Surfaces and Nanoparticles", Lausanne, CH, 9-11/3/11 (http://www.cecam.org/workshop-2 -548.html)

PUBLICATIONS
37 papers in international peer-reviewed journals. H-index = 17; 1 book chapters