Dott. Giuseppe Pellicane (PhD)

Nato a Pavia, Italia, il 10/10/1971.

Cittadinanza italiana. Residente permanente del Sud Africa dal giugno 2011.

POSIZIONI PERMANENTI RICOPERTE

01 January 2018- current

*Associate Professor (*equipollente a Professore Associato in Italia in accordo alla tabella allegata al D.M. Universita' e Ricerca dell' 1 settembre 2016, n. 662*)*, School of Chemistry and Physics, University of Kwazulu-Natal, Sud Africa.

1 Gennaio 2013 – 31 December 2017

Senior Lecturer (equipollente a Professore Associato in Italia in accordo alla tabella allegata al D.M. Universita' e Ricerca del 2 maggio 2011, n. 236/2011), School of Chemistry and Physics, University of Kwazulu-Natal, Sud Africa.

1 Gennaio 2011 – 31 Dicembre 2012

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

ASSOCIAZIONI NEL CAMPO DELLA RICERCA E METRICA

Abilitazione scientifica nazionale docente universitario di seconda fascia in Italia, nel settore 02/B2 (fisica teorica della materia), valida dal 26/07/2017 al 26/07/2023.

Membro ordinario del Istituto Nazionale di Fisica Teorica (NITheP), Sud Africa.

Membro ordinario della Societa' Sudafricana di Fisica (SAIP).

Membro del Comitato Editoriale della rivista *Journal Applied Mathematics*, Hindawi (https://www.hindawi.com/journals/jam/).

Rating della Fondazione Nazionale di Ricerca (NRF) del Sud Africa (vedi document allegato al curriculum: C1 per il periodo 2012-2017; C1 per il periodo 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.")

h-index (indice di Hirsch): **19**.

SERVIZIO MILITARE

Luglio -Novembre 1996

Allievo ufficiale dell' esercito italiano, arma di Fanteria.

Dicembre 1996 – Ottobre 1997

Ufficiale di complemento dell' esercito italiano, arma di Fanteria.

EDUCAZIONE

9 Giugno 2006

Diploma di specializzazione nell' insegnamento secondario della Matematica e Fisica (classe di concorso A049) conseguito presso l'Universita' di Messina, Italia. Voto: 79/80

25 Maggio 2002

Diploma di specializzazione nell' insegnamento secondario della Fisica (classe di concorso A038) conseguito presso l'Universita' di Messina, Italia. Voto: 78/80

26 Febbraio 2001

Dottore di ricerca in Fisica.

Universita' degli studi di Messina (Italia).

19 Marzo 1996

Laurea quadriennale in Fisica

Universita' degli studi di Messina (Italia). Voto: 110/110 e lode.

TRAINING DI RICERCA

27-7 Agosto/Settembre 2007

"Scuola estiva di calcolo avanzato"

Scuola CASPUR, Villa Florio, Grottaferrata, Roma, Italia.

1-5 Marzo 2004

"Tutorial PWscf su proprieta' elettroniche, strutturali e dinamiche di materiali"

CINECA, Bologna, Italia.

6-13 dicembre 2001

"The Nuts and Bolts of First Principles Simulation"

Sviluppatori del pacchetto CASTEP, Durham, Regno Unito.

10-21 Settembre 2001

Scuola estiva su “functional density theory’”

Caramulo, Portogallo.

10-21 September 2001

“Scuola estiva di Calcolo Parallelo”

CINECA school, Bologna, Italy.

18-27 Giugno 2000

Scuola estiva su “Methods in computer simulation”

Manchester, Regno Unito.

7-17 Settembre 1999

Scuola Istituto Nazionale di Fisica della Materia (INFM) su “Teoria della materia condensata”

7-17 Luglio 1998

Scuola NATO-ASI su “New approaches to problems in liquid state theory”

Patti Marina, Italia.

INTERESSI DI RICERCA

In generale, i miei interessi si focalizzano sulla teoria e simulazione al computer di sistemi della materia condensata e soffice nello stato fluido. Tali sistemi includono un ampio spettro di materiali con un certo numero di applicazioni nel campo della bio-tecnologia, ingegneria delle superfici, medicina, e risorse energetiche rinnovabili quali, ad esempio, miscele polimeriche, sistemi colloidali, soluzioni di proteine, e fluidi confinati all’ interno di strutture porose o di strutture geometriche semplici.

