

Prof. Giuseppe Pellicane
Italian (by birth)-South African (by naturalisation since 11 September 2020) citizenship.

ACADEMIC POSITIONS

31 October 2022 – present

Associate Professor, Department of Biomedical, Odontoiatric Sciences and Morpho-Functional Imaging (BIOMORF), University of Messina, Italy

31 October 2019 – 30 October 2022

Assistant Professor, Department of, Biomedical, Odontoiatric Sciences and Morpho-Functional Imaging (BIOMORF), University of Messina, Italy

1 November 2019- 31 October 2024

Honorary Associate Professor, School of Chemistry and Physics, University of Kwazulu-Natal, South Africa.

01 January 2018-31 October 2019

Associate Professor, School of Chemistry and Physics, University of Kwazulu-Natal, South Africa.

01 January 2013- 31 December 2017

Senior Lecturer, School of Chemistry and Physics, University of Kwazulu-Natal, South Africa.

01 January 2011- 31 December 2012

Lecturer, School of Chemistry and Physics, University of Kwazulu-Natal, South Africa.

ACADEMIC MEMBERSHIPS

Individual Associate (since 2015) of the *National Institute for Theoretical Physics* (NITheP), now National Institute for Theoretical and Computational Sciences (NITheCS) South Africa.

Ordinary member (since 2015) of the *South African Institute of Physics* (SAIP), South Africa.

Individual Associate (2020-2022) of the Institute for Chemical-Physical Processes (IPCF), National Research Council (CNR), Italy

Editorial Board Member (since 2019) of the journals *Advances in Mathematical Physics*, *Advances in Condensed Matter Physics*, Hindawi (<https://www.hindawi.com/journals/acmp/> <https://www.hindawi.com/journals/amp/>).

Guest Editor (2021) of the issue “Smart nanostructured materials: from molecular self-assembly to advanced applications” for the Journal of Nanomaterials (Hindawi-Wiley).

Rated *CI* by the National Research Foundation (NRF), South Africa, for the period 2018-2023

(“It is the firm belief of all of the reviewers that you are a well-established researcher that is recognized nationally and internationally by your peers with a body of high quality research output in the area of Condensed Matter Physics and a sound international standing in your field. Your reviewers have acknowledged you for having made important contributions to the field of Condensed Matter Physics, in particular your application of Statistical mechanics and Molecular simulation to the study of Biomolecules, with particular emphasis in proteins.”).

Rated *CI* by the National Research Foundation (NRF), South Africa, for the period 2012-2017.

SERVICE-MAN

July-November 1996

Officer cadet of the Italian Army.

December 1996 - October 1997

Officer (second lieutenant) of the Italian Army.

EDUCATION

March 2017

Academic Development Program (Assessing Learning in Higher Education; Supervising Research in higher Education; Designing and Evaluating Curricula in Higher Education; Teaching and Learning in higher Education)
University of Kwazulu-Natal (South Africa).

9 June 2006

Secondary Maths and Physics teaching post-graduate diploma (Masters in Education)
- 1 year course.
University of Messina, (Italy). Mark: 79/80

25 May 2002

Secondary Physics teaching post-graduate diploma (Masters in Education)
- 2 years course.
University of Messina (Italy). Mark: 78/80

26 February 2001

PhD in Physics.
University of Messina (Italy). Mark: none

19 March 1996

Master Degree in Physics.
University of Messina (Italy). Mark: 110/110 cum laude

TRAINING

27-7 August/September 2007

“Summer school on advanced computing”
CASPUR school, Villa Florio, Grottaferrata, Rome, Italy.

1-5 March 2004

“PWscf tutorial on electronic, structural and dynamical properties of materials”
CINECA, Bologna, Italy.

6-13 December 2001

“The Nuts and Bolts of First-Principles Simulation”
Durham, United Kingdom.

10-21 September 2001

“School of parallel computing”
CINECA school, Bologna, Italy.

28-1 August/September 2001

“Summer school on density functional theory” school
Caramulo, Portugal.

18-27 June 2000

“Methods in computer simulation” summer school
Manchester, United Kingdom.

7-17 September 1999

“INFM school on condensed matter theory”
Torino, Villa Gualino, Italy.

7-17 July 1998

“New approaches to problems in liquid state theory” NATO ASI school
Patti Marina, Italy.

RESEARCH INTERESTS

Broadly speaking, my interests are in the theory and computer simulation of soft and condensed matter systems in the fluid state. The latter include a range of fluid materials of interest in biotechnology, surface engineering, medicine, and renewable energy sources such as protein solutions, polymer blends, colloidal systems, and fluids in porous media.

HONOURS

On the top of the description reported below, I also routinely reviewed bursary applications by PhD/MSc students and research projects upon request of the National Research Foundation (NRF) of South Africa. I also participated as a panel member in many committees to evaluate applicants to academic positions inside my former university (University of Kwazulu-Natal). From 2013 to 2019, I also was a member of the Committee “Research and Higher degrees” School of Chemistry and Physics, University of Kwazulu-Natal, South Africa.

2022

Referee for the European Research Council (ERC) for Consolidator Grant 2021 proposals.

2021

Referee for the National Agency for the Evaluation of Performance of Higher Degree Institutions and Research (ANVUR), within the Evaluation of Research Quality (VQR) of the period 2015-2019.

NRF (National Research Foundation of South Africa) Panel Member for Physics and Astronomy

American Chemical Society (ACS) Petroleum Research Fund reviewer

Member of the Technical Committee of the 3rd Ieee International Conference on Design & Test of Integrated Micro & Nano-systems (7-10 July 2021) http://www.dts-conf.org/DTS_2021/Technical_Committees.php

Member of the Technical Committee of the 3d World Nanotechnology Conference (19-21 April 2021) - <https://worldnanotechnologyconference.com/2021>.

2020

Invitation to be a member of NRF (National Research Foundation of South Africa) Standing Panel for Physics, Astronomy, Mathematics and ICT in the period 2020-2023

2019

Scientific habilitation to function as full professor in Italian Universities for the scientific grouping 02/B2 (Theoretical Condensed Matter Physics).

Institute of Physics (IOP) Outstanding Reviewer award (Physica Scripta).

2017

Scientific habilitation to function as associate professor in Italian Universities for the scientific grouping 02/B2 (Theoretical Condensed Matter Physics).

Member of the Local Committee of the 2017 EMN (Energy, Materials and Nanotechnology) Mauritius Meeting (26-30 November, Port Louis, Mauritius).

2016

NITheP (National Institute of Theoretical Physics of South Africa) Panel member at the 2016 Bursary Workshop.

NRF (National Research Foundation of South Africa) Panel Member for Review of South African Research Chairs (SARCHI Chair).

2015

Acting Academic Leader, Physics cluster, Pietermaritzburg, School of Chemistry and Physics, University of Kwazulu-Natal, South Africa.

Representative of the Department of Physics at the University of Kwazulu-Natal in the National Strategic Planning Meeting on Implementing Recommendations from Review of Undergraduate Physics Training in South Africa.

2014

NRF (National Research Foundation of South Africa) Panel Member for Physical Science applications related to the Doctoral Fellowships Programme.

American Chemical Society (ACS) Petroleum Research Fund reviewer

2013

NRF (National Research Foundation of South Africa) Panel Member for Physical Science applications related to Competitive Programme for Rated Researchers (CPRR) and Competitive Support for Unrated Researchers (CSUR).

NRF (National Research Foundation of South Africa) Panel Member for Physical Science applications related to the Doctoral Fellowships Programme.

ACTIVITY AS A REFEREE FOR INTERNATIONAL JOURNALS

Nature Physics (Springer)

Frontiers Molecular Biosciences (Frontiers)

Polymers (MDPI)

Polymer (Elsevier)

Results in Physics (Elsevier)

Journal of Smart and Nano Materials (Taylor & Francis)

Journal of Physical Chemistry C (American Chemical Society)

Chemical Physics Letters (Elsevier)

Journal of the Royal Society Interface (Royal Society Publishing)

Journal of Physics A (Institute of Physics)

Physica Scripta (Elsevier)

Molecular Physics (Taylor & Francis)

Physical Review Letters (American Physical Society)

Soft Matter (Royal Society of Chemistry)

Physical Chemistry Chemical Physics (Royal Society of Chemistry)

Journal of Physical Chemistry B (American Chemical Society)

Journal of Chemical Physics (American Institute of Physics)

Physical Review E (American Physical Society)

Journal of Physics: Condensed Matter (Institute of Physics)

European Journal of Physics (Institute of Physics)

New Journal of Chemistry (Royal Society of Chemistry)

Crystal Growth and Design (American Chemical Society)

Thermochimica Acta (Elsevier)

TEACHING ACTIVITY

November-December 2022

Applied Physics

Lecturer, Department of Experimental Medicine, University of Messina (Italy) – 1 CFU

October-December 2022

Physics and fundamentals of Maths

Lecturer, Department of Biomedical and Odontoiatric Sciences and Morpho-Functional Imaging, University of Messina (Italy) – 8 CFU

March-May 2022

Applied Physics to Biological Systems and Systems of Livestock Production

Lecturer, Department of Veterinary Sciences, University of Messina (Italy) – 10 CFU

March-May 2022

Cryptography

Lecturer, Department of Electronic and Computer Science Engineering, University of Messina (Italy) – 6 CFU

October-November 2021

Applied Physics

Lecturer, Department of Experimental Medicine, University of Messina (Italy) – 1 CFU

March-May 2021

Applied Physics to Biological Systems and Systems of Livestock Production

Lecturer, Department of Veterinary Sciences, University of Messina (Italy) – 10 CFU

March-May 2021

Cryptography

Lecturer, Department of Electronic and Computer Science Engineering, University of Messina (Italy) – 6 CFU

October-November 2020

Applied Physics

Lecturer, Department of Experimental Medicine, University of Messina (Italy) – 1 CFU

March-May 2020

Applied Physics to Biological Systems and Systems of Livestock Production

Lecturer, Department of Veterinary Sciences, University of Messina (Italy) – 10 CFU

April 2020

Complex analysis, inverse Laplace transforms and applications to the solution of partial differential equations relevant to heat propagation

Lecturer, PhD course in Civil Engineering, University of Messina (Italy) – 1 CFU

March 2020

General Statistics

Lecturer, PhD course in Bioengineering, University of Messina (Italy) – 2 CFU

July-October 2019

Statistical Physics (PHYS367)

Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

July-October 2019

Computational Mechanics and Symbolic Programming (CPHY212)

Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

February-May 2019

Statistical Physics (PHYS741)

Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

July-October 2018

Mathematical methods (PHYS752)

Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

February-May 2018

Statistical Physics (PHYS741)

Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

September-October 2017

Mathematical methods (PHYS752)

Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

July-October 2017

Statistical Physics (PHYS362)

Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

February-May 2017

Statistical Physics (PHYS741)

Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

September-October 2016

Modern Physics for Life Sciences & Agriculture (PHYS133)

Lecturer in charge of the laboratory activities, College of Agriculture, Engineering and Science, University of Kwazulu-Natal (UKZN, South Africa).

September-October 2016

Mathematical methods (PHYS752)

Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

July-October 2016

Statistical Physics (PHYS362)

Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

February-May 2016

Statistical Physics (PHYS741)

Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

February-March 2015

Intro Physics for Life Sciences & Agriculture (PHYS131)

Lecturer in charge of the laboratory activities, College of Agriculture, Engineering and Science, UKZN (South Africa).

February-May 2015

Statistical Physics (PHYS741)

Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

September-October 2014

Thermal Physics (PHYS212)

Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

September-October 2014

Mathematical methods (PHYS752)

Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

July-October 2014

Statistical Physics (PHYS362)

Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

February-May 2014

Intro Physics for Life Sciences & Agriculture (PHYS131)

Lecturer in charge of the laboratory activities, College of Agriculture, Engineering and Science, UKZN (South Africa).

February-May 2014

Statistical Physics (PHYS742)

Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

September-October 2013

Thermal Physics (PHYS212)

Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

September-October 2013

Mathematical methods (PHYS752)

Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

July-October 2013

Modern Physics for Life Sciences & Agriculture (PHYS133)

Lecturer in charge of the laboratory activities, College of Agriculture, Engineering and Science, UKZN (South Africa).

July-October 2013

Statistical Physics (PHYS362)

Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

February-May 2013

Intro Physics for Life Sciences & Agriculture (PHYS131)

Lecturer in charge of the laboratory activities, College of Agriculture, Engineering and Science, UKZN (South Africa).

February-May 2013

Statistical Physics and Superfluidity (PHYS742)

Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

September-October 2012

Thermal Physics (PHYS212)

Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

September-October 2012

Mathematical methods (PHYS752)

Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

July-October 2012

Statistical Physics (PHYS362)

Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

February-May 2012

Statistical Physics and Superfluidity (PHYS742)
Lecturer, College of Agriculture, Engineering and Science, UKZN (South Africa).

September-October 2011
Mathematical methods (PHYS752)
Lecturer, Faculty of Science and Agriculture, UKZN (South Africa).

July-October 2011
Statistical Physics and Superfluidity (PHYS742)
Lecturer, Faculty of Science and Agriculture, UKZN (South Africa).

April-May 2011
Thermal Physics (PHYS131)
Lecturer, Faculty of Science and Agriculture, UKZN (South Africa).

February-May 2011
Statistical Physics and Thermodynamics (PHYS306)
Lecturer, Faculty of Science and Agriculture, UKZN (South Africa).

April-May 2009
Advanced studies of condensed matter Physics for third year students of the bachelor degree course in Physics
Lecturer, Faculty of Sciences, University of Messina (Italy).

April-May 2009
Advanced studies of Statistical Physics for third year students of the bachelor degree course in Physics
Lecturer, Faculty of Sciences, University of Messina (Italy).

March-June 2009
Computer science for first year students of the bachelor degree courses in
Chemistry and Pharmaceutical Technology - Pharmacy
Lecturer, Faculty of Pharmacy, University of Messina (Italy).

March-June 2008
Computer science for first year students of the bachelor degree course in
Chemistry and Pharmaceutical Technology
Lecturer, Faculty of Pharmacy, University of Messina (Italy).

September-October 2007
Analytical Mechanics for second year students of the bachelor degree course in Physics
Lecturer, Faculty of Sciences, University of Messina (Italy).

January-February 2007
Advanced studies of Statistical Physics for third year students of the bachelor
degree course in Physics
Lecturer, Faculty of Sciences, University of Messina (Italy).

March-June 2007
Computer science for first year students of the bachelor degree course in
Chemistry and Pharmaceutical Technology
Lecturer, Faculty of Pharmacy, University of Messina (Italy).

June-July 2006
Computer Science for first year students of the bachelor degree course in Physics
Lecturer, Faculty of Sciences, University of Messina (Italy).

March-May 2006
Computer science for first year students of the bachelor degree course in Nursing
Lecturer, Faculty of Medicine, University of Messina (Italy).

June-July 2005
Statistical Physics for third year students of the bachelor degree course in Physics
Lecturer, Faculty of Sciences, University of Messina (Italy).

COMPLETED STUDENT SUPERVISION

2019 Supervisor of NITheP Internships for Mr Aluwani Guga (Hons) from Nelson Mandela University, Ms Angel Mbedzi (Hons) from University of the Witwatersrand and Ms Valencia Marandela (BSc) from University of Venda.

2015–2018 Mr Francis M. Gaitho, PhD in Physics (UKZN, South Africa)

2016–2018 Mr Anele Mkanya, PhD in Physics (UKZN, South Africa)

2012-2015

Ms Mireille Megnidio-Tchoukouegno, PhD in Physics (UKZN, South Africa – cosupervision with Prof. G T Mola).

2014-2015

Mr Anele Mkanya, Masters in Physics (UKZN, South Africa)

2013-2015

Mr Berhanu Aragie Woldetsadik, PhD in Physics (UKZN, South Africa)

2017 Ms Cindy Mphara, Honours project in Physics (UKZN, South Africa).

2016 Mr Jashan Naicker, BSc Honours in Physics (UKZN, South Africa)

2015

Mr Verlan Moodley, Honours Research Project in Physics (UKZN, South Africa)

2013-2014

Mr Owen Daniel Pandaram, Masters in Physics (UKZN, South Africa)

2014

Mr Mdusumeni Isaac Nxumalo, BSc Honours in Physics (UKZN, South Africa).

2012

Dr Miguel Cavero, post-doctoral fellow in Physics (UKZN, South Africa).

2011

Mr Lizwe Wandile Mdakane, BSc Honours in Physics (UKZN, South Africa).

2010-2011

Mr Bruno Russo, Masters in Physics (University of Messina, Italy – co-supervision with Prof P V Giaquinta).

External examiner for MSc/PhD theses

External examiner of the PhD thesis of the Addis Ababa University (Ethiopia) “Translocation of Homogeneous Linear and Star Structures of Polymer chains into Spherical Cavity Subject to Pulling Force. A 3D Langevin Dynamics Simulation Study” by Mr Fikre Jida Urgessa

External examiner of the UKZN (South Africa) PhD thesis “The Effects of Nano-composites in Bulk Heterojunction Thin-film Organic Solar Cells.” by Mr Mohammed Saeid Gebreel.

External examiner of the UKZN (South Africa) PhD thesis “Fabrication and Characterization of Solution Processed Thin Film Solar Cells” by Mr Patrick Tonui.

External examiner of the PhD thesis of Stellenbosch University (South Africa): “The role of cytoskeletal networks in the elastic response of cells” by Ms Somicalo Azote

External examiner of the PhD thesis of the Addis Ababa University (Ethiopia) “A 3D Simulation Model of Tumor Growth” by Anley Gesese Tesfaye.

External examiner of the PhD thesis of the Addis Ababa University (Ethiopia) “Effect of tacticity on the structure and glass transition temperature of polystyrene thin films adsorbed onto graphite and hydroxylated α -quartz surfaces” by Solomon Negash

External examiner of the UKZN (South Africa) PhD thesis “Bulk heterojunction organic cell and thin film electrode buffer layers: synthesis, preparation and characterization” by Alhadi Abdalla Adam Arbab.

External examiner of the UKZN (South Africa) MSc thesis “Single and Double Layer Heterojunction Organic Solar Cell” by Mpumelelo H. Hlongwane.

External examiner of the University of Stellenbosch MSc thesis “One-dimensional fluid model with oscillating, exponentially decaying pair interactions” by G. M. Maziya

External examiner of the UKZN (South Africa) MSc thesis “Generation and detection of Bessel beams” by Thandeka Mhlanga.

External examiner of the UKZN (South Africa) MSc thesis “Bulk heterojunction organic solar cell” by Wiseman Mpilo Dlamini.

External examiner of the UKZN (South Africa) MSc thesis “Quantum dynamics in classical-temperature baths” by Nkosinathi Dlamini.

External examiner of the UKZN (South Africa) MSc thesis “Monitoring the States of Single Quantum Systems” by Kevin Garapo.

TALKS

8-10 July 2022

“Numerical Studies of Morphology of Polymeric materials at the interface”
International Online Conference on Foamed Polymers (ICFP 2022) 8-10 July 2022 at Mahatma Gandhi University, Kottayam, Kerala, India – Invited Plenary talk

7-10 June 2022

“Unveiling the role of topology in the interfacial properties of polymeric materials via molecular dynamics simulations”
Horizon 2020 RISE project "Effects of confinement on inhomogeneous systems" (CONIN), Serock, Poland – Invited talk

16-19 August 2021

“Nano-structuring of polymer blends at the interface driven by topology”
The 8th Global Conference on Polymer and Composite Materials (<http://www.cpcmconf.org/Speaker>) – Invited talk

05-07 July 2021

“Computer Simulation of Polymeric Materials at the Interface”
International Conference on Polymer Science and Composite Materials (<https://polymersconference.yuktan.com/featured-speakers>) – Keynote talk

20-25 June 2021

“Construction of a Composite-Sphere Model for Molecules of Tetrahedral Symmetry”
21st Symposium on Thermophysical Properties, Boulder, USA

19-20 April 2021

“Nano-structuring of polymer blends at the interface driven by topology”
2nd World Nanotechnology Conference (<https://worldnanotechnologyconference.com/speakers/2021>) – Keynote talk

30 November – 2 December 2020

“Interfacial and Morphological phase transitions in Polymeric Materials”
14th CHPC National Conference (<https://chpcconf.co.za/home-2>)

10-13 December 2019

“Colloidal interactions in molecular simulations of globular protein solutions” – Keynote talk
African Materials Research Society conference, Arusha, Tanzania.

02-04 October 2019

“Molecular dynamics simulations of coarse-grained models of polymer blends” – Invited talk
Workshop “Smart nanostructured materials: from molecular self-assembly to advanced applications”, Montelibretti-Rome, Italy

18-19 March 2019

“Topology as a surface-active agent for nano-structured polymers at the interface”- Invited talk
International Conference on Polymer-Biopolymer Chemistry, Amsterdam, Netherlands

4 – 6 March 2019

“Polymer blends on the nanoscale: topology as a surface-active agent“ – Invited talk
International conference on Biopolymers and Bioplastics, Baltimore, Maryland, USA

2 – 6 Dicembre 2018

“The role of the interface in binary polymer blends”
CHPC National Conference 2018, Cape Town, South Africa.

4 – 7 Novembre 2018

“The importance of polymer topology in surface absorption” – Invited Talk
Sustainable industrial Processing Summit & Exhibition (SIPS), Rio de Janeiro, Brasil.

25 Febbraio – 1 Marzo 2018

“Polymer topology in surface absorption of binary blends”
41th Annual Meeting of The Adhesion Society, San Diego, California, USA.

11th-14th December 2017

“Polymer topology in surface absorption of binary blends”
African Materials Research Society (AMRS) 2017 conference, Gaborone, Botswana.

03rd – 04th September 2017

“Exploiting polymer topology for surface modification of thermoplastics”
European Conference on Thermophysical Properties, ECTP 2017, Graz, Austria..

18th – 23rd June 2017

“Exploiting polymer topology for surface modification of thermoplastics”
ICMAT 2017, 9th International conference on Materials for Advanced Technologies, Singapore.

26th February – 1st March 2017

“Understanding the role of polymer topology in surface absorption”, Keynote Lecture.
40th Annual Meeting of The Adhesion Society, St. Petersburg, Florida, USA.

13 Marzo – 17 Marzo 2017

“Unravelling the surface composition of topologically-different polymer blends” – Invited Talk
EMN Meeting on Polymer 2017, Auckland, New Zealand.

5th – 9th December 2016

“Computational studies of binary polymer blends”
CHPC National Meeting 2016, East London, South Africa.

2nd – 6th October 2016

“Interfacial properties of linear-cyclic polymer blends”
The 11th Asian Thermophysical Properties Conference, Yokohama, Japan.

18th -22nd July 2016

“Interfacial properties of linear-cyclic polymer blends”
ICPAC 2016 “Emerging Trends in Chemical Sciences”, Mauritius.

28th September-2nd October 2015

“Anomalous adsorption of linear-cyclic polymer blends”
FISMAT 2015, University of Palermo, Palermo (Italy).

21-26th June 2015

“Interfacial properties of linear-cyclic polymer blends”

Nineteenth Symposium on thermophysical properties, Boulder, Colorado (USA)

31-04 september 2014

“Interfacial Properties and Dynamics of linear-cyclic polymer blends”

ECTP 2014 – *European Conference on Thermophysical Properties*, Porto (Portugal)

24-29 june 2012

“Effective interactions in atomistic studies of lysozyme solutions”

18th Symposium on thermo-physical properties, Boulder, Colorado (USA)

15-17 June 2010

“Effective interactions in globular protein solutions”

Translational Access Meeting 2010, Helsinki, Finland.

15-18 July 2009

“Effective protein interactions underlying crystal contacts in aqueous solutions”

“*New Trends in Simulating Colloids: from Models to Applications*” workshop,
CECAM, Lausanne, Switzerland.

15-17 December 2008

“A numerical assessment of solvated protein interactions underlying hydrophobic patches”

Translational Access Meeting 2008, Stuttgart, Germany.

22-26 November 2008

“Nonequilibrium MD as a probe of protein interactions in aqueous solutions”

Final Arrested Matter Conference, Taormina, Italy (<http://www.arrestedmatter.net/>).

16-19 June 2008

“Molecular dynamics characterization of protein-protein crystal contacts in aqueous solutions”

Polyelectrolytes 2008, Coimbra, Portugal.

5-7 July 2007

“Phase diagram of binary, athermal mixtures: theoretical and simulation results”

“*Fluid phase behaviour and critical phenomena from liquid state theories and Simulation*” workshop, CECAM, Lyon, France.

20-24 January 2007

“Phase diagram of binary, athermal mixtures: theoretical and simulation results”

“*Dynamical Arrest of Soft Matter and Colloids*” workshop, Bad Gastein, Austria.

29-31 August 2006

“Structure and Phase Equilibria of Fluid Mixtures in random pores: simulation and theoretical results”

“*Computational aspects of building blocks, nucleation, and synthesis of porous materials*” workshop,
CECAM, Lyon, France.

2-4 December 2005

“Thermodynamic stability of fluid-fluid phase separation in binary, athermal mixtures: the role of nonadditivity”

CRS-SOFT meeting, L'Aquila, Italy.

22-25 June 2005

“Stripe phases in systems with core-corona molecular architecture”

“*Materials, Matter and Devices (MMD) meeting*”, Genova, Italy.

8-12 May 2005

“Stripe phases from isotropic repulsive interactions”

“*NANOTECH 2005*” conference, Anaheim, California USA.

6-8 April 2005

“Stripe phases in systems with core-corona molecular architecture”

“*Thermodynamics 2005*” conference, Sesimbra, Portugal.

12-15 July 2004

“Theoretical phase diagram determination of globular protein solutions”
“Disorder, Complexity and Biology” STATPHYS 22 satellite conference,
Varanasi (India).

8-10 June 2004

“Microscopic Determination of the Phase Diagrams of Lysozyme and gamma-Crystallin Solutions”
“INFM meeting” (conference of the National Institute of Condensed Matter Physics), Genova, Italy.

20-26 July 2003

“Liquid-liquid phase equilibria of gas mixtures in nanoporous media and effects of confinement”
Tenth Annual International Conference on Composites/Nano Engineering ICCE-10, New Orleans (USA).

17-19 February 2003

“Simulation and theoretical study of athermal mixtures in random matrices”
“PanAmerican Workshop on Molecular and Materials Sciences; Theoretical and Computational Aspects”, Cuernavaca,
Mexico.

PEER-REVIEWED PUBLICATIONS:

1. C. Caccamo and G. Pellicane
“RY theory investigation of phase separation in binary hard sphere mixtures”
Physica A **235**, 149 (1997). 10.1016/S0378-4371(96)00336-6
2. C. Caccamo, G. Pellicane and E. Enciso
“PY bridge functions in a thermodynamic self-consistent theory of hard sphere mixtures”
Physical Review E **56**, 6954 (1997).
3. C. Caccamo, D. Costa and G. Pellicane
“A comprehensive study of the phase diagram of symmetric hard core Yukawa mixtures”
Journal of Chemical Physics **109**, 4498 (1998).
4. C. Caccamo, D. Costa and G. Pellicane
“Theoretical and simulation study of model protein solutions”
NATO ASI School proceedings on “New Approaches to Old and New Problems in Liquid State Theory -
Inhomogeneities and Phase Separation in Simple, Complex and Quantum fluids”
Vol. **529**, 421 (1999).
5. M. Björling, G. Pellicane and C. Caccamo
“On the Flory-Huggins and integral equation theory application to hard sphere mixtures”
Journal of Chemical Physics **111**, 6884 (1999).
6. C. Caccamo, G. Pellicane, D. Costa, D. Pini and G. Stell
“Thermodynamically self-consistent theories of fluids interacting through short-range forces”
Physical Review E **60**, 5533 (1999).
7. C. Caccamo, G. Pellicane and R. Ricciari
“Generalized Mean Spherical Approximation with internal thermodynamic consistency constraints: an application to
hard sphere mixtures”
Nuclear and Condensed Matter Physics, Vol. **513**, 55 (2000) .
8. C. Caccamo, G. Pellicane, R. Ricciari and G. Faggio
“Generalized Mean Spherical description of highly asymmetric hard sphere mixtures”
Journal of Physics: Condensed Matter **12**, 2613 (2000).
9. C. Caccamo, D. Costa and G. Pellicane
“Theoretical investigations of simple model protein solutions”
Nuclear and Condensed Matter Physics, Vol. **513**, 51 (2000) .

10. C. Caccamo, G. Pellicane and D. Costa
“Phase transitions in hard-core Yukawa fluids: toward a theory of phase stability in protein solutions”
Journal of Physics: Condensed Matter **12**, A437 (2000).
11. G. Malescio and G. Pellicane
“Simple fluids with complex phase behavior”
Physical Review E **63**, 020501 (R) (2001).
12. M.C. Abramo, C. Caccamo, D. Costa and G. Pellicane
“Phase diagram of model C_n>70 fullerenes”
Europhysics Letters **54**, 468 (2001).
13. G.Malescio, G.Franzese, G.Pellicane, A.Skibinsky, S.V.Buldyrev and H.E.Stanley
“Liquid-liquid transition in one-component systems”
Journal of Physics: Condensed Matter **14**, 2193 (2002).
14. C. Caccamo and G. Pellicane
“Microscopic theories of model macromolecular fluids and fullerenes: the role of thermodynamic consistency”
Journal of Chemical Physics **117**, 5072 (2002).
15. G. Malescio and G. Pellicane
“Stripe phases from isotropic repulsive interactions”
Nature Materials **2**, 97 February 2003.
16. G. Pellicane, D. Costa and C. Caccamo
“Phase coexistence in a DLVO model of globular protein solutions”
Journal of Physics: Condensed Matter **15**, 375 (2003).
17. D. Costa, G. Pellicane, M.C. Abramo and C. Caccamo
“Free energy determination of phase coexistence in model C60: A comprehensive Monte Carlo study”
Journal of Chemical Physics **118**, 304 (2003).
18. D. Costa, G. Pellicane, C. Caccamo, M. Pashinger, G. Kahl
“Theoretical description of phase coexistence in model C60”
Physical Review E **68**, 021104 (2003).
19. G. Pellicane, D. Costa and C. Caccamo
“Cloud and solubility temperatures versus ionic strength in model lysozyme solutions”
Journal of Physics: Condensed Matter **15**, S3485 (2003).
20. M.C. Abramo, C. Caccamo, D. Costa, G. Pellicane and R. Ruberto
“Atomistic vs two-body central potential models of C60: A comparative molecular dynamics study”
Physical Review E **69**, 031112 (2004).
21. G. Pellicane, C. Caccamo, D. S. Wilson and L. L. Lee
“A replica Ornstein-Zernike self consistent theory of mixtures in random pores ”
Physical Review E **69**, 061202 (2004).
22. B. Pellicane, G. Pellicane and G. Malescio
“Polymorphism in simple liquids: a Gibbs Ensemble Monte Carlo study”
Journal of Chemical Physics **120**, 8671 (2004).
23. G. Malescio and G. Pellicane
“Stripe patterns in two-dimensional systems with core-corona molecular architecture”
Physical Review E **70**, 021202 (2004).
24. G. Pellicane, D. Costa and C. Caccamo
“Microscopic determination of the phase diagrams of lysozyme and γ -crystallin solutions”
Journal of Physical Chemistry B **108**, 7538 (2004).

25. G. Pellicane, D. Costa and C. Caccamo
 “Theory and simulation of phase coexistence in short-range models of globular protein solutions”
Journal of Physics: Condensed Matter **16**, S4923 (2004).
26. G. Pellicane, F. Saija, C. Caccamo and P.V. Giaquinta
 “Thermodynamic stability of fluid-fluid phase separation in binary athermal mixtures:
 The Role of nonadditivity”
Journal of Physical Chemistry B **110**, 4539 (2006).
27. G. Pellicane and L.L. Lee
 “Phase separation of model adsorbates in random matrices ”
Physical Chemistry Chemical Physics **9**, 1064 (2007).
28. G. Pellicane, F. Saija, C. Caccamo and P.V. Giaquinta
 “Virial coefficients and demixing of athermal nonadditive mixtures”
Journal of Physical Chemistry B **111**, 4503 (2007).
29. G. Pellicane, R. L. C. Vink, C. Caccamo and H. Löwen
 “Colloid-polymer mixtures in the presence of quenched disorder: a theoretical and computer simulation study”
Journal of Physics: Condensed Matter **20**, 115101 (2008).
30. P.G. De Sanctis-Lucentini and G. Pellicane
 “Critical behavior of symmetrical fluid mixtures in random pores ”
Physical Review Letters **101**, 246101 (2008).
31. G. Pellicane, G. Smith and L. Sarkisov
 “Molecular dynamics characterization of protein crystal contacts in aqueous solutions”
Physical Review Letters **101**, 248102 (2008).
32. M.C. Abramo, C. Caccamo, D. Costa, G. Pellicane and R. Ruberto
 “Molecular Dynamics of an Embedded Charge Model of Lysozyme Aqueous Solutions”
Journal of Physical Chemistry B **114**, 9109 (2010).
33. L.L. Lee, G. Pellicane and W. Chapman
 “A star-function based density functional theory using the local density approach”
Journal of Supercritical Fluids **55**, 524 (2010).
34. M.C. Abramo, C. Caccamo, M. Calvo, V. Conti Nibali, D. Costa, R. Giordano, G. Pellicane, R. Ruberto and U. Wanderlingh
 “Molecular dynamics and small-angle neutron scattering of lysozyme aqueous solutions”
Philosophical Magazine **91**, 2066 (2011).
35. L.L. Lee and G. Pellicane
 “A potential distribution induced mapping of free energies and their wetting behaviour for simple fluids”
Condensed Matter Physics **14**, 33601 (2011).
36. L.L. Lee and G. Pellicane
 “A potential distribution induced mapping of free energies for simple fluids”
Physica A **391**, 1942 (2012).
37. M.C. Abramo, C. Caccamo, D. Costa, G. Pellicane, R. Ruberto and U. Wanderlingh
 “Effective interactions in lysozyme aqueous solutions: a small-angle neutron scattering and computer simulation study”
Journal of Chemical Physics **136**, 035103 (2012).
38. G. Pellicane
 “A colloidal model of lysozyme aqueous solutions: a computer simulation and theoretical study”
Journal of Physical Chemistry B **116**, 2114 (2012).
39. M.C. Abramo, C. Caccamo, M. Cavero, D. Costa, G. Pellicane, R. Ruberto and U. Wanderlingh
 “Effective protein-protein interaction from structure factor data of a lysozyme solution”

Journal of Chemical Physics **139**, 054904 (2013).

40. G. Pellicane and M. Cavero
“Theoretical study of interactions of BSA protein in a NaCl aqueous solution”
Journal of Chemical Physics **138**, 115103 (2013).

41. G. Pellicane, R.L.C. Vink, B. Russo and P.V. Giaquinta
“Fluids in porous media: The case of neutral walls”
Physical Review E **88**, 042131 (2013).

42. G. Pellicane and O. D. Pandaram
“Gibbs ensemble Monte Carlo of nonadditive hard-sphere mixtures”
Journal of Chemical Physics **141**, 044508 (2014).

43. G. Fiumara, O. D. Pandaram, G. Pellicane and F. Saija
“Theoretical and computer Simulation study of phase coexistence of nonadditive hard-disk mixtures”
Journal of Chemical Physics **141**, 214508 (2014).

44. G. Pellicane and L. Sarkisov
“Effective interactions in molecular dynamics simulations of lysozyme solutions”
European Physical Journal B **87**, 191 (2014).

45. A. Mkanya, G. Pellicane and L. L. Lee
“Adsorption of Yukawa fluids on a hard wall”
Molecular Physics **113**, 1097 (2015).

46. R S. Bhatta, G. Pellicane, and M. Tsige
“Tuning range-separated DFT functionals for accurate orbital energy modeling of conjugated molecules”
Computational and Theoretical Chemistry **1070**, 14 (2015).

47. G. Pellicane, M. Tsige, and B. Aragie
“Thermodynamics of a stochastic three level elevator model”
European Physical Journal B, **88**, 150661 (2015).

48. G. Pellicane, M. M. Tchoukouegno, G. T. Mola, M. Tsige
“Surface enrichment driven by polymer topology”
Physical Review E Rapid Communications, **93**, 050501 (2016).

49. Lloyd L. Lee and G. Pellicane
“Towards composite spheres as building blocks for structured molecules”
Journal of Physics: Condensed Matter, **28** 414008 (2016).

50. G. Pellicane and C. Caccamo
“A thermodynamically self-consistent theory of hard-core Yukawa mixtures”
Journal of Physics: Condensed Matter, **28**, 414009 (2016).

51. M. M. Tchoukouegno, G. Pellicane, G., M. Tsige, and G. T. Mola
“Nano-scale morphology dependent performance of thin film organic solar cells”
Journal of Material Science: Materials in Electronics, **28**, 214 (2017).

52. M. M. Tchoukouegno, F. M. Gaitho, G. T. Mola, G., M. Tsige, and G. Pellicane
“Unravelling the surface composition of symmetric linear-cyclic polymer blends”
Fluid Phase Equilibria, **441**, 33 (2017).

53. X. G. Mbuyise, E. A.A. Arbab, K. Kaviyarasu, G. Pellicane, M. Maaza, G. T. Mola
“Zinc oxide doped single wall carbon nanotubes in hole transport buffer layer”
Journal of Alloys and Compounds, **706**, 344 (2017).

