

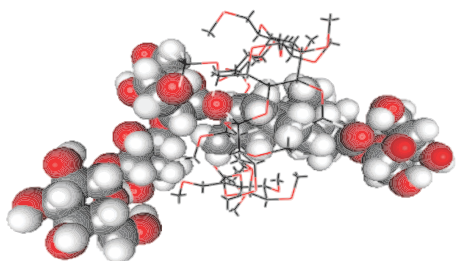


DURBAN UNIVERSITY OF TECHNOLOGY
INYUVESI YASETHEKWINI YEZOBUCHWEPHESHE

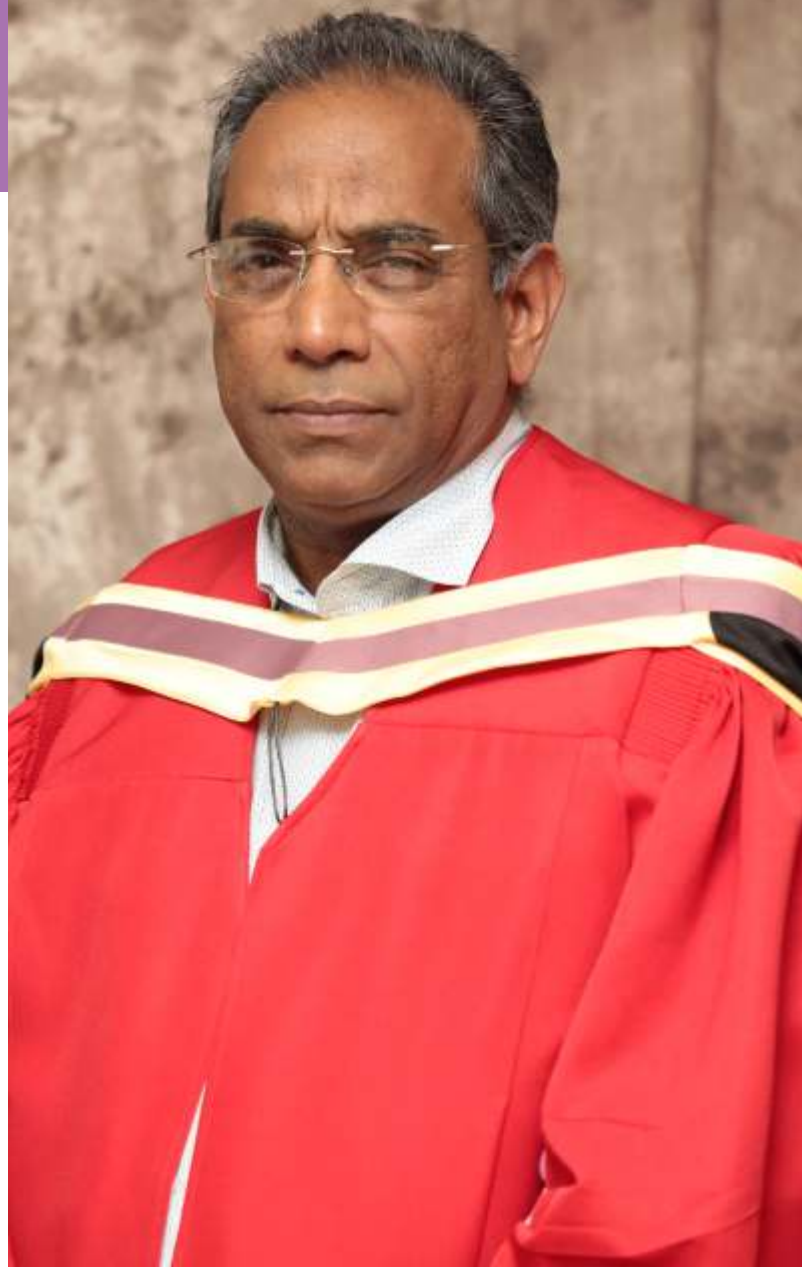
FACULTY OF
APPLIED
SCIENCES

INAUGURAL LECTURE OF
PROFESSOR KRISHNA BISETTY

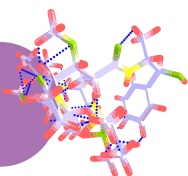
COMPUTATIONAL MODELLING:
A CHEMISTS PERSPECTIVE



1 OCTOBER 2021
17:00 - 18:30



PROGRAMME



PROGRAMME DIRECTOR

Professor Megandhren Govender

Full Professor in Mathematics at DUT

WELCOME AND OPENING REMARKS

Professor Sibusiso Moyo

Deputy Vice-Chancellor: Research, Innovation and Engagement

INTRODUCTION OF INAUGURAND

Professor Suren Singh

Executive Dean: Faculty of Applied Sciences

INAUGURAL LECTURE

Professor Krishna Bisetty

Computational Modelling: *A Chemists Perspective*

CLOSING REMARKS AND VOTE OF THANKS

Professor Nokuthula Sibiya

Deputy Vice-Chancellor: Teaching and Learning

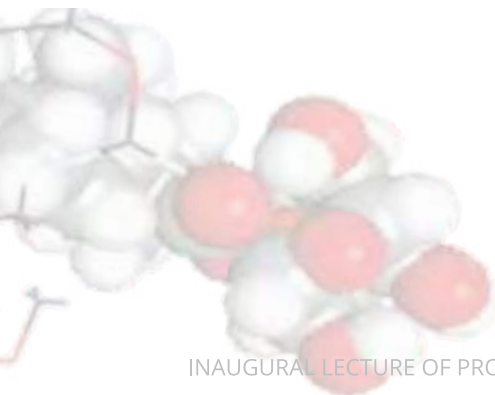
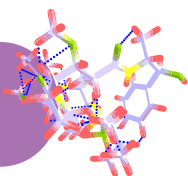


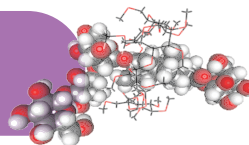
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BIOGRAPHY: PROFESSOR K BISETTY



Krishna Bisetty is a Professor of Chemistry and a seasoned educator with 30 years of experience in higher education, during this period he also served as HoD from 2014-2017.

Prior to joining the ML Sultan Technikon in 1991, he spent 3 years as a lecturer in chemistry at the Springfield College of Education. The experience gained in the training of high school teachers in Physical Science paved the way for a sound career path in chemistry. His passion for Chemical Education has had a major impact on both his teaching and research. He is currently an NRF C1 rated researcher and leader of the Computational Modelling and Bioanalytical Research Group at DUT, a flagship project registered at the Centre for High Performance Computing (CHPC).

He is a co-author of over 100 published papers in peer-reviewed journals, 8 book chapters and has over 1600 citations with an H-index of 24 (Scopus). He supervised over 20 masters and doctoral students, and more than 5 post-doctoral fellows. He served on several Conference Organizing Committees and actively participated at local and international conferences.

In addition to his postdoctoral work undertaken in Barcelona in the early 1990's, he also held visiting positions at the Jamia Islamia University (A Central University) in India, the University of Valencia in Spain, the University of Mauritius and the University of Latvia.

SUMMARY OF INAUGURAL LECTURE

COMPUTATIONAL MODELLING: A CHEMISTS PERSPECTIVE

In his inaugural lecture, a glimpse of his cutting-edge research will be showcased in trying to understand the synergy between experimental and computational approaches in addressing the design and mechanism of electrochemical sensing of specific nanobiosensors and identifying the contributing factors in order to enhance the sensing capabilities, with applications in the food and health sectors.

RESEARCH EXPERTISE

Prof Bisetty has a keen interest in establishing synergies between electroanalytical chemistry and computational chemistry focussing on biosensing devices using state-of-the-art experimental and computational methodologies, with the latter used as a design technique that provides models to explain the experimental findings.

The broader goals are to design, model and fabricate doped smart engineered nanomaterials to improve human health and biosensor technology.