SERVIZI ALLA COMUNITA’ ACCADEMICA

Oltre alla descrizione sintetica sotto riportata, svolgo regolare attivita’ di revisore di applicazioni di studenti per borse di studio a livello di Masters/Dottorato e di progetti di ricerca, su richiesta della Fondazione di Ricerca Nazionale (NRF) del Sud Africa. Ho anche revisionato progetti di ricerca sottomessi alla Societa’ di Chimica Americana (ACS, Stati Uniti) e fatto parte di diverse commissioni per valutare l’idoneita’ di candidati per posizioni accademiche all’interno della mia attuale universita’ in Sud Africa (University of

Kwazulu-Natal). Dal 2013 sono membro della commissione “Ricerca e lauree di grado superiore (Masters, Dottorato)” nella School of Chemistry and Physics, University of Kwazulu-Natal, Sud Africa.

2016

Membro della commissione per la valutazione dei premi assegnati al Workshop annuale dei borsisti dell’ Istituto Nazionale di Fisica Teorica del Sud Africa (NITheP).

Membro della commissione per la valutazione dei rinnovi delle posizioni sudafricane di Research Chair (SARCHI chair) della Fondazione di Ricerca Nazionale (NRF) del Sud Africa.

2015

Line Manager reggente, raggruppamento di Fisica del campus di Pietermaritzburg, School of Chemistry and Physics, University of Kwazulu-Natal, Sud Africa.

Rappresentante del raggruppamento di Fisica della University of Kwazulu-Natal nella conferenza di pianificazione strategica nazionale per implementare le raccomandazioni del comitato di revisione dell’insegnamento della Fisica a livello universitario (Sud Africa).

2014

Membro della commissione per la assegnazione delle borse di studio di Dottorato di ricerca, settore di Scienze Fisiche, della Fondazione di Ricerca Nazionale (NRF) del Sud Africa.

2013

Membro della commissione per la valutazione dei progetti di ricerca del settore di Scienze Fisiche nell’ambito del programma competitive per ricercatori con rating (CPRR) della Fondazione di Ricerca Nazionale (NRF) del Sud Africa.

Membro della commissione per la assegnazione delle borse di studio di Dottorato di ricerca, settore di Scienze Fisiche, della Fondazione di Ricerca Nazionale (NRF) del Sud Africa.

ATTIVITA’ DI REVISORE (REFEREE) PER RIVISTE SCIENTIFICHE INTERNAZIONALI

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)

IDONEITA'/PREMI - BORSE DI STUDIO DA CONCORSI PER TITOLI ED ESAMI (PERIODO ANTECEDENTE POSIZIONE PERMANENTE)

Luglio 2008 – Marzo 2010

Assegno di ricerca universitario press il Dipartimento di Fisica, Universita; degli studi di Messina (Italia).

2009

Borsa di studio nell' ambito del network europeo HPC-Europa (High Performance Computing – Europa: http://www.hpc-europa.eu/)

2008

Borsa di studio nell' ambito del network europeo HPC-Europa (High Performance Computing – Europa: http://www.hpc-europa.eu/)

2007

Borsa di studio nell' ambito del network europeo HPC-Europa (High Performance Computing – Europa: http://www.hpc-europa.eu/)

Idoneita' a ricercatore di terzo livello presso l' Istituto di Biofisica del Consiglio Nazionale delle Ricerche (CNR).

Luglio 2004 – Giugno 2008

Assegno di ricerca universitario presso il Dipartimento di Fisica, Universita' degli studi di Messina (Italia).

2005

Cultore della materia nel settore scientifico-disciplinare FIS03, Facolta' di Scienze, Universita' degli studi di Messina (Italia).

2004

Premio per Giovani Ricercatori per eccellenza nella ricerca del settore scientifico-tecnologico, Universita' degli studi di Messina (Italia).

Fondi di ricerca per Giovani ricercatori per il progetto "Teoria e Simulazione al Computer di fluidi bulk e non-omogenei" presso Universita' degli studi di Messina (Italia).

Febbraio 2002 – Gennaio 2004

Borsa di studio post-dottorato, Universita' degli studi di Messina (Italia).