54. A. Mkanya, G. Pellicane, D. Pini and C. Caccamo
“Theory and computer simulation of hard-core Yukawa mixtures: thermodynamical, structural and phase coexistence properties”
Journal of Physics: Condensed Matter, **29**, 365102 (2017).

55. S. Prestipino, G. Munao', D. Costa, G. Pellicane, and C. Caccamo
"Two-dimensional mixture of amphiphilic dimers and spheres: Self-assembly behaviour"
Journal of Chemical Physics, **147**, 144902 (2017).
56. G. Fiumara, F. Saija, G. Pellicane, M. Lopez de Haro, A. Santos, and Santos B. Yuste
"Virial coefficients, equation of state, and demixing of binary asymmetric nonadditive hard-disk mixtures"
Journal of Chemical Physics, **147**, 164502 (2017).
57. F. M. Gaitho, G. T. Mola, and G. Pellicane
"Computational approach to the study of morphological properties of polymer/fullerene blends in photovoltaics"
Physical Sciences Reviews, **3**, 20170102 (2018).
58. F. M. Gaitho, M. Tsige, G. T. Mola, G., and G. Pellicane
"Surface Segregation of Cyclic Chains in Binary Melts of Thin Polymer Films: The Influence of Constituent Concentration", *Polymers*, **10**, 324 (2018).
59. S. O. Oseni, K. Kaviyarasu, M. Maaza, G. Sharma, G. Pellicane, G. T. Mola
"ZnO:CNT assisted charge transport in PTB7:PCBM blend organic solar cell"
Journal of Alloys and Compounds, 748, 216-222 (2018).
60. M. C. Abramo, D. Costa, G. Malescio, G. Munao', G. Pellicane, S. Prestipino, and C. Caccamo
"Accurate molecular dynamics determination of liquid-vapor coexistence in molten alkali halides"
Physical Review E Rapid Communications, **98**,010103 (2018).
61. A. Mkanya, G. Pellicane, F. S. Ramos, A. M. Ramos, L.L. Lee
"On the structure, property, and phase behavior of the symmetric Yukawa mixtures: Testing of the consistent integral equation theories"
Molecular Physics, **117**,784 (2019).
62. F. M. Gaitho and G. Pellicane
"Adsorption of binary polymer mixtures with different topology on a wall"
Results in Physics, **12**, 975 (2019).
63. G. Pellicane, L.L. Lee, C. Caccamo
"Integral equation theories of fluid phase equilibria in simple fluids"
Fluid Phase Equilibria, **521**, 112665 (2020).
64. M.C. Abramo, D. Costa, G. Malescio, G. Munao', G. Pellicane. S. Prestipino, and C. Caccamo
"Structure factors and x-ray diffraction intensities in molten alkali halides"
J. Phys. Commun., **4**, 07501 (2020).
65. Z. Workineh, G. Pellicane, M. Tsige
"Tuning solvent quality induces morphological phase transitions in miktoarm star polymer films"
Macromolecules, **53**, 15, 6151 (2020).
66. D. Lombardo, M. A. Kiselev, L. Pasqua, G. Pellicane, and P. Calandra
"Smart Nanostructured Materials: From Molecular Self-Assembly to Advanced Applications"
Journal of Nanomaterials, **2021**, 6482857 (2021).
67. F. S. Ramos, A. M. Ramos, G. Pellicane, and L.L. Lee
"Construction of a composite-sphere model for molecules of tetrahedral symmetry"
Molecular Physics, **119**, e1913254 (2021).
68. N. Dlamini, S. Prestipino, and G. Pellicane
"Self-Assembled Structures of Colloidal Dimers and Disks on a Spherical Surface"
Entropy, **23**, 585 (2021).
69. S. T. Mamba, D. S. Perry, M. Tsige, and G. Pellicane
"Toward the rational design of organic solar photovoltaics: Application of molecular structure methods to donor polymers"
Journal of Physical Chemistry A, **125** 10593-10603 (2021).

70. B. Aragie, M. Bekele, and G. Pellicane
“Noise formed triple-well potential and stochastic resonance of charge carriers”
Pramana Journal of Physics, **96**, 59 (2022).
71. G. Pellicane, E. Lomba, and F. Saija
“Theory and equation of state of two-component nonadditive hard-disks: an application in the colloidal regime”
Physics and Chemistry of Liquids, **60**, 463 (2022).
72. B. Aragie, T. Daba, and G. Pellicane
“A stochastic model for diffusion in a semiconductor layer under the effect of an external potential and nonuniform temperature”
Physica A, **596**, 127197 (2022).

REPORTS

- 1 G. Pellicane, G. Smith and L. Sarkisov
“Molecular dynamics studies of protein-protein interactions: linking atomistic and mesoscales”
Science and Supercomputing in Europe, edited by HPC-Europa, Pan-European Infrastructure on High Performance Computing, ISBN 978-88-86037-22-8 (2008).
- 2 G. Pellicane, G. Smith and L. Sarkisov
“Molecular dynamics studies of protein-protein interactions: linking atomistic and mesoscales”
Science and Supercomputing in Europe, edited by HPC-Europa, Pan-European Infrastructure on High Performance Computing, ISBN 978-88-86037-22-8 (2009).
- 3 G. Pellicane and L. Sarkisov
“Towards a new generation of efficient polyelectrolyte membranes: computer simulation of composite silica/nafion materials”
Science and Supercomputing in Europe, edited by CINECA, ISBN 978-88-86037-23-5 (2010).