

# **CURRICULUM VITAE, CORPORATE AND RESUMÉ**

## **NITHAYA CHETTY**

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*Nithaya Chetty  
Physics Department, University of Pretoria  
and  
National Research Foundation of South Africa  
January 2017*

**JANUARY 2017**

# CURRICULUM VITAE

**Nithaya Chetty**  
**University of Pretoria**  
**and**  
**National Research Foundation of South Africa**  
**January 2017**

## Personal Data

Name: CHETTY, Nithayanathan (preferred name Nithaya)  
Date of Birth: 25 September 1963  
Citizenship: South African  
South African ID: 6309255219080  
Work Address1: Department of Physics, University of Pretoria, 0001, South Africa  
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Present positions: Full Professor of Physics, University of Pretoria; Seconded to NRF as DCEO: Astronomy  
NRF rating: C2  
H-index: 15

## Pre-doctoral

- Represented South Africa at the International Youth Science Fortnight, London (1980)
- Placed first in national matriculation examinations (1980)
- BSc (*cum laude*) University of Natal, Pietermaritzburg, South Africa (1981-1983)
- BSc (Hons) (*cum laude*) University of Natal, Pietermaritzburg, South Africa (1984)
- Awarded University of Natal undergraduate scholarship, CSIR undergraduate bursary (1981-1984)
- Elected to Students Representative Council, University of Natal (1982-1983)
- Employed at CSIR as a researcher (1985)

## Graduate

- Selected as principal candidate for American Fulbright fellowship (1985)
- Masters degree, University of Illinois at Urbana-Champaign, USA, GPA 4.968 (1985-1986)
- Doctoral degree, University of Illinois at Urbana-Champaign, USA, (1986-1990), Thesis advisor: Prof. Richard M. Martin, Thesis title: First principles energy density and its applications to selected polar surfaces and interfaces

## Post-doctoral positions

- Technical University of Denmark (1990-1992)
- Brookhaven National Laboratory, USA (1992-1995)

## Academic positions

- Lecturer at University of South Africa (1995-1996)
- Senior Lecturer at University of Natal (1997-2005)
- Associate Professor at University of Kwa-Zulu Natal (2005-2008)
- Associate Professor at University of Pretoria (2009-2012)
- Full Professor at University of Pretoria (2013-current)

## Management and leadership positions

- Inaugural Deputy Director National Institute for Theoretical Physics (2006-2008)
- President South African Institute of Physics (2007-2009)
- Deputy Head of School of Physics, UKