Prof Giuseppe Pellicane
Italian citizenship. *South-African permanent resident* since July 2011.

ACADEMIC POSITIONS

1 November 2019 – current
Assistant Professor, Department of, Biomedical, Dental, Morphological and Functional images Sciences (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 (2020-2021) 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 ***C1*** 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 ***C1*** by the National Research Foundation (NRF), South Africa, for the period *2012-2017*.

h-index (Hirsch index): ***23***.

SERVICE-MAN

July-November 1996
Officer cadet of the Italian Army.

December 1996 - October 1997
Officer (lieuteneant) 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 with a number of applications in bio-technology, 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 to a number of 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.

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/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

NIThePP (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

2021 – present Frontiers Molecular Biosciences (Frontiers)

2020 – *present* Polymers (MDPI)

2018 – *present* Polymer (Elsevier)

2020 – *present* Results in Physics (Elsevier)

2015 – present Journal of Smart and Nano Materials (Taylor & Francis)

2015 – present Journal of Physical Chemistry C (American Chemical Society)

2015 - present Chemical Physics Letters (Elsevier)

2014 - present Journal of the Royal Society Interface (Royal Society Publishing)

2013 - present Journal of Physics A (Institute of Physics)

2012 – present Physica Scripta (Elsevier)

2011 – present Molecular Physics (Taylor & Francis)

2009 – present Physical Review Letters (American Physical Society)

2008 – present Soft Matter (Royal Society of Chemistry)

2007 – present Physical Chemistry Chemical Physics (Royal Society of Chemistry)

2006 – present Journal of Physical Chemistry B (American Chemical Society)

2009 – present Journal of Chemical Physics (American Institute of Physics)

2007 – present Physical Review E (American Physical Society)

2008 – present Journal of Physics: Condensed Matter (Institute of Physics)

2009 – present European Journal of Physics (Institute of Physics)

2010 – present New Journal of Chemistry (Royal Society of Chemistry)

2009 – present Crystal Growth and Design (American Chemical Society)

2005 Thermochimica Acta (Elsevier)

RESEARCH POSITIONS and AWARDS (before permanent)

July 2008 – March 2010
19-months research fellowship (national competition – "assegno di ricerca")
Department of Physics, University of Messina (Italy).

2009

Bursary of the European Network HPC-Europa (High Performance Computing – Europa: http://www.hpc-europa.eu/).

2008

Bursary of the European Network HPC-Europa (High Performance Computing – Europa: http://www.hpc-europa.eu/).

2007

Bursary of the European Network HPC-Europa (High Performance Computing – Europa: http://www.hpc-europa.eu/).

Habilitation as a researcher, Biophysical Institute, Italian Research Council (CNR) (national competition).

July 2004 - June 2008
4-years research fellowship (national competition – "assegno di ricerca")
Department of Physics, University of Messina (Italy).

2005
Expert on the subject FIS03/Structure of Condensed Matter, named by the Faculty of Sciences, University of Messina, Italy.

2004

Young researchers' award for excellence in research - scientific-technological section, University of Messina (Italy) (local competition).

Young researchers' grant for the project "Theory and computer simulation of bulk and inhomogeneous fluids" University of Messina (Italy) (local competition).

February 2002 - January 2004
post-doc fellowship (national competition)
Department of Physics, University of Messina (Italy).

2002
National Council of Research (CNR) fellowship (national competition)
School of Chemical Engineering and Materials Science, University of Oklahoma (USA).

Foundation "Angelo Della Riccia" grant for research activities in foreign countries (national competition).

2001
INFM (Italian Institute of Physics of Matter) research fellowship
Research Unit of the University of Messina (Italy).

1998 - 2000
PhD studentship (national competition), Department of Physics, University of Messina (Italy).

SHORT-TERM VISITING PERIODS

February 2001
visiting scientist at the Department of Chemical & Materials Engineering
California State University, Pomona (USA).
Host Contact: Prof Lloyd L. Lee.

December 2016 – January 2017
Visiting researcher at the Dipartimento di Science Matematiche ed Informatiche, Scienze Fisiche e Science della Terra. Universita' di Messina, Italy.
Host Contact: Prof. C. Caccamo

July-August 2010
visiting scientist at the Department of Chemical & Materials Engineering,
California Polytechnic University, Pomona, USA.
Host contact: Prof Lloyd L. Lee.

September-November 2009
HPC-Europa (http://www.hpc-europa.eu/) visitor at the Centre of Materials and Processes
School of Engineering and Electronics, University of Edinburgh (UK).
Host contact: Dr Lev Sarkisov.

January-March 2008
HPC-Europa visitor at the Centre of Materials and Processes,
School of Engineering and Electronics, University of Edinburgh (UK).
Host contact: Dr Lev Sarkisov.

October-December 2007
HPC-Europa visitor at the Centre of Materials and Processes,
School of Engineering and Electronics, University of Edinburgh (UK).
Host contact: Dr Lev Sarkisov.

June 2007
visiting scientist at the Theoretische Physik II,

Heinrich-Heine-Universität, Düsseldorf (GE).
Host contact: Prof Hartmut Löwen.

May 2007
visiting scientist at the Centre of Materials and Processes,
School of Engineering and Electronics, University of Edinburgh (UK).
Host contact: Dr Lev Sarkisov.

June-August 2001
visiting scientist at the School of Chemical Engineering and Materials Science,
University of Oklahoma (USA).
Host Contact: Prof Lloyd L. Lee.

April 2001
Department of Physics, University of Modena and Reggio-Emilia (Italy).
Host contact: Prof Mauro Ferrario.

January-February 2000
Bio-Spectroscopy Laboratory, University of Milan (Italy).
Host contact: Prof Giuseppe Chirico

TEACHING ACTIVITY

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 NIThePInternships 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).

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 Somiéalo 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 this 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.

INVITED SEMINARS

29 October 2020
"Nano-structuring of polymer blends at the interface driven by topology"
Nanotechnology Virtual 2020 (https://www.magnuswebinars.com/nanotechnology-virtual)

14-15 July 2020
"Polymer blends at the interface"
International Webinar "Materials for current trend and future challenges" – Invited talk Government Arts College for Women, Salem, Tamil Nadu. India.

30 Novembre 2017
"Computational studies of complex fluids"
Department of Chemistry, University of Mauritius, Port Luis, Mauritius.

10th february 2015
"Physics of polymer blends: a microscopic approach"
Department of Physics, University of Indonesia, Jakarta, Indonesia.

28 september 2011
"Effective interactions in atomistic studies of lysozyme solutions"
NITheP, Stellenbosch, South Africa.

06 settembre 2010
"A computational insight of protein interactions"
School of Physics, Trinity College, Dublin, Ireland.

29 Luglio 2010
"Critical behaviour of binary fluid mixtures in random pores"
Department of Chemical & Materials Engineering, California State Polytechnic University, Pomona, USA.

8 July 2010
"A computational approach to the study of globular protein solutions"
Department of Chemical & Materials Engineering, California State Polytechnic University, Pomona, USA.

16 December 2008
"Coarse graining of complex fluids: two case-studies"
Institute of Theoretical Physics, University of Göttingen, Germany.

24 October 2008
"Modeling of globular protein solutions: the computational challenge"
School of Physics, University of Kwazulu-Natal, Durban, South Africa.

21 October 2008

"Modeling of globular protein solutions: the computational challenge"
School of Physics, University of Kwazulu-Natal, Pietermaritzburg, South Africa.

13 June 2007
"Colloidal models and phase transitions of complex fluids"
Theoretische Physik II, Heinrich-Heine-Universität, Düsseldorf, Germany.

24 May 2007
"Simple modeling of complex fluids: what amount of information can we get from?"
Institute for Materials and Processes, University of Edinburgh, United Kingdom.

TALKS

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 – 0thd 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, Anheim, 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 confiment"
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.