2002

Borsa di studio di un anno del CNR presso istitutuzioni scientifiche estere (School of Chemical Engineering and Materials Science, University of Oklahoma (USA).)

Borsa di studio "Angelo della Riccia" per attivita' di ricerca in paesi stranieri (School of Chemical Engineering and Materials Science, University of Oklahoma (USA).)

2001

Borsa di studio Istituto Nazionale di Fisica della Materia (INFM) presso Universita' degli studi di Messina (Italia).

1998-2000

Borsa di studio di Dottorato di Ricerca presso Universita' degli studi di Messina (Italia).

PERIODI DI RICERCA DI BREVE DURATA FUORI SEDE

Dicembre 2016 – Gennaio 2017

"Visiting Researcher" presso il Dipartimento di Science Matematiche ed Informatiche, Scienze Fisiche e Science della Terra, Universita' degli studi di Messina (Italia).
Contatto: Prof C. Caccamo

Luglio-Agosto 2010

"Visiting Scientist" presso il Department of Chemical & Materials Engineering, California Polytechnic University, Pomona, Stati Uniti.
Contatto: Prof Lloyd L. Lee

Settembre-Novembre 2009

HPC-Europa (http://www.hpc-europa.eu/) visitor presso il Centre of Materials and Processes School of Engineering and Electronics, University of Edinburgh (UK).
Contatto: Dr Lev Sarkisov

Gennaio-Marzo 2008

HPC-Europa (http://www.hpc-europa.eu/) visitor presso il Centre of Materials and Processes School of Engineering and Electronics, University of Edinburgh (UK).
Contatto: Dr Lev Sarkisov

Ottobre-Dicembre 2007

HPC-Europa (http://www.hpc-europa.eu/) visitor presso il Centre of Materials and Processes School of Engineering and Electronics, University of Edinburgh (UK).
Contatto: Dr Lev Sarkisov

Giugno 2007

"Visiting Scientist" presso il Theoretische Physik II,
Heinrich-Heine-Universität, Düsseldorf (GE).
Contatto: Prof Hartmut Löwen.

Maggio 2007

Visiting Scientist presso il Centre of Materials and Processes,
School of Engineering and Electronics, University of Edinburgh (UK).
Contatto: Dr Lev Sarkisov.

Giugno-Agosto 2001

Visiting Scientist presso la School of Chemical Engineering and Materials Science,
University of Oklahoma (USA).
Contatto: Prof Lloyd L. Lee.

Aprile 2001

Dipartimento di Fisica, Universita' degli studi di Modena e Reggio-Emilia (Italia)
Contatto: Prof Mauro Ferrario.

Gennaio-Febbraio 2000

Laboratorio di Bio-Spettroscopia, Universita' degli studi di Milano (Italia).
Contatto: Prof Giuseppe Chirico

ATTIVITA' DI INSEGNAMENTO

Luglio-Ottobre 2018

Fisica Statistica (PHYS362)
College of Agriculture, Engineering and Science, UKZN (Sud Africa).

Luglio-Ottobre 2018
Meccanica computazionale e programmazione simbolica (CPHY212)
College of Agriculture, Engineering and Science, UKZN (Sud Africa).

Settembre-Ottobre 2018
Metodi Matematici (PHYS752)
College of Agriculture, Engineering and Science, University of Kwazulu-Natal (UKZN, Sud Africa).

Febbraio-Maggio 2018
Fisica Statistica avanzata (PHYS741)
College of Agriculture, Engineering and Science, UKZN (Sud Africa).

Luglio-Ottobre 2017
Fisica Statistica (PHYS362)
College of Agriculture, Engineering and Science, UKZN (Sud Africa).

Settembre-Ottobre 2017
Metodi Matematici (PHYS752)
College of Agriculture, Engineering and Science, University of Kwazulu-Natal (UKZN, Sud Africa).

Febbraio-Maggio 2017
Fisica Statistica avanzata (PHYS741)
College of Agriculture, Engineering and Science, UKZN (Sud Africa).

Settembre-Ottobre 2016
Metodi Matematici (PHYS752)
College of Agriculture, Engineering and Science, University of Kwazulu-Natal (UKZN, Sud Africa).

