| PHUTI NGOEPE |

TOP THREE AWARDS

- National Order of Mapungubwe, 2008
- NRF Presidential Transformation of the Science Cohort Award, 2008
- The prizes his students have received at conferences

DEFINING MOMENT

When his father intervened to send him 250 km away from home to a school where he could study mathematics and science.

WHAT PEOPLE DO NOT KNOW

Every member of his immediate family holds a PhD. His wife Junia holds a PhD in English from North-West University, son Noko a PhD in chemical engineering from the University of Cape Town and daughter Malebogo, a PhD in mechanical engineering from the University of Oxford.

A DIPLOMAT OF NOTE

When Prof Phuti Ngoepe was a first-year BSc physics student in 1972, it was still the very early days of supercomputers and computational number-crunching in a big way. The personal computer had not yet been invented, and there was only one large calculator available in the Department of Physics that only his professors at the then University of the North (now University of Limpopo) could use.

Today, the University of Limpopo is home to the Materials Modelling Centre, of which Ngoepe has been the dedicated Director since its inception in 1996.

Over the past three decades, this passionate researcher has become a leader in computational modelling in South Africa, a regular speaker on the topic around the world and a much-loved mentor of students. He has guided new initiatives, helped shape science policy and cement South Africa's international research relationships.

In 2007, the centre's efforts were strengthened considerably. Ngoepe was awarded a research chair on computational modelling of materials as part of the then new South African Research Chair Initiative (SARChI) of the Department of Science and Technology (DST) and the National Research Foundation (NRF).

"The SARChI Chair has provided us with an excellent opportunity to extend computational modelling into high-performance computing at the University of Limpopo," he acknowledges. "It has been enabled by the establishment of the Centre for High Performance Computing in Cape Town, and has made South Africa competitive."

RESEARCH ENDEAVOURS

Ngoepe, his colleagues and postgraduate students use so-called third-emerging scientific methods of computational modelling to develop computing methods and models. These are used to predict properties of minerals, light and precious metal alloys, and energy storage materials used mostly in lithium-ion batteries.

Research about high-energy density batteries has become increasingly important in the development of electric vehicles, solar energy storage and to support the electricity grid. Better performance and better storage capacity of such batteries are crucial. It can, in part, be provided by materials on the nanoscale, for instance, through nanoparticle, nanorod, nanosheet, nanoporous structured electrodes.

Ngoepe's team has contributed novel work on the simulated synthesis of nanostructures for lithium-ion and newer lithium-air batteries to these efforts. It is used to predict the performance of such structures, by calculating their voltage profiles, microstructures and mechanical properties. These computerised models make it possible to estimate the lifetimes of related batteries before their design is executed practically.

In this, the Materials Modelling Centre participates in the DST's National Energy Storage Programme. It also networks internationally with American national laboratories and through meetings of the International Battery Association.

These are among the many collaborations Ngoepe has fostered over the years, among others through the centre's membership of international software development consortia. Notably he has also worked with several researchers from the United Kingdom through the support of the NRF and the Royal Society, London. Other links are in the European Union and Japan.

The centre's focus on modelling minerals such as platinum and manganese is a logical extension to the University of Limpopo's close proximity to some of South Africa's most valuable mining areas.

Together with South African mining companies and other research institutions the centre looks at efficient mineral processing approaches that address challenges of water, energy and environmental conservation.

"These are becoming imperative in the mining sector," explains Ngoepe, who guides his students to study minerals and mineral surfaces properties through quantum mechanical, semi-empirical and empirical methods. Large-scale simulations are conducted thanks to the empirical potential

models of mineral sulphides in platinum ores they have derived and validated. This has ushered in accurate studies of the surface properties of large systems, including nanoparticles.

The centre also works on the phase stabilities of precious and light metal alloys, and in particular their thermodynamic, elastic and vibrational properties and related high-temperature studies.

"The approach has provided valuable information for aerospace applications, shape memory devices and powder metallurgy processing," Ngoepe elaborates on the work that is part of the DST's effort to beneficiate titanium and precious metals.

EARLY YEARS

It wasn't easy to set up and run a research-driven centre at an institution with a historical disadvantage in terms of resources and funding. Through determination and a belief in especially the abilities of his students, colleagues and collaborators, Ngoepe has made it work.

No wonder that of him has been said: "He was born for a big purpose and turned an academic desert into a paradise. He is a serial promoter, researcher, and academic traveller".

Ngoepe was born on 7 January 1953 in Polokwane, and matriculated from Setotolwane High School in 1971. His career choice was influenced by his father, an English teacher and headmaster, who often told him about groundbreaking black South African scientists.

In Ngoepe's first year, Prof Bob Seretlo of the University of Fort Hare became the first black person in South Africa to receive a PhD in physics.

"That really motivated me and made me realise what is possible," Ngoepe reflects.

After receiving his BSc and BSc Hons (physics) from the University of the North, Ngoepe considered studying engineering. However, he was offered a junior lecturing position at his *alma mater* in 1977 – his academic home ever since. In 1981, he received the MSc (physics) with distinction from the University of South Africa, and in 1988 the PhD (physics) from the University of the Witwatersrand (Wits).

Ngoepe, who became Professor in 1992 and a Senior Professor in 2006, counts serving as Dean of the then Faculty of Mathematics and Natural Sciences and as Acting Deputy Vice-Chancellor Academic among the leadership roles he fulfilled at his institution.

UNITED KINGDOM COLLABORATION

A conference in Spain in 1986 changed his life's course from experimental physics to computational modelling.

At the time, he was completing his PhD research under the guidance of Prof Darrell Comins at Wits, and was one of the first researchers in the country working in the field of experimental Brillouin scattering techniques. A vast amount of data churning was needed to really get to grips with his results, but such facilities were not yet available in South Africa.

At the Europhysical Conference on Defects in Insulating Crystals in Madrid, Ngoepe met Prof Richard Catlow, now a Fellow of the Royal Society based at the University College London in the UK. In the 1980s, Catlow was already renowned for his computational modelling work.

When Ngoepe was a British Council Visiting Research Fellow in 1988 and 1989, he visited Catlow at the University of Keele to learn more about computer simulation techniques. He subsequently also spent three months at the University of Bath for ultrasonic studies on condensed matter. A shorter stay at the University of Pennsylvania in the US extended his computational modelling experience and helped him get to grips with non-linear optic techniques.

Since that first Spanish conference Ngoepe and Catlow have become colleagues and collaborators who have provided many of their respective students with shared learning experiences in South Africa and England.

Their combined efforts included a series of materials modelling conferences hosted jointly by the University of Limpopo between 1997 and 2008.

"It helped to promote the awareness of this new field in South Africa," Ngoepe elaborates on their working relationship of more than 27 years, made possible through support by the NRF and The Royal Society, London.

SHAPING STUDENTS

Of his involvement in shaping students' lives over the past 40 years, Ngoepe says philosophically: "There are moments of shared sorrow, when computational data of researchers disappear or experiments break down, but there are so many moments of joy on making new discoveries and when researchers go to conferences and win prizes."

His influence stretches further than just his own students. In the early 1990s, Ngoepe was a driving force behind his institution's Science Teacher In-Service (UNIST) diploma and Science Foundation Year (UNIFY) bridging programme for first-year students who struggled with mathematics and science.

IN SERVICE OF SCIENCE

This great believer in the sharing of ideas and networking has helped arrange many workshops, summer schools and conferences related to the computational modelling of materials. In 2000, for instance, he co-chaired the International Conference on Defects in Insulating Materials in South Africa and still serves on its advisory committee. In 2011, Ngoepe helped with an International Battery Association Conference in South Africa and subsequently co-chaired workshops on energy storage with international partners.

As Chair of the Council for Geosciences – a position he has held since 2003 – he supports the organising of the 2016 International Geology Conference.

He has served on the governing boards of entities such as Mintek, the National Research Foundation, the South African Minerals to Metals Research Institute, the South African Power Utility Research Advisory Board and the Council of the South African Institute of Physics. As part of its science advisory council he was also involved in the formative years of the CSIR's Centre for High Performance Computing. Ngoepe is a Founder Member of the Academy of Science of South Africa and was a CSIR Fellow.

Despite so many leadership positions, this diplomat of note has never had the inclination to go into politics or government, no matter how hard others have tried to persuade him to leave academia behind.

"I'm just too passionate about research," is his reasoning.

Ngoepe has met them halfway through his involvement in the politics of science. He served on the African National Congress Science Policy Foundation Task Force set up between 1993 and 1994. Since then he has helped develop national science green and white papers, national foresight exercises, as well as strategies looking into establishment of nanotechnology, energy, South Africa's hydrogen economy, advanced metals and mineral processing research and innovation. He also helped review government initiatives such as the National Advisory Council on Innovation and the DST Ministerial Review Committee on Innovation. He is currently involved in coordinating projects about the beneficiation of certain South African minerals to products in energy storage. Participation in bilateral science and technology missions have taken Ngoepe to among others the USA, Russia, Japan, China and countries in the European Union.

Ngoepe has seized the opportunities that have come his way, and has worked hard in the process. The support of his family has been invaluable in this regard.

In 2013, a conference was held to celebrate his 60th birthday. At the time, Dr Reuel Khoza, Chancellor of the University of Limpopo, summed up Ngoepe's career as such: "Phuti's odyssey through the territory of mathematics, materials science and physics has been a delightful cruise characterised by regular distinctions and awards. Phuti's accomplishments as a professional and practitioner in physics and technological innovation, fundamentally redefined such descriptive concepts as dedication, dilligence and discipline, putting them unquestionably in the superlative".