RESEARCH GRANTS

2011 UKZN Competitive Research Grant (R20.000)

2011 Faculty of Science and Agriculture (UKZN) grant for research development (R55.000)

2012 DoHET Infrastructure and Efficiency funding (R65.000)

2012 School of Chemistry and Physics (UKZN) strategic funding (R100.000)

2012-2017 NRF Incentive funding (Principal Investigator. Budget: R240.000).

2014 NRF Blue Skies Concept Notes "Microscopic Theoretical Study of DNA-Grafted Colloidal Structures" (Principal Investigator. Budget: R194500).

2014-2016 NRF Competitive grant for Rated Researchers "Multiscale theoretical and experimental modelling of electrochemical energy storage and conversion" (Principal Investigator. Budget: R 864000).

2016 NRF Knowledge, Interchange, Collaboration (KIC) grant for mobility (R 40.000).

2015-2017 NRF Competitive grant for Rated Researchers "Investigation of bulk Heterojunction organic solar cell" (Co-investigator. Budget: R 455000).

2015-2017 NRF Blue Skies grant "Microscopic theoretical study of bulk and inhomogeneous Colloidal Structures" (Principal Investigator. Budget: R 260000).

2017-2019 NRF Competitive grant for Rated Researchers "Computational and Experimental Study of Structure-Property Relationships in Organic Solar Cell Materials" (Principal Investigator. Budget: R 515000).

2018-2020 NRF Competitive grant for Rated Researchers "Organic and Hybrid Perovskite based thin film solar cells: Experimental and theoretical investigation" (Co-investigator. Budget: R 513000).

2016 - ongoing South African Center for High Performance Computing (CHPC) grant "Computational Study of Structure-Property Relationships in polymer blends relevant to OPV devices" (Principal Investigator. Budget: 45000000 CPU hours equivalent to R 2025000).

PEER-REVIEWED PUBLICATIONS:

1. C. Caccamo and G. Pellicane
"RY theory investigation of phase separation in binary hard sphere mixtures"
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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 an 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 Cn>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
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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"
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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"
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18. D. Costa, G. Pellicane, C. Caccamo, M. Pashinger, G. Kahl

"Theoretical description of phase coexistence in model C60"
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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"
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21. G. Pellicane, C. Caccamo, D. S. Wilson and L. L. Lee
"A replica Ornstein-Zernike self consistent theory of mixtures in random pores "
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22. B. Pellicane, G. Pellicane and G. Malescio
"Polymorphism in simple liquids: a Gibbs Ensemble Monte Carlo study"
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23. G. Malescio and G. Pellicane
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"Microscopic determination of the phase diagrams of lysozyme and γ-crystallin solutions"
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25. G. Pellicane, D. Costa and C. Caccamo
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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
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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
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35. L.L. Lee and G. Pellicane
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41. G. Pellicane, R:L.C. Vink, B. Russo and P.V. Giaquinta
"Fluids in porous media: The case of neutral walls"
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"Effective interactions in molecular dynamics simulations of lysozyme solutions"
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45. A. Mkanya, G. Pellicane and L. L. Lee
"Adsorption of Yukawa fluids on a hard wall"
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46. R S. Bhatta, G. Pellicane, and M. Tsige
"Tuning range-separated DFT functionals for accurate orbital energy modeling of conjugated molecules"
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47. G. Pellicane, M. Tsige, and B. Aragie
"Thermodynamics of a stochastic three level elevator model"
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48. G. Pellicane, M. M. Tchoukouegno, G. T. Mola, M. Tsige
"Surface enrichment driven by polymer topology"
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49. Lloyd L. Lee and G. Pellicane
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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
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"Unravelling the surface composition of symmetric linear-cyclic polymer blends"
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"Zinc oxide doped single wall carbon nanotubes in hole transport buffer layer"
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"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
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"Computational approach to the study of morphological properties of polymer/fullerene blends in photovoltaics"
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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"
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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"
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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. B. Aragie, M. Bekele, and G. Pellicane
"Noise formed triple-well potential and stochastic resonance of charge carriers"
Accepted by Pramana Journal of Physics, PRAM-D-21-00219 (2021).

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
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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).