Settembre-Ottobre 2016
Fisica Moderna per le Scienze della Vita ed Agrarie (PHYS133)
Supervisore delle ativita' di Laboratorio, College of Agriculture, Engineering and Science,
UKZN (South Africa).

Luglio-Ottobre 2016
Fisica Statistica (PHYS362)
College of Agriculture, Engineering and Science, UKZN (Sud Africa).

Febbraio-Maggio 2016 February-May 2016
Fisica Statistica avanzata (PHYS741)
College of Agriculture, Engineering and Science, UKZN (Sud Africa).

Febbraio-Maggio 2015 February-March 2015
Introduzione alla Fisica per le Scienze della Vita ed Agrarie (PHYS131)
Supervisore delle ativita' di Laboratorio, College of Agriculture, Engineering and Science,
UKZN (South Africa).

Febbraio-Maggio 2015
Fisica Statistica avanzata (PHYS741)

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

Settembre-Ottobre 2014
Termodinamica (PHYS212)
College of Agriculture, Engineering and Science, UKZN (South Africa).

Settembre-Ottobre 2014
Metodi Matematici (PHYS752)
College of Agriculture, Engineering and Science, UKZN (Sud Africa).

Luglio-Ottobre 2014
Fisica Statistica (PHYS362)
College of Agriculture, Engineering and Science, UKZN (Sud Africa).

Febbraio-Maggio 2014
Introduzione alla Fisica per le Scienze della Vita ed Agrarie (PHYS131)
Supervisore delle ativita' di Laboratorio, College of Agriculture, Engineering and Science, UKZN (Sud Africa).

Febbraio-Maggio 2014
Fisica Statistica avanzata (PHYS742)
College of Agriculture, Engineering and Science, UKZN (Sud Africa).

Settembre-Ottobre 2013
Termodinamica (PHYS212)
College of Agriculture, Engineering and Science, UKZN (Sud Africa).

Settembre-Ottobre 2013
Metodi Matematici (PHYS752)
College of Agriculture, Engineering and Science, UKZN (Sud Africa).

Luglio-Ottobre 2013
Fisica Moderna per le Scienze della Vita ed Agrarie (PHYS133)
Supervisore delle ativita' di Laboratorio, College of Agriculture, Engineering and Science, UKZN (Sud Africa).

Luglio-Ottobre 2013
Fisica Statistica (PHYS362)
Lecturer, College of Agriculture, Engineering and Science, UKZN (Sud Africa).

Febbraio-Maggio 2013
Introduzione alla Fisica per le Scienze della Vita ed Agrarie (PHYS131)
Supervisore delle ativita' di Laboratorio, College of Agriculture, Engineering and Science, UKZN (Sud Africa).

Febbraio-Maggio 2013
Fisica Statistica e Superfluidita' (PHYS742)
College of Agriculture, Engineering and Science, UKZN (Sud Africa).

Settembre-Ottobre 2012
Termodinamica (PHYS212)

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

Settembre-Ottobre 2012
Metodi Matematici (PHYS752)
College of Agriculture, Engineering and Science, UKZN (Sud Africa).

Luglio-Ottobre 2012
Fisica Statistica (PHYS362)
College of Agriculture, Engineering and Science, UKZN (Sud Africa).

Febbraio-Maggio 2012
Fisica Statistica e Superfluidita' (PHYS742)
College of Agriculture, Engineering and Science, UKZN (Sud Africa).

Settembre-Ottobre 2011
Metodi Matematici (PHYS752)
Faculty of Science and Agriculture, UKZN (Sud Africa).

Luglio-Ottobre 2011
Fisica Statistica e Superfluidita' (PHYS742)
Faculty of Science and Agriculture, UKZN (Sud Africa).

Aprile-Maggio 2011
Termodinamica (PHYS131)
Faculty of Science and Agriculture, UKZN (Sud Africa).

Febbraio-Maggio 2011
Fisica Statistica e Termodinamica (PHYS306)
Faculty of Science and Agriculture, UKZN (Sud Africa).

Aprile-Maggio 2009
Fisica avanzata della materia condensata per studenti del terzo anno del corso di laurea di primo livello in Fisica.
Facolta' di Scienze, Universita' degli studi di Messina (Italia).