PATENT

Development of a Chili-based Electrochemical Sensor
Patent No: 2017/07307



AWARDS

External Awards

- Certificate received for Best oral presentation on a paper entitled, "A Theoretical Study of Cage Peptides." presented at the 36th Convention SA Chemical Institute held in Port Elizabeth, July 2002.
- First prize Gold Poster award received for the best Poster presentation, "M.I. Sabela, P. Singh, N.J. Gumede, K. Bisetty and S. Sagrado. "Evaluation of enantioresolution of catechin using electrokinetic chromatography and molecular docking", Separation Science 2012, held in Kuala Lumpur (Malaysia) from 22-27 June 2012.

Institutional Awards

- Council Achievement Award, in recognition of being an outstanding University Publisher in 2012
- Council Award, in recognition of NRF C3 Rating in 2015
- Top Researcher in the Faculty of Applied Science (2012; 2015; 2016)
- Top University Publisher in 2016
- Innovator of the Year Award in 2017
- Research & Innovation Award: Top Impact Researcher, Dec 2020
- Research & Innovation Award: Re-Rated NRF C1 Researcher, Dec 2020

EXTERNAL GRANTS

- NRF/SPAIN-RSA Bilateral Agreement Grant (Barcelona Group) (2006-2008) R300 K
- NRF/SPAIN-RSA Bilateral Agreement Grant (Valencia Group) (2006-2010) R200 K
- NRF-NEP Equipment Grant: Capillary Electrophoresis (2010) R600 K
- CHIETA- Structural Infra Structure Projects (SIPs) (2015) R500 K
- TIA- Development of a Biosensor for the detection of Capsaicin (2016) R495 K
- Spectro-Electrochemistry instrument (2017) R320 K
- NRF-NEP Grant for FFF/UHPLC/ICP-MS (2017) R12 M

MEMBERSHIP TO BOARD AND COMMITTEES

Chemistry Advisory Board

Faculty Board (FAS)

Faculty Research Committee (FRC)

Faculty of Applied Sciences Rep for Shortlisting and Interview Panel (2013-2017)

Higher Degrees Committee (2013-2017)

Professorial Committee (FAS)

Senate

LOCAL ORGANIZING COMMITTEES

- SACI 2006 International conference, held from 3-8 December 2006, at UKZN.
- SACI 2015 International conference, held from 3-8 December 2015, at Elangeni Hotel, Durban.
- NanoAfrica2018 International conference, held from 25-28 April 2018, Salt Rock Hotel, Durban.
- 70th Annual Meeting of the International Society for Electrochemistry (ISE): held from 4-9 August 2019, ICC Durban. Symposium 15: "Computational Electrochemistry and Simulation: from Prediction of Properties to Optimization of Devices"

MEMBERSHIP TO PROFESSIONAL SOCIETIES

South African Chemical Institute (SACI)

American Chemical Society (ACS)

Royal Society of Chemistry (RSC)

International Society of Electrochemistry (ISE)



INTERNATIONAL/LOCAL/INDUSTRIAL COLLABORATION

- Prof. Juan Jesus Perez, Universitat de Catalunya, Barcelona, Spain;
- Prof. Salvador Sagrado, Bioanalytical Research, University of Valencia, Spain;
- Prof. Ashutosh Tiwari, Materials Science, Linköping University, Sweden;
- Prof. Imtiyaz Hassan Centre for Interdisciplinary Research in Basic Sciences, Jamia Milia Islamia, Jamia Nagar, New Delhi;
- Prof. Mikhael Bechelany, Institut Européen des Membranes, University of Montpellier, France;
- Prof Ponnadurai Ramasami, Computational Chemistry Group, University of Mauritius
- Dr Florian Meier, Research Scientist, Postnova Analytics, Germany;
- Prof Bonex Wakufwa Mwakikunga, CSIR- National Centre for Nano-Structured Materials, Pretoria.
- Dr Njabulo Joyful Gumede, Department of Chemistry, Mangosuthu University of Technology;
- Dr Tony Pfaffe, Instrument Engineering, Postnova Analytics, Germany;
- Dr Helmut Ernstberger, Application Specialist, PerkinElmer, Italy;
- Mr Achim Schmottlach, Senior Experten Service (SES), Project: ZA-DUTCHEM, Germany;
- Mr Tys van der Merwe, PerkinElmerSA

REVIEWER OF ISI JOURNALS

South African Journal of Chemistry;
 Journal of Analytical Letters;
 Journal of Molecular Simulations;
 Organic Chem Letters;
 Current Drug Metabolism;
 Computational and Structural Biology;
 Electrochimica Acta;
 Chem Physics Lett;
 Biosensors and Bioelectronics; Sensors;
 Sensors and Actuators B: Chemical;
 International Journal of Biomacromolecules;
 Material Science and Semiconductor processing;
 Superlattices and Microstructures;
 Journal of Theoretical Biology

INVITED CONFERENCE TALKS

- “An overview of Computational studies at DUT” during the 1st International Congress on Materials Science 2011, May13-16 hosted by the University of Jinan at Shandong, China.
- “Smart Electrochemical Signalling of Bisphenol A with Silver-doped ZnO on Screen Printed Electrodes”, at the International Conference on Nanosciences & Nanotechnologies (NN17), held in Thessaloniki, Greece from 3-7 July 2017.
- “Computational Modelling Research @DUT”, Invited Speaker at University of Latvia from 31 June-2July 2017.

KEY-NOTE CONFERENCE TALKS

- “Computational Modelling to support the development of biosensing devices”, CHPC National Conference 2017 which will be held on 3-7 December 2017 at Velmoré Hotel Estate, Pretoria.
- K Bisetty, A Darumas and B Tri Murti, “Experimental and computational studies on sensing of DNA damage in Alzheimer's disease” 70th Annual Meeting of the International Society of Electrochemistry (ISE), 4-9 August 2019 Durban, South Africa
- Keynote Speaker at Virtual Conference on Chemistry and its Applications Topic: “A Computational Investigation into the Selectivity of Enzymatic Biosensing of Sweeteners”. VCCA-2020 (1st to 31st August 2020)



PhD STUDENTS GRADUATED

1. Mr Paul Mokoena; "Conformational analysis of peptide folding by computational techniques". (Sept 2010)
2. Ms Parul Sharma; "An assessment of the conformational profile of Bombesin and its mammalian analogues using computational chemistry methods". (April 2011)
3. Mr Ayyappa; "Development of electrophoretic and biosensor methods applied to high intensity sweeteners". (April 2015)
4. Mr Faiz Khan; "Experimental and computational studies of a fungal chitinase". (Sept 2015)
5. Mr NJ Gumede; "Computational and micro-analytical techniques to study the in vitro and in silico models of novel therapeutic drugs". (Sept 2016)
6. Mr. Md. Shahbaaz; "Computational and experimental studies of putative virulence factor in the genome of mycobacterium tuberculosis H37Rv". (April 2017)
7. Mr MI Sabela; "Interaction studies of nanomaterials with plasma proteins using experimental and computational methods". (May 2018)
8. Mrs L Madhura; "Quality management strategies for the improvement of wastewater by using engineered nanomaterials" (Sept 2019)
9. Ms Thishana Singh; "Ab initio studies of Pentacyclo-undecane Cage lactam" (2012)