17/2/4
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Dear Dr Pellicane

OUTCOME OF EVALUATION AND RATING PROCESS

I have pleasure in informing you that after a rigorous evaluation by peers your application for evaluation and rating has been finalised. Based on the quality and the impact of your research outputs and the comments of the reviewers you have been placed in the **C** category at level **C1**.

The **C** category and **C1** sub-category are defined as follows:

C: Established researchers with a sustained recent record of productivity in the field who are recognised by their peers as having: • produced a body of quality work, the core of which has coherence and attests to ongoing engagement with the field • demonstrated the ability to conceptualise problems and apply research methods to investigating them.

C1: All of the reviewers are firmly convinced that the applicant is an established researcher as described and who, on the basis of the high quality and impact of his/her recent research is regarded by:
Some reviewers as already enjoying considerable international recognition;
OR
The overriding majority of reviewers as being a scholar who has attained a sound/solid international standing in their field, but not yet considerable international recognition;
OR
The overriding majority of reviewers as being a scholar whose work focuses mainly on local and/or regional issues and who as a scholar at a nationally leading level has substantially advanced knowledge and understanding in the field by contributing to new thinking, a new direction and/or a new paradigm.*

Your rating will be valid for administrative purposes from **01 January 2018** to **31 December 2023**.

Should you have indicated that you wished to receive feedback it is included as an attachment to this letter (see Annexure A). To contextualise the feedback the Evaluation and Rating Feedback Policy Guidelines is attached for your information. Please take note that these are the opinions of your peers and do not reflect an NRF view.

In the event of an **appeal** being lodged by your institution on your behalf against the outcome of the evaluation result, such an appeal should reach the NRF's Reviews and Evaluation directorate within three months of the date of this letter. For the guidelines on the appeals process please consult the following link on the NRF website: http://www.nrf.ac.za/rating.

Kindly note that you will be required to submit documents for re-evaluation and rating in **2023**. You will be sent a reminder in this regard during **2022** when a formal invitation to re-submit documents for evaluation and rating will be extended to you. Should you fail to do so your rating will **lapse** on **31 December 2023**.

In making this rating award, the NRF anticipates that you, as a rated researcher, will actively participate in the peer review process to strengthen and expand quality research in South Africa.

Should you require additional information on the evaluation and rating process kindly access the website at http://www.nrf.ac.za/rating (rating link). You are also most welcome to contact me directly via e-mail at joyce.olivier@nrf.ac.za or by telephone on (012) 481-4106.

Yours sincerely

Joyce Olivier
DIRECTOR: REVIEWS AND EVALUATION
cc. A copy of this letter has been sent to the relevant designated authority at your institution.\par

Annexure A

FEEDBACK: DR G PELLICANE

Reviewer Profile:

Total number of reviewers approached*:

Number approached nominated by applicant	3
Number approached nominated by Specialist Committee	12

Total number of reports received:

Number of reports from reviewers nominated by the applicant	3
Number of reports from reviewers nominated by the Specialist Committee	4
Number of reports from reviewers based in South Africa	2
Number of reports from reviewers based outside South Africa	5
Total number of reports used:	**6**

*Includes reviewers who declined to assist, who indicated that they are not to be approached on the system, who did not respond to the invitation to review or who were not approached because they were marked as inappropriate by the members of the Specialist Committee.

Narrative justification of outcome (See attached the Definition of NRF Rating Categories document):

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. Reviewers complimented you concerning the number of papers that you have published in national and international journals (3 articles per annum), as well as the number of papers in conference proceedings. They were impressed by the quality of your work. You are selecting appropriate venues for your work and should continue to target the top international outlets in the field.

Points raised by reviewers which you may wish to consider:

Continue publishing in the top ranked journals as this will be important in extending your international profile and the international impact of your work. Continue to build your network of local and international collaborators, especially funding opportunities involving international collaborates.

Some reviewers recommended that your future research might (within the limits of available material /human resources) benefit from extending QC calculations to first principle molecular dynamics, including approaches such as Parrinello's metadynamics and neural network effective interactions, which might expand the possibilities to deal with complex quantum systems.