Aprile-Maggio 2009
Fisica statistica avanzata per studenti del terzo anno del corso di laurea di primo livello in Fisica.
Facolta' di Scienze, Universita' degli studi di Messina (Italia).

Marzo-Giugno 2009
Informatica per studenti del primo anno del corso di laurea di primo livello in Chimica e Tecnologia Farmaceutica – Farmacia
Facolta' di Farmacia, Universita' degli studi di Messina (Italia).

March-June 2008
Informatica per studenti del primo anno del corso di laurea di primo livello in Chimica e Tecnologia Farmaceutica – Farmacia
Facolta' di Farmacia, Universita' degli studi di Messina (Italia).

Settembre-Ottobre 2007
Meccanica Analitica per student del secondo anno del corso di laurea di primo livello in Fisica

Facolta' di Scienze, Universita' degli studi di Messina (Italia).

January-February 2007
Fisica statistica avanzata per studenti del terzo anno del corso di laurea di primo livello in Fisica.
Facolta' di Scienze, Universita' degli studi di Messina (Italia).

March-June 2007
Informatica per studenti del primo anno del corso di laurea di primo livello in Chimica e Tecnologia Farmaceutica
Facolta' di Farmacia, Universita' degli studi di Messina (Italia).

June-July 2006
Informatica per studenti del primo anno del corso di laurea di primo livello in Fisica.
Facolta' di Scienze, Universita' degli studi di Messina (Italia).

March-May 2006
Informatica per studenti del primo anno del corso di laurea di primo livello in Infermieristica
Facolta' di Medicina, Universita' degli studi di Messina (Italia).

June-July 2005
Fisica statistica avanzata per studenti del terzo anno del corso di laurea di primo livello in Fisica.
Facolta' di Scienze, Universita' degli studi di Messina (Italia).

RELATORE DI TESI DI LAUREA/DOTTORATO

2017 – attuale Sig.re Tapiwa Musunga, Masters in Fisica (UKZN, Sud Africa).

2016 – attuale Sig.re Sandile T. Mamba, Dottorato di Ricerca in Fisica (UKZN, Sud Africa).

2016 – attuale: tesi consegnata al College in data 23/11/2018 Sig.re Anele Mkanya, Dottorato di Ricerca in Fisica (UKZN, Sud Africa).

2015 – attuale: tesi consegnata al College in data 09/11/2018 Sig.re Francis M. Gaitho, Dottorato di Ricerca in Fisica (UKZN, Sud Africa).

2017
Sig.rina Cindy Mphara, Tesi di laurea di Honours in Fisica (UKZN, Sud Africa).

2016
Sig.re Jashan Naicker, Tesi di laurea di Honours in Fisica (UKZN, Sud Africa).

2012-2015
Sig.ra Mireille Megnidio-Tchoukouegno, Dottorato di Ricerca in Fisica (UKZN, Sud Africa).

2014-2015
Sig.re Anele Mkanya, Masters in Fisica (UKZN, Sud Africa).

2013-2015

Sig.re Berhanu Aragie Woldetsadik, Dottorato di Ricerca in Fisica (UKZN, Sud Africa).

2015
Sig.re Verlan Moodley, Tesi di laurea di Honours in Fisica (UKZN, Sud Africa).

2013-2014
Sig.re Owen Daniel Pandaram, Masters in Fisica (UKZN, Sud Africa).

2014
Sig.re Mdusumeni Isaac Nxumalo, Tesi di aurea di Honours in Fisica (UKZN, Sud Africa).

2012
Dr Miguel Cavero, borsista post-dottorato in Fisica (UKZN, Sud Africa).

2011
Sig.re Lizwe Wandile Mdakane, Tesi di laurea di Honours in Fisica (UKZN, Sud Africa).

2010-2011
Sig.re Bruno Russo, Masters in Fisica (Universita' degli studi di Messina (Italia).
– correlatore con il Prof P V Giaquinta).

ESAMINATORE ESTERNO DI TESI DI DOTTORATO/MASTERS

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 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 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 MSc thesis "Generation and detection of Bessel beams" by Thandeka Mhlanga.

External examiner of the UKZN MSc thesis "Bulk heterojunction organic solar cell" by Wiseman Mpilo Dlamini.