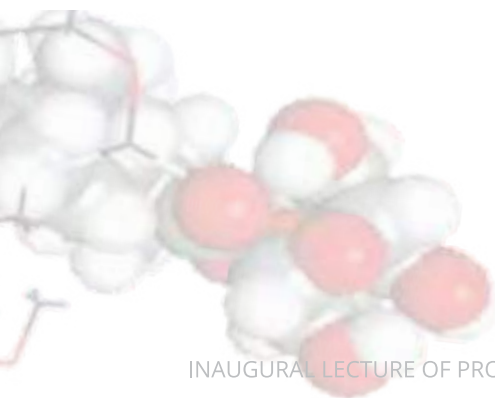
MASTERS STUDENTS GRADUATED

1. Ms Thishana Singh; "Ab initio studies of a Pentacycloundecane Cage Lactam". (June 2004)
2. Ms Poomani Penny Govender; "A computational study of trishomocubane amino acid dipeptide". (June 2004)
3. Mr NJ Gumede; "Speciation studies using Electrochemical techniques". (Sept 2008)
4. Mr MI Sabela; "A study of interactions between polyphenolic compounds and proteins using computational and electrophoretic techniques". (April 2013)
5. Mrs G. Neha Manhas; "Computational studies of anti-cancer Aurein peptide". (April 2014)
6. Mrs. S. Khulu; "Interaction studies of chiral Non-Steroidal Anti-Inflammatory Drugs (NSAIDs) using Capillary Electrophoresis Frontal Analysis and Electrokinetic Chromatography". (April 2015)
7. Mr. Thabani M; "Determination of Capsaicin using Carbon Nanotubes based Electrochemical Biosensors". (Sept 2016)
8. Mr Bayu Tri Murthi; "Experimental and Computational Studies of Chemical Biosensing of DNA Damage in Alzheimer's Disease". (Sept 2017)
9. Ms Athika Durmas; "Fabrication of Graphene Based Aptasensors for Early Detection of Prostate Cancer by Experimental and Computational Techniques". (Sept 2017)
10. Ms Nocepho Cele; "Computational studies in the identification and the analysis of p53 cancer associated mutations". (Sept 2017)
11. Ms Kwanele Kunene; "Fabrication of electrochemical biosensors for the determination of phenolic compounds by experimental and computational methods". (May 2018)
12. Ms LeeAnne Ramsuroop; "An investigation of the voltammetric behaviour of antioxidants in flavanoids". (June 2020)
13. Mr Calvin Carl Harilal; "Development of an electrochemical immunosensor for detection of tau protein: Computational and experimental studies". (June 2020)
14. Mr P Hloma; "Development of an electrochemical immunosensor for the detection of steviol glycosides by experimental and computational methods". (June 2020)
15. Ms N Jiyane; "Implementation of a third-generation sensor for oxygen detection and power generation cell". (June 2020)
16. Ms M Lephala; "Electrochemical enzymatic biosensing of neotame in sweeteners by experimental and computational methods" (June 2021)
17. Mr L Naidoo; "Analysis of nanoscale ingredients in commercial food and cosmetic products by FFF coupled with ICP-MS (June 2021)

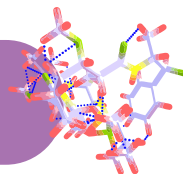


SUPERVISION OF POSTDOCTORAL/RESEARCH FELLOWS

Dr Parvesh Singh (PDF)	2007 - 2010
Dr Parvesh Singh (RA)	2010 - 2013
Dr Parvesh Singh (RF)	2013 - 2014
Dr S. Kanchi (PDF)	2012 - 2014
Dr D. Sharma (PDF)	2014 - 2016
Dr S. Kanchi (RA)	2014 - 2016
Dr S. Kanchi (RF)	2017 - 2020
Dr Olayide Arodola	2018 - 2019
Dr Bahareh Honarparvar	2018 - 2019
Dr G. Uwaya	2021 - current



DVC: RESEARCH, INNOVATION & ENGAGEMENT

**Prof S Moyo**

DVC Research, Innovation and Engagement

A congratulatory note to, Professor Krishna Bisetty, Full Professor in the Chemistry Department of the Faculty of Applied Sciences at the Durban University of Technology.

According to Google Scholar, Professor Bisetty has 2703 citations with an H-index of 28 since 2004 and holds an NRF C-Rating. See [Krishna Bisetty - Google Scholar](#) for further information.

Today marks a very important day in the life of the university, as we come together, as a university community with our quad-helix partners, to celebrate the ascension of Prof Krishna Bisetty to the status of full professorship at DUT. It is a celebration of academic excellence, which has not only been evidenced in the University attaining its first entry in the Times Higher Education World University Ranking tables for 2021, but also shows the achievements made by Professor Bisetty as a researcher, a teacher, supervisor of future researchers in his field and mentor. Not only has he had to do his research with excellence, but he is also an excellent teacher and mentor, albeit with much generosity to emerging researchers he has mentored to they themselves become established.

Today also reminds us to reflect on the DUT strategy, ENVISION2030, and the four perspectives on Stewardship, Systems and Processes, Sustainability and Society. Inaugural lectures form part of our stewardship perspective as an Engaged University to demonstrate to the public what it is that we hold most important in terms of our values and purpose. Excellence, research ethics and integrity are dear to our pursuit of knowledge and ensuring we can translate research into commercialisation. Prof Bisetty was able to register a patent which should be the case for Universities of Technology.

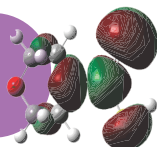
The Inaugural lecture, apart from being the most important milestone of an outstanding academic, also represents the official recognition by the University of the outstanding achievements made through a rigorous process of appointing a Professor at DUT. This way we also ensure that our professors become part of a global community of senior academics and scholars.

Today Prof Bisetty will also share with us the body of research and innovation that he has constituted in progressing towards full professorship. His research has touched on a number of areas in Chemistry including his most highly cited review paper on the "Biogenic synthesis of nanoparticles". Having worked very closely with Prof Bisetty, over the years, I have noted in hard work, persistence and his generosity in helping students, even incentivising them when they publish and sharing his publication units with them.

Congratulations once again Prof Bisetty for being a great example and Leader in Chemistry and for also supporting our capacity building programmes and actively applying for grants since our paths met in 2010. Our Province, KwaZulu-Natal and Country, South Africa, needs many more Scientists like you and we look forward to your continued focus on training the next generation of Scientists!



DVC: TEACHING & LEARNING



Professor Nokuthula Sibiyi

DVC: Teaching and Learning
Durban University of Technology

It is indeed an immense pleasure for me to congratulate Prof Krishna Bisetty.

His research production, teaching excellence and passion for Chemical Education has had a major impact on both his teaching and research. As a C1 NRF rated researcher, Professor Bisetty currently leads the Computational and BioAnalytical Research Group at DUT, and holds a flagship project at the Centre for High Performance Computing (CHPC).

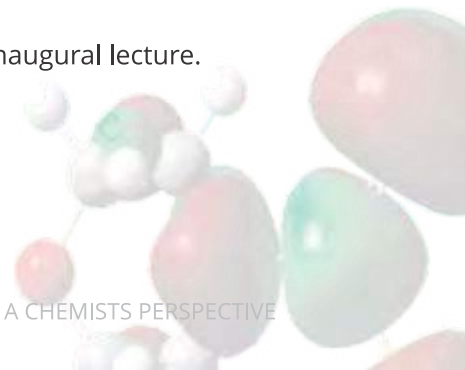
His Google Scholar H-index is 22 with over 1200 citations. He is a co-author of over 90 published papers in peer-reviewed journals, 8 book chapters. He supervised over 20 masters and doctoral students, and more than 5 post-doctoral fellows.

He is not only recognized nationally but also internationally as he has held visiting positions at the Jamia Islamia University (A Central University) in India, the University of Valencia in Spain, the University of Mauritius and the University of Latvia.

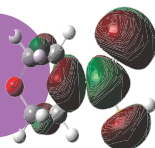
Prof Bisetty, your dedication, enthusiasm and insight are really inspiring. Congratulations to you and your future successes!

The university salutes you. We wish you many years of great achievements.

I look forward to your inaugural lecture.



EXECUTIVE DEAN: FAS



Professor Suren Singh

Executive Dean: Faculty of Applied Sciences

With three decades of service to the university, Prof Krishna Bisetty has been a teaching, learning and research stalwart. It is important to note that Prof Bisetty is a well-rounded academic, and only one of a select cohort of Professors at DUT.

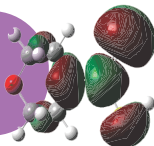
From a science educator to a Full Professor and a NRF C1 rated scientist in a span of 15 years is a success trajectory that few of us can attain. The Faculty of Applied Sciences has its vision deeply embedded in "Educate Engage Innovate" and to this end, I must state that Prof Bisetty has been a champion embodying all of these values. His contributions as a lecturer at all levels in Chemistry have been exemplary and this has also spanned across to his postgraduates.

This includes his outstanding contributions in the development of undergraduate curricula, with his lead contribution in the most recent Chemistry degree submitted to the CHE for approval. His headship of chemistry for more than three years elevated the department to a faculty and university powerhouse and demonstrated his exceptional academic leadership. On the international front, Prof Bisetty has expanded his collaborations for more than a decade with sustained high-impact outputs. In addition, he has also been at the forefront in facilitating staff and student mobility to expand their research expertise with many of whom have become emerging researchers in the faculty. This exemplifies the ability of this outstanding individual to create opportunities for both staff and students and to drive the research agenda of the faculty and university. The metrics related to his research (web of science: h - index 24; Scopus: h - index 24; 111 publications) as leader of the Computational and Bioanalytical Research Group at DUT, places him as one of the most esteemed and high achieving Professors of the Faculty and University, signifying the great strides he has made. Innovations have been forthcoming from his research as well and the royalties will soon be pouring to acknowledge the final product of his chemical reactions.

On behalf of the Faculty and University, I wish to express my sincere gratitude for placing us on the global map and steering us to such a high level of catalysis in your research endeavours. May you continue to soar to higher levels of success and create greater research inertia in your career, and may this inaugural lecture inform the community of your greatness as a professor.



PhD SUPERVISOR



Professor Gert Kruger

UKZN, Catalysis and Peptide Research Unit

Prof Bisetty is a good friend and colleague for more than 20 years. I met Vincent first at Howard College when he was looking for a PhD supervisor.

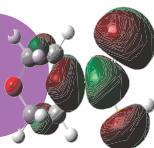
He was my first PhD student and he wanted to model polymers. I told him if he is interested in biopolymers (peptides) we are willing to assist - with the full knowledge that we have no experience in modeling of larger molecules. He managed to independently secure funding to visit Spain in order to learn from Professor Jesus Perez how AMBER works. He opened up AMBER research in South Africa and we collaborated for several years. He expanded his research focus to include Bioanalytical research, and he now enjoys international recognition for his work.

During the years he was extremely supportive towards many research grants that we have applied for. We were also serving together on organising committees for several SACI events and conferences.

I have the utmost respect for him and several of his colleagues that were able to complete their PhD studies while doing full time teaching at DUT. It is an extreme challenge to do research with the high teaching loads at DUT (at least when he started there). Becoming one of the leading research scientists at DUT is therefore a huge honour.

Our research group wishes Vincent well with his future role as professor in Chemistry.

INTERNATIONAL



Professor Juan Jesus Perez
UPC Barcelona, Spain

Dear Vincent,

It is an honor and a satisfaction to congratulate you in this special occasion. From the time we met first in Barcelona back in the 90s, I feel emphatic with the enthusiasm you have always demonstrated to discuss chemical problems. I have good memories of the periods you spent with us, involved in computer simulations trying hard to understand the structure-activity relationships of a special class of peptides.

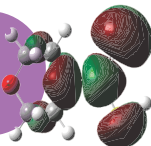
After your dissertation and establishment in DUT we were awarded with a grant funded by a collaboration agreement between the Spanish and South African governments that permitted a fruitful collaboration between the two laboratories for the following few

years. Hard worker, never giving up, we learnt together the importance to include an interdisciplinary approach to tackle real problems. Indeed, successfully applied these ideas in your lab, where you have demonstrated the potential of combining computational and experimental studies on proteins.

I can only congratulate you for your successful studies of recognized impact, reported in diverse prestigious specialized journals. However, I cannot finish this short note without underlining the great heart behind the scientist, always worried for all those that surround you. Vincent, my best wishes for success in your brilliant young carrier.



INTERNATIONAL


Professor Mikhael Bechelany

Chargé de recherche CNRS
Institut Européen des Membranes, Montpellier, France

Dear Prof Bisetty,

My warmest congratulations for your achievement! It is an honor for me to collaborate with you and with your group in topics focusing on biosensing with applications in the food and health sectors.

Well done in your achievement in the fields of electroanalytical chemistry and computational chemistry with the target to continuously improve human health and biosensor technology. We are all beneficiaries from your outstanding achievement and I am looking forward our continued faithful collaboration.


Professor Salvador Sagrado

Facultad de Farmacia, Departamento de Química Analítica
Universidad de Valencia, Spain

Dear Professor Bisetty,

Congratulations on reaching this significant milestone in your career in the Department of Chemistry at Durban University of Technology. I would also like to congratulate your institution for providing resources for your capacity.

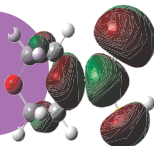
I have worked with you in Chemistry research at Durban and here in Valencia and thereafter in discussions on how we can improve the essential international collaborative work and I believe that this award is well earned.

Well done on your established position in the multi-disciplinary research including bioanalytical chemistry, nano-chemistry, computational chemistry and drug-receptor interaction studies.

I must acclaim you for your scientific efforts to merge experimental and computational domains as reflected by your brilliant publication record.

We are now all receivers of your scientific feats. I look forward to the next finding from you and to our continued co-operation.

INTERNATIONAL



Professor Ponnadurai Ramasami,
Computational Chemistry Group, Department of Chemistry,
Faculty of Science, University of Mauritius

Dear Professor Krishna Bisetty,

I would like to congratulate you for your award and for your scientific achievements in the Department of Chemistry at Durban University of Technology. The award is well deserved for your fruitful contributions to the field of computational chemistry. I am looking forward that we sustain our collaborations which we started years back. In addition to our scientific collaborations, your participations as keynote, invited and plenary speakers in conferences I organised have been well appreciated.

I am interested that we join together to promote computational chemistry in Africa and I wish you all the best for the way ahead.



Dr. Ashutosh Tiwari

Director, Institute of Advanced Materials, Secretary General,
International Association of Advanced Materials, Sweden

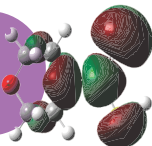
Dear Professor Bisetty,

I applaud the publication of your wonderful book on computational modelling. Nevertheless, you must have done an excellent contribution in book "Computational Modelling: A Chemists Perspective", which reflect your long-lasting research work.

Understanding the computational approaches in electrochemical sensing of nanobiosensors and several other contributing factors was important hard-work in the book. I knew that eventually researcher would see logical sense and your research will definitely reach a wider chemical science community. I trust this book will soon be popular with applications in the food and health sectors.



INTERNATIONAL



Prof Alberto Araújo
University of Porto

Dear Prof Bisetty,

Thank you for remembering me in this special event and happy to read you are safe. Please consider the text below, which the best I can foresee regarding good friends: It immediately came into my mind to quote Epictetus when knowing this special occasion, because I'm certain: you will "make the best use of what is in your power, and take the rest as it happens." I was one more having had the privilege to collaborate with Prof. Vincent Bisetty in fruitful research activities.

Congratulations!

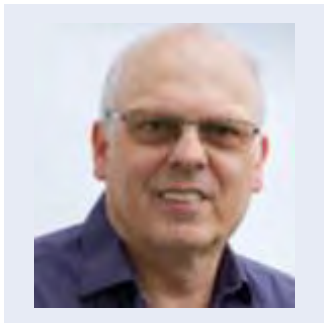
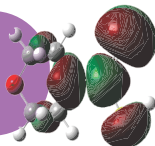


Dr Helmut Ernstberger
PerkinElmer Field Application Specialist,
Inorganic, EMT & Spain/Pt

Dear Prof Bisetty,

I am very pleased to hear about your promotion, Vincent! Congratulations! It has been a pleasure collaborating with you on nanoparticulate analysis in the past and I wish you and your workgroup much success in your research in the years to come. Best wishes.

INTERNATIONAL

**Achim Schmottlach**

INDIKATOR GmbH, Wuppertal,
Germany

Dear Prof Bisetty,

I congratulate you most warmly on your appointment as a full professor. Working with you has been both an honor and a pleasure. I wish you further successful and exciting years at the university. I am pleased with you that your achievements at the University have received this traditional and dignified form of recognition.

Best regards.

**Dr Florian Meier**

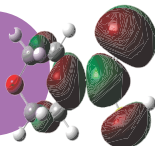
Dear Prof Bisetty,

My sincere congratulations to you on your promotion to the rank of a full professor at The Durban University of Technology! What an achievement and well-deserved!

We got to know each other in a time, where face-to-face meetings were practically impossible and where we had to build not only our professional, but also our personal relationship solely via online video-conferencing tools or via the very old-school exchange of e-mails. Despite these difficult circumstances, I got to know you as a dedicated researcher, who is not afraid of new challenges and who is eager to dive into new scientific endeavors. Also sharing the same passion for mentoring young students on their way to scientific excellence, I'm really looking forward to continuing and expanding our fruitful collaboration!

I wish you all the best from Germany and waiting for the day, when we can finally meet in person!





Professor Vincent O. Nyamori
(PhD; FRSC; FSACI)

A big Congratulations Prof Krishna Bisetty. I am so happy and excited for you! This is the biggest milestone in your academic career, and you have made it. This is as a result of your commitment and excellent positive strides that you have made over the years, and, even more important, a true reflection of your dedication to science, in particular chemistry, and your impact on this world to be a better place.

I am glad to be associated with you and your accomplishments. Maybe there are reasons why we share the name "Vincent". Nonetheless, I have worked with you in many different bodies of the chemistry community, and truly you have been a role model for many. In your quiet and humble manner, you have made many positive contributions to various entities, of which you can be truly proud. Through your leadership

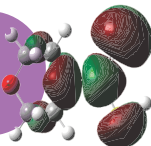
and direction at Durban University of Technology (DUT), we have seen the growth and widespread recognition of the Department of Chemistry. As a South African Chemical Institute (SACI) member and Executive member of the KZN Coordinating Committee, you have been instrumental in moving the organisation forward in your participation on several Conference Organizing Committees, and your work was presented at both local and international conferences. You are a well-rated and experienced scientist, and you are acknowledged for your involvement in various panels of the National Research Foundation (NRF). Your research on Computational Modelling and Bioanalytical Chemistry has led to you having a well-established research group at DUT with strong national and international collaborations. Also, your numerous solid publications in recognised international publications, including the high citations, have contributed to this great achievement. In addition to this are your top research awards within DUT and prestigious external ones too!

The auspicious inaugural event is indeed a proud and joyful one, yet a landmark moment for you and your loved ones, colleagues at DUT, and peers in higher education in South Africa and beyond the borders.

I am pleased to salute you and congratulate you on your inauguration as a Full Professor at the Durban University of Technology. Please accept my best wishes for continued success.

My warm congratulations!

NATIONAL

**Professor Ndeke Musee**

University of Pretoria

Congratulations Prof Bisetty as you celebrate your appointment and well deserved Full Professorship at DUT.

Your dedication to research, work ethics for the last one year I have interacted with you, and humane spirit clearly I find them as hallmarks of your success in your career. Further, it is evident that students are the centre of your being, given the dedication I have closely observed as you pour hours if not days to mentor, teach, and guide besides making funding applications to support research and postgraduate students' studies.

I look forward to the collaboration beginning from 2022 where the focus will be to apply computational

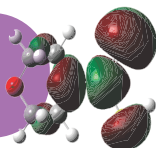
modelling in an endeavour to improve risk assessment of chemicals in the aquatic environment.

Based on the impact you have made in variant domains of research you have previously worked on using computational modelling techniques, I am confident your expertise will serve as a catalytic driver for improving chemicals management in South Africa, and globally.

And, as I join you and others to celebrate your achievements, it is heart-warming to point out that one of your striking traits is humility, an amenable person, and deeply caring human being.



NATIONAL


Dr Sreekanth B. Jonnalagadda

Senior Professor of Chemistry
University of KwaZulu-Natal

Dear Professor Bisetty,

My sincere congratulations on your appointment as Professor at Durban Institute of Technology, and I am delighted to know about your inaugural talk scheduled for 1st October 2021. It is appropriate and due recognition for your contributions to science for over 25 years. Your vast experience encompassing computation, bio and electroanalytical chemistry, and environmental chemistry will benefit the academic community. Your humble approach and leadership qualities will indeed profit society. I firmly believe that this promotion will positively contribute to accelerated growth in your research productivity, student mentorship and social engagement.

With all best wishes!


Professor Bhekhe Mamba

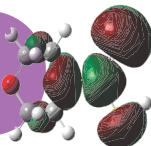
Executive Dean, College of Science Engineering and Technology, University of South Africa

Professor Krishna Bisetty's ascension to the level of Full Professor needs to be celebrated as it embodies excellence, fortitude and resilience that should be emulated by any aspiring academic. Prof Bisetty has mentored fellow academics, supervised lots of Postgraduate students, some of whom are pursuing academic careers which suggests that he has been an excellent role model.

His publications research outputs in his chosen field of research which is Computational and Electrochemistry have appeared in high impact journals where they have attracted a high number of citations as attested by his google scholar h-index of 28. I therefore wish to congratulate Prof Bisetty on his recognition by the university and promotion to the level of Full Professor at Durban University of Technology and wish him well as he progresses in his academic career.

Best regards.

NATIONAL

**Professor Emmanuel I. Iwuoha**

HonFRSC (DSI/NRF SARCHI)

Chair: NanoElectrochemistry & Sensor Technology,
University of the Western Cape)

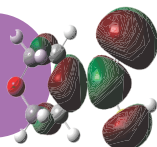
Congratulations Krishna Bisetty for your well-deserved promotion to Full Professor of Chemistry at the Durban University of Technology.

Your high impact research work on computational and experimental nano-electroanalytical chemistry has earned you national and international recognition and respect, and has also, brought great prestige to South Africa.

I wish you all the best in your future endeavours.



INDUSTRY

**Kesun Govender**

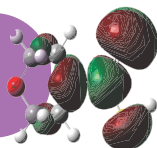
Sen Operations Manager
Lonza Wood Protection SA

It is an honour and privilege to congratulate Professor Bisetty on this extremely significant occasion for him in his personal capacity, Durban University of Technology, the Academic Community and our Country. He lectured to me for about three years and they were important years for me because it was during this time that I developed an appreciation of the broader role that Chemistry had to play in ensuring a more sustainable existence. I saw the need to apply my knowledge and understanding of Chemistry in order to reduce the negative impact of our existence on our environment. The impact of our teachers and lecturers, hardwires values that we carry with us through our journey of life. Professor Bisetty had a profound influence on me and on my understanding of importance of using Science to benefit mankind.

As we develop new technologies, products and processes, we need to be grounded in understanding the importance of our initiatives in improving the lives of mankind, the protection and preservation of our environment and in ensuring that we contribute positively to our existence. It is precisely when considering this that I am reminded of the impact of Professor Bisetty on my growth and development. He, together with other lecturers at DUT have packaged humility, loyalty, hard work and dedication as part and parcel of their service offering. He belongs to generation of lecturers that approached academia in a manner that placed the student as the central focus but also allowed the student to become a conduit through which the field of Chemistry could be developed, humanity can benefit, the Institution can receive the necessary accolades and it can continue to act as a repository of knowledge for future generations to benefit from.

Therefore, it is indeed befitting that he takes his rightful place amongst the giants of this illustrious institution, past and present. As my lecturer, a colleague and a fellow researcher, he continues to inspire and motivate us. I want to congratulate Professor Bisetty on this great achievement and may he continue to robustly develop, shape and mould students and academics so that they too can contribute to a better world. May his dedication, devotion and exemplary conduct continue to guide and inspire future researchers, academics and students of Chemistry.

INDUSTRY

**Chreeson Moodley**

CEO,
Gotec Group

Congratulations Prof Krishna Bisetty!

Sincere congratulations Krishna on your appointment as a full Professor in Chemistry.

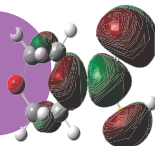
This is an incredible achievement. I always knew that you were a high achiever and a dedicated person. You have always been innovative and your numerous academic accolades is certainly proof.

From humble beginnings you broke through various barriers and your sheer determination resulted in your dreams becoming reality. I will always appreciate your support and encouragement that you offered me during my academic studies and for that I am always grateful.

You have managed to achieve a wonderful balance between excelling in the academic world and having a beautiful family.

Wishing you all the very best in the future and may you continue to excel.

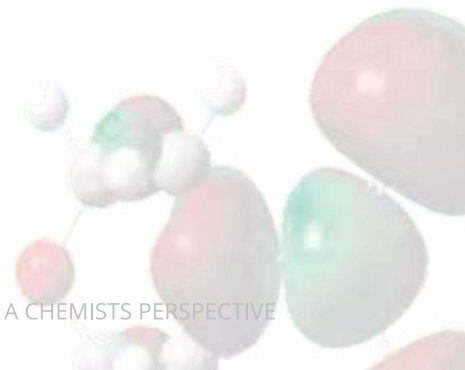


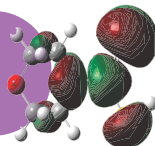
**Professor K Permaul**

Biotechnology and Food Technology

I had the pleasure of interacting with Professor Krishna Bisetty for over 20 years now as colleagues at DUT. Prof Bisetty is a well-respected and accomplished scientist with international recognition in his field. He has garnered an impressive track record of publications and other research recognitions that is well-deserved due to the dedication and sheer hard work he has devoted to his research career. While he's usually measuring analytes at minute concentrations using cutting-edge equipment and biosensors – his passion for his research area must surely be immeasurable!

It has been pleasing to see his research career rising meteorically, especially in the last decade and I am glad that we have been involved in a few joint projects recently. In addition to his academic achievements, Prof Bisetty is also a genuinely upstanding individual, proud family man and pillar of strength to fellow colleagues. Thank you, Vincent, for being a good friend and someone I can always rely on for advice and good company. Congratulations on your long-overdue inaugural lecture and best wishes for the future.





I have known Prof Bisetty for many years and clearly his passion for science and his subject area is reflected in his outstanding achievements over time.

He has been an excellent role model for young scientist.

I do take this opportunity to wish him all the best in his inaugural lecture.

Professor Faizal Bux

Director: Institute for Water and Waste Water Technology



Testaments to Professor Bisetty's scholarship will be found elsewhere in this booklet. I choose therefore to congratulate him on being an exemplar of a good human being.

Notwithstanding his many accomplishments, he remains a gentle, humble and approachable person. Under his leadership within the Department of Chemistry, the department has grown in its research impact, curriculum renewal, novel approaches to community engagement and contribution to the Faculty's equity and transformation.

Professor Darren Lortan

HoD: Mathematics





Professor Ian Lazarus

Physics

Congratulations Prof Bisetty on your achievement. Your contributions and the significant impact of your research in the field of Computational and BioAnalytical Chemistry is nothing short of exemplary. The impressive high quality of your research productivity reflects well and brings deserved recognition to DUT.

These achievements are attributed to your dedication and perseverance within your research field. I have had the pleasure of being your colleague for almost 30 years and have admired your dedication towards your teaching and research and wish you continued success.

Well done Prof Bisetty!



Professor Megan Govender

Mathematics

To describe Professor Bisetty in a few lines is as absurd as trying to fit the entire Universe into a singular point - such is his stature as an internationally recognised researcher, a brilliant teacher and humble human being.

I am extremely proud to call him a friend whom I can approach on various disciplines.

Congratulations!



Dr Prinavin Govender

Information Technology

Congratulations Prof Bisetty,

It's an honour and a privilege to consider you both as a friend and a colleague.

You are a respected, humble, highly qualified, professor extraordinaire. I thank you for your friendship, expertise and above all role model status that we may emulate to reach your stardom.

Congratulations and may you go on to acquire even greater accolades.

Your colleague and friend.





Professor Gan Redhi
Chemistry

I have known Vincent from my undergraduate days at the UDW campus. He has always had a keen interest in computers, and it's no surprise that his research focus area has become computational chemistry.

He's also been a stalwart and pacesetter both in terms of teaching and research in the Chemistry Department, and indeed has made a sterling contribution to the Department's administration, growth, leadership and eminence.

Sincere congratulations and good wishes Professor Bisetty on your inauguration, and all the best in your future endeavours.



Dr Vimla Paul
Chemistry

My heartfelt congratulations on your inauguration. I wish you much success and personal fulfilment in your role as professor.

Thank you for being my mentor and an amazing colleague.

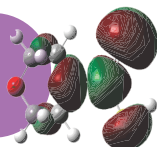


Mr Naresh Ramnarian
Chemistry

Prof. K. Bisetty is a long standing academic and colleague of 19 years. He has excelled in the field of research during his illustrious tenure at the Durban University of Technology. During this tenure he has served at the Head of Department with distinction whilst in the pursuit of his research excellence. Not only has he served himself with adulation for his research work but also for his leadership skills.

He has added value to the Chemistry department in particular and the Durban University of Technology in general. Congratulations on your Inaugural Lecture. A profound moment in your academic career.





Dr Njabulo Gumede, MUT

Thanks for the invite on your inaugural lecture. I would like to congratulate you on these two milestones for being NRF C1 rated researcher and your full professorship at DUT.

I have known you for the past 19 years, firstly as a National Diploma student in Analytical Chemistry from 2002-2005 after the university merger.

At BTech level in 2006 you started supervising me on my project, if I remember very well it was on nitrate determination in water. In 2007, you convinced me to come and do my MTech under your supervision, which turned out to be the best decision I ever took in my career.

My first flight experience was through your Spanish grant, where I got an opportunity to go to University of Valencia on a study visit for 3 months in 2008. My research career took off from there and it never landed as we are still collaborating up to now. It was a great experience to learn about our collaborator's cultures in Spain and also the exposure to their way of doing things in their labs.

I subsequently registered for my PhD under your supervision in 2009 thereafter. This experience opened my third eye, this in turn helped me to succeed in my PhD. It is evident that internationalization and globalization plays a huge role in academia, for professional development purposes.

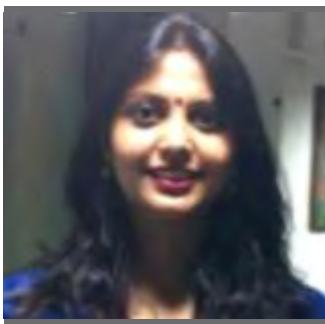
In closing, in IsiZulu they say "Ukwanda kwaliwa umthakathi" – which simply means a wicked heart hates it when others succeed. I thank you for your humility on a personal level and I have learned a lot from you professionally, be blessed more abundantly.



Dr Ayyappa B

My heartfelt congratulations to Prof. K. Bisetty for his outstanding achievement. With his vast teaching and research experience, guided and helped the number of students to achieve their dreams and careers. As his former student, I always wanted to thank him and learnt from him "be passionate, never give up and be enthusiastic towards work".

Once again congratulations for your Inaugural lecture and strongly believing that this will benefit for researchers to understand both experimental and computational methodologies.



Dr Parul Sharma

Prof Bisetty, my PhD mentor is one of the few people who inspired me to achieve greater heights in research with diligence and hard work.

His drive and passion for research and development is infectious. He believes in constant learning and acquiring new skills. I would like to congratulate him on his achievements. Do enjoy your moment of pride!



Dr Faez Khan

Wishing you great days ahead. Thank you and God bless you.

As the best teacher, I know you've played an important role in my life, thank you very much for being my friend and mentor.

So, I am wishing you, my amiable teacher more wins in your career.



Dr Mohd Shahbaaz, PhD
 Post Doctoral Researcher
 South African National
 Bioinformatics Institute
 (SANBI)

Sincere congratulations regarding the commencement of your Inaugural Lecture in Durban University of Technology (DUT).

I am so proud to be an alumnus of your lab and of the strides that you made in the research over the years, and, even more important, to be working for you!