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

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

SEMINARI SU INVITO

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

10 Febbraio 2015
“Physics of polymer blends: a microscopic approach”
Department of Physics, University of Indonesia, Jakarta, Indonesia.

28 Settembre 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 Luglio 2010
“A computational approach to the study of globular protein solutions”
Department of Chemical & Materials Engineering, California State Polytechnic University, Pomona, USA.

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

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

21 Ottobre 2008
“Modeling of globular protein solutions: the computational challenge”
School of Physics, University of Kwazulu-Natal, Pietermaritzburg, South Africa.

13 Giugno 2007
“Colloidal models and phase transitions of complex fluids”

Theoretische Physik II, Heinrich-Heine-Universität, Düsseldorf, Germany.

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

RELAZIONI ORALI PRESSO CONFERENZE INTERNAZIONALI

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" – Invited Talk (e Chairman di sessione parallela)
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" (anche Chairman di sessione parallela)
ICMAT 2017, 9th International conference on Materials for Advanced Technologies, Singapore.

13 Marzo – 17 Marzo 2017
"Unravelling the surface composition of topologically-different polymer blends" – Invited Talk
EMN Meeting on Polymer 2017, Auckland, New Zealand.

26 Febbraio – 1 Marzo 2017
"Understanding the role of polymer topology in surface absorption" – Keynote Lecture (Invited Talk)
40th Annual Meeting of The Adhesion Society, St. Petersburg, Florida, USA.

5 – 9 Dicembre 2016
"Computational studies of binary polymer blends"
CHPC National Meeting 2016, East London, South Africa.

2 – 6 Ottobre 2016
"Interfacial properties of linear-cyclic polymer blends"
The 11th Asian Thermophysical Properties Conference, Yokohama, Japan.

18 -22 Luglio 2016
"Interfacial properties of linear-cyclic polymer blends"
ICPAC 2016 "Emerging Trends in Chemical Sciences", Mauritius.

28 Settembre-2 Ottobre 2015
"Anomalous adsorption of linear-cyclic polymer blends" (Invited Talk)
FISMAT 2015, University of Palermo, Palermo (Italy).

21-26 Giugno 2015
"Interfacial properties of linear-cyclic polymer blends"
Nineteenth Symposium on thermophysical properties, Boulder, Colorado (USA)

31 Agosto-04 Settembre 2014
"Interfacial Properties and Dynamics of linear-cyclic polymer blends"
ECTP 2014 – *European Conference on Thermophysical Properties*, Porto (Portugal)

24-29 Giugno 2012
"Effective interactions in atomistic studies of lysozyme solutions"
18th Symposium on thermo-physical properties, Boulder, Colorado (USA)

15-17 Giugno 2010
"Effective interactions in globular protein solutions"
Translational Access Meeting 2010, Helsinki, Finland.

15-18 Luglio 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 Dicembre 2008
"A numerical assessment of solvated protein interactions underlying hydrophobic patches"
Translational Access Meeting 2008, Stuttgart, Germany.

22-26 Novembre 2008
"Nonequilibrium MD as a probe of protein interactions in aqueous solutions"
Final Arrested Matter Conference, Taormina, Italy (http://www.arrestedmatter.net/).

16-19 Giugno 2008
"Molecular dynamics characterization of protein-protein crystal contacts in aqueous solutions"
Polyelectrolytes 2008, Coimbra, Portugal.

5-7 Luglio 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 Gennaio 2007
"Phase diagram of binary, athermal mixtures: theoretical and simulation results"
"*Dynamical Arrest of Soft Matter and Colloids*" workshop, Bad Gastein, Austria.

29-31 Agosto 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 Dicembre 2005
"Thermodynamic stability of fluid-fluid phase separation in binary, athermal mixtures: the role of nonadditivity"
CRS-SOFT meeting, L'Aquila, Italy.

22-25 Giugno 2005
"Stripe phases in systems with core-corona molecular architecture"
"*Materials, Matter and Devices (MMD) meeting*", Genova, Italy.

8-12 Maggio 2005
"Stripe phases from isotropic repulsive interactions"
"*NANOTECH 2005*" conference, Anheim, California USA.

6-8 Aprile 2005
"Stripe phases in systems with core-corona molecular architecture"
"*Thermodynamics 2005*" conference, Sesimbra, Portugal.

12-15 Luglio 2004
"Theoretical phase diagram determination of globular protein solutions" (Invited Talk)
"*Disorder, Complexity and Biology*" STATPHYS 22 satellite conference,
Varanasi (India).

8-10 Giugno 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 Luglio 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 Febbraio 2003
"Simulation and theoretical study of athermal mixtures in random matrices"
"*PanAmerican Workshop on Molecular and Materials Sciences; Theoretical and Computational Aspects*", Cuernavaca, Mexico.

PROGETTI DI RICERCA FINANZIATI

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

2018-2020 NRF Competitive grant per Ricercatori con rating "Organic and Hybrid Perovskite based thin film solar cells: Experimental and theoretical investigation" (Co-investigatore. Budget: R 513000).

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

2015-2017 NRF Competitive grant per Ricercatori con rating “Investigation of bulk Heterojunction organic solar cell” (Co-investigator. Budget: R 455000).

2016 Fondi KIC per mobilita’ fra strutture di ricerca (R 40.000).

2014-2016 NRF Competitive grant per Ricercatori con rating “Multiscale theoretical and experimental modelling of electrochemical energy storage and conversion” (Principal Investigator. Budget: R 864000).

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

2012-2017 Fondi di incentivazione NRF (Principal Investigator. Budget: R240.000).

2013 Fondi Knowledge, Interchange, Collaboration (KIC) dell’ NRF per mobilita’ fra strutture di ricerca (R 20.000)

2012 Fondi strategici della School of Chemistry and Physics (UKZN) (R100.000).

2012 Fondi per miglioramento dell’ efficienza ed infrastruttura DoHET (R65.000).

2011 Grant per sviluppo di attivita’ di ricerca della Faculty of Science and Agriculture, UKZN (R55.000).

2011 Grant per ricerca competitiva UKZN (R20.000).

PUBLICAZIONI SU RIVISTE INTERNAZIONALI:

1. C. Caccamo and G. Pellicane
“RY theory investigation of phase separation in binary hard sphere mixtures”
Physica A **235**, 149 (1997).

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"
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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
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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 "
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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
"Stripe patterns in two-dimensional systems with core-corona molecular architecture"
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"Microscopic determination of the phase diagrams of lysozyme and □-crystallin solutions"
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"Theory and simulation of phase coexistence in short-range models of globular protein solutions"
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"Thermodynamic stability of fluid-fluid phase separation in binary athermal mixtures:
The Role of Nonadditivity"
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"Virial coefficients and demixing of athermal nonadditive mixtures"
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"Colloid-polymer mixtures in the presence of quenched disorder: a theoretical and computer simulation study"

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"Molecular dynamics characterization of protein crystal contacts in aqueous solutions"
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"Effective protein-protein interaction from structure factor data of a lysozyme solution"
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40. G. Pellicane and M. Cavero
"Theoretical study of interactions of BSA protein in a NaCl aqueous solution"
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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"
Molecular Physics **113**, 1097 (2015).

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"Tuning range-separated DFT functionals for accurate orbital energy modeling of conjugated molecules"
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"Thermodynamics of a stochastic three level elevator model"
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"Surface enrichment driven by polymer topology"
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"Towards composite spheres as building blocks for structured molecules"
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"Nano-scale morphology dependent performance of thin film organic solar cells"
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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"
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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"
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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"
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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, 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 (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, https://doi.org/10.1080/00268976.2018.1542165 *(*2018).

62. F. M. Gaitho and G. Pellicane
"Adsorption of binary polymer mixtures with different topology on a wall"
Results in Physics (RINP_2018_2462), accepted for publication.

RAPPORTI DI RICERCA SU VOLUMI INTERNAZIONALI

1 G. Pellicane, G. Smith and L. Sarkisov
"Molecular dynamics studies of protein-protein interactions: linking atomistic and mesoscales"
Science and Supercomputing in Europe, edito da 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, edito da 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, edito da CINECA, ISBN 978-88-86037-23-5 (2010).

17/2/4
Pellicane G
30 January 2018

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National Research Foundation | RISA Research and Innovation Support and Advancement

Dr G Pellicane
School of Chemistry and Physics
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pellicane@ukzn.ac.za

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.