As an alumnus, I cannot begin to express how moving it has been to witness your career progression, from working as Lecturer to Head of the Department- how inspiring!

Equally significant, is your demeanour with those with whom you interact. You are always gracious, respectful and truly a wonderful person. I am so blessed to know you and to be able to finish my PhD under your supervision. I wish you all the best during your next chapter at DUT.



Dr Thishana Singh
 UKZN

It is a great pleasure to congratulate Prof Bisetty on attaining this milestone.

I have known Prof Bisetty since 1991 when I was a second year diploma student at the former ML Sultan Technikon. Since then I have gone on to work with him at the former technikon, running his Physical Chemistry practicals. So, it's no coincidence that he eventually became a mentor, encouraging me to pursue postgraduate studies. I think I was his first postgrad student!

Prof, you didn't just teach me a new subject, you opened my eyes to a whole new world. You have been instrumental in developing and promoting Computational Chemistry in South Africa and I am proud to have been part of that transformation.

As you cherish the fruits of your hard work, I wish that success keeps following you in everything that you do.



Professor Penny Govender
University of Johannesburg

Dear Prof Bisetty, wishing you the very best on this wonderful day of your inaugural lecture.

Congratulations once again for this great achievement! Well done and proud of you as always.



Dr Suvadhan Kanchi

With your leadership as you guided the Department both in Research, Teaching, and Learning through the next phase to achieve unforgettable milestones, and I have followed your leadership activities and am very proud of them.

Congratulations on your Inaugural Lecture!



Dr GE Uwaya

Prof K Bisetty is such an “amiable and approachable” person, recalling from my first conversation with him on phone, arrival and stay in DUT.

I could see dedication, commitment, discipline and excellence in his words and deeds which is worthy of emulation. He is an inspirer and motivator to explore new horizon.

I feel privilege to be mentored under a seasoned expert in computational chemistry and electroanalytical chemistry. I am confident that his inaugural lecture will be successful and impactful.

Congratulations Prof!





Bayu Tri Murti

PhD student in the College of Biomedical Engineering,
Taipei Medical University, Taiwan

Congratulations and many blessings to you, Prof. Krishna Bisetty, on your inaugural lecture!

You have achieved a historical milestone in your esteemed academic and research career, particularly in the field of electroanalytical sensing and computational chemistry. Your keen sense of research and education are source of inspiration to me and whomever interact with you in person. I was truly glad to be advised by you during my master's study in the Department of Chemistry, DUT.

I wish you all the best.



Ms Lee-Ann Chunilall

Metrom SA

I extend my heartfelt congratulations to Professor Bisetty on his inaugural lecture. Thank you Prof for your mentorship and guidance throughout my academic journey. You encouraged me to think smart and work hard.

With your teaching skills you have the ability to take a daunting subject and make it more approachable.

Your expertise in the field of Computational and BioAnalytical Research is prominent, pivotal and promising.



Ms Kwanele Kunene

Dear Prof Bisetty I am very happy for you to hear that you have been selected to deliver this auspicious lecture. For sure, delivering such a concise lecture on a vast topic requires high level of intelligence and vast hands on experiences. And you are the person who can deliver it. Your inspirations in human form that keeps inspiring me to pursue chemistry to the highest cadre, you own a slot Prof. I can vividly remember our first encounter ten years back at the physical chemistry lecture. Your humility is inexplicable; I shall continue to appreciate those words of advice and encouragement. You inspire a lot of us. Do wish you a great inaugural lecture Prof."

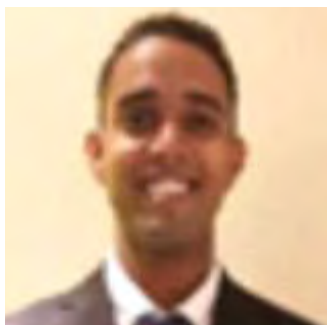


Ms Matshidiso Lephala

Having dreams is one thing but taking action to turn those dreams into a reality is another.

You are a doer, not only a dreamer. You are one of those people who inspire others to achieve greatness. Your drive and passion are infectious.

Congratulations on your achievement!



Mr Lyndon Naidoo

Congratulations Professor Bisetty on this remarkable accolade, an award fitting of an individual whose career embodies years of passion, hard work and dedication in the field of chemistry.

As a young student, it was always important to be set on a positive path. I greatly appreciate you shepherding me through the trials and tribulations of a novice researcher. Your continuous support has proven invaluable not just from an academic perspective, but in my personal development as well.

Best regards for the future!



Ms Khethiwe Mthiyane

Halala!

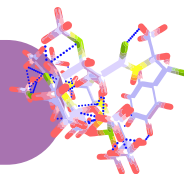
Congratulations to Professor Krishna Bisetty on your best achievement.

The contribution you have place in my learning and research skills proceed to excellent foundation for my journey. The dedication and availability that you have provide has proven to be an outstanding result for my study.

Continue with the good work and inspirations.



PUBLICATIONS IN PEER REVIEWED JOURNALS



2021

1. Ayyappa, B., Kanchi, S., Sabela, M., I and **Bisetty, K.** 2021. Separation of Sucralose in Food Samples using Amines as Background Electrolyte Supported with DFT Calculations. *Current Analytical Chemistry*, 17 (7): 989-1002.
2. **Bisetty, K.**, Kanchi, S. and Hloma, P. 2021. Evaluation of the Catalytic Activity of Graphene Oxide and Zinc Oxide Nanoparticles on the Electrochemical Sensing of T1R2-Rebaudioside A Complex supported by In Silico Methods. *Pure and Applied Chemistry*, <https://doi.org/10.1515/pac-2020-1104>
3. Kanchi, S., Sabela, M., I, Shahbaaz, M. and **Bisetty, K.** 2021. Sensitivity Enhancement of Pre-Capillary Chelation Method for the Separation of Metal Ions: Experimental and DFT Study. *Current Analytical Chemistry*, 17 (6): 839-848.
4. Madhura, L., Singh, S., Kanchi, S., Sabela, M., I, **Bisetty, K.** and Inamuddin*. 2021. Removal of Targeted Pharmaceuticals and Personal Care Products from Wastewater Treatment Plants using QSAR Model. *Current Analytical Chemistry*, 17 (7): 1003-1015.
5. Naidoo, L., Kanchi, S., Drexel, R., Meier, F. and **Bisetty, K.** 2021. Measurement of TiO₂ Nanoscale Ingredients in Sunscreens by Multidetector AF4, TEM, and spICP-MS Supported by Computational Modeling. *ACS Applied Nano Materials*, 4 (5): 4665-4675.

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6. Arodola, O. A., Kanchi, S., Hloma, P., **Bisetty, K.**, Asiri, A. M. and Inamuddin. 2020. An in-silico layer-by-layer adsorption study of the interaction between Rebaudioside A and the T1R2 human sweet taste receptor: modelling and biosensing perspectives. *Scientific Reports*, 10(1)
7. Bathinapatla, A., Kanchi, S., Sabela, M. I., Ling, Y. C., **Bisetty, K.** and Inamuddin. 2020. Experimental and Computational Studies of a Laccase Immobilized ZnONPs/GO-Based Electrochemical Enzymatic Biosensor for the Detection of Sucralose in Food Samples. *Food Analytical Methods*, 13(11): 2014-2027.
8. Gumede, N. J., Nxumalo, W., **Bisetty, K.**, Escuder Gilabert, L., Medina-Hernandez, M. J. and Sagrado, S. 2020. Prospective computational design and in vitro bio-analytical tests of new chemical entities as potential selective CYP17A1 lyase inhibitors. *Bioorganic Chemistry*, 94
9. Kunene, K., Sabela, M., Kanchi, S. and **Bisetty, K.** 2020a. High Performance Electrochemical Biosensor for Bisphenol A Using Screen Printed Electrodes Modified with Multiwalled Carbon Nanotubes Functionalized with Silver-Doped Zinc Oxide. *Waste and Biomass Valorization*, 11 (3): 1085-1096.
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11. Lephalala, M., Kanchi, S., Sabela, M. I. and **Bisetty, K.** 2020. Electrochemical Enzymatic Biosensing of Neotame Supported by Computational Methods. *Electroanalysis*, 32 (12): 2669-2680.
12. Naidoo, L., Suvadhan, K., Sabela, M. I. and **Bisetty, K.** 2020. Multivariate optimization of field-flow fractionation of nanoscale synthetic amorphous silica in processed foods supported by computational modelling. *New Journal of Chemistry*, 44 (40): 17542-17551.
13. Shahbaaz, M., Potemkin, V., **Bisetty, K.**, Hassan, M. I. and Hussien, M. A. 2020a. Classification and functional analyses of putative virulence factors of Mycobacterium tuberculosis: A combined sequence and structure based study. *Computational Biology and Chemistry*, 87.
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15. Torrinha, Á., Jiyane, N., Sabela, M., **Bisetty, K.**, Montenegro, M. C. B. S. M. and Araújo, A. N. 2020. Nanostructured pencil graphite electrodes for application as high power biocathodes in miniaturized biofuel cells and bio-batteries. *Scientific Reports*, 10 (1)
16. Viter, R., Kunene, K., Genys, P., Jevdokimovs, D., Erts, D., Sutka, A., **Bisetty, K.**, Viksna, A., Ramanaviciene, A. and Ramanavicius, A. 2020. Photoelectrochemical Bisphenol S Sensor Based on ZnO-Nanoroads Modified by Molecularly Imprinted Polypyrrole. *Macromolecular Chemistry and Physics*, 221 (2).

2019

17. Honarparvar, B., Kanchi, S. and **Bisetty, K.** 2019. Theoretical insights into the competitive metal bioaffinity of lactoferrin as a metal ion carrier: A DFT study. *New Journal of Chemistry*, 43 (41): 16374-16384.
18. Jiyane, N., Sabela, M. I., Kanchi, S., Mdluli, P. S., Xhakaza, M., Arodola, O. A. and **Bisetty, K.** 2019. MWCNTs-Fe₂O₃ nanoparticle nanohybrid-based highly sensitive electrochemical sensor for the detection of kaempferol in broccoli samples. *Turkish Journal of Chemistry*, 43 (5): 1229-1243.
19. Madhura, L., Singh, S., Kanchi, S., Sabela, M., **Bisetty, K.** and Inamuddin. 2019. Nanotechnology-based water quality management for wastewater treatment. *Environmental Chemistry Letters*, 17 (1): 65-121.
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21. Sabela, M. I., Kunene, K., Kanchi, S., Xhakaza, N. M., Bathinapatla, A., Mdluli, P., Sharma, D. and **Bisetty, K.** 2019. Removal of copper (II) from wastewater using green vegetable waste derived activated carbon: An approach to equilibrium and kinetic study. *Arabian Journal of Chemistry*, 12 (8): 4331-4339.
22. Sharma, D., Kanchi, S. and **Bisetty, K.** 2019. Biogenic synthesis of nanoparticles: A review. *Arabian Journal of Chemistry*, 12 (8): 3576-3600.



2018

23. Kanchi, S., Sabela, M. I., Mdluli, P. S., Inamuddin and **Bisetty, K.** 2018a. Smartphone based bioanalytical and diagnosis applications: A review. *Biosensors and Bioelectronics*, 102: 136-149.
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ACADEMIC RESEARCH VISITS

The CRMD encourages academics to undertake study visits in order to catalyse networking and collaboration and to enhance research output. In 2004, two of DIT's researchers, Dr. K. Bisetty and Mr. A. Tekukdaris spent time in laboratories in Spain and the USA, respectively. The following is an account of their experiences.

Dr. K. Bisetty from the Department of Chemistry undertook research at the Universitat de Politècnica de Catalunya (UPC) in Barcelona, Spain from 13 September to 17 December 2004.

Dr Bisetty's collaboration with the Computational Chemistry research group at the UPC, dates back as far as 1999, where he spent 3 months in their research laboratory working on the application of computational techniques in the field of peptide and molecular design towards his PhD studies. His latest study visit abroad was based on the development of forcefield parameters for the bioactive cage peptides. The primary aim was to extend the scope of study to include biological and organic molecules. With the utilization of the supercomputer facilities along with the molecular modelling software tools configured for parallel computing, novel research findings worthy of publication have been produced.

The computational study was based on Metenkephalin, which is a 5-residue opiate peptide with an amino acid sequence of Tyr-Gly-Gly-Phe-Met. Here molecular dynamics (MD) and simulated annealing (SA) simulation protocols were used to assess the bioactive conformations of this pentapeptide, in gas phase as well as in different solvents including dimethyl sulfoxide, methanol and water. On average, each system comprise of about 3 500 molecules, resulting in the simulation being computationally expensive, and often time consuming. For this purpose high performance computers are essential. This laboratory is equipped with state-of-the-art computational facilities. All the simulations were carried out on 3 separate dual processor LINUX machines, plus the supercomputer with 8 of the 64 processors dedicated for the MD simulation. For publication purposes, it is expected that molecular dynamics simulations of up to 50 nanoseconds are required. Periodic sampling of the simulation involved viewing the structures in 3D as well as analysis of their thermodynamic properties.

As this is a long-term study, the broader goals are as follows:

- To compare the theoretical results with known experimental studies such as Nuclear Magnetic Resonance (NMR) spectroscopy, and infra-red (IR) spectroscopy;
- To contribute to the understanding of the conformation of short peptides in solution; and
- To undertake a methodological approach with regard to the simulation protocols used by SA and MD approaches.



Francisco Garcia and Vincent Birkby



Molecular Modelling group in Barcelona
Left to right: Arnan, Josep, Vincent, David, Arnie and Martha

A manuscript titled "A conformation analysis of Metenkephalin" is currently in preparation, and will be submitted for publication to an international journal. In addition, some work was also done on the development of new force field parameters for the cage peptide. This is quite an extensive study and is expected to last for 6 months. By accessing the supercomputers remotely, the work will be continued on a part-time basis.

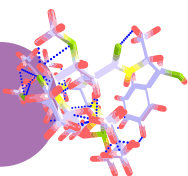
The experience gained from this study visit has been very rewarding, in the sense that it has strengthened Dr. Bisetty's collaboration with the group in Spain. As he is part of this research group, all the necessary computational facilities are at his disposal, and he is able to access them. It is hoped that in the future such high performance computing facilities would be established in the KZN region.

The highlight of this visit is that, as from January 2005, the world's secondmost powerful supercomputer comprising 4 500 processors is to be hosted in Barcelona. It is very pleasing to note that as part of the on-going collaboration, Dr. Bisetty would be able to remotely utilize one of the most powerful computers in Europe. Finally, the knowledge and the experience gained from this visit will contribute significantly towards the understanding of biologically/pharmaceutically important compounds, using computational techniques.

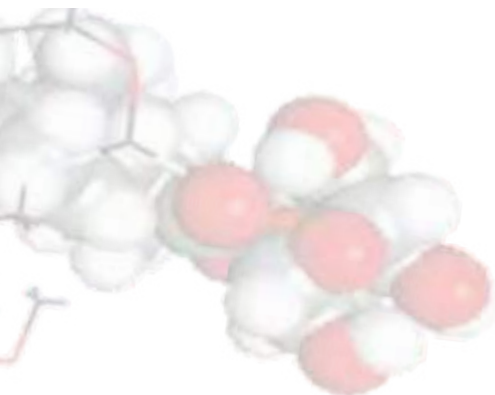
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COMPUTATIONAL MODELLING & BIO-ANALYTICAL CHEMISTRY RESEARCH GROUP

WHAT WE DO

WE DESIGN, MODEL AND FABRICATE DOPED ENGINEERED NANOMATERIALS TO IMPROVE HUMAN HEALTH AND BIOSENSING SYSTEMS, BY CREATING SYNERGIES BETWEEN EXPERIMENTAL AND COMPUTATIONAL CHEMISTRY METHODS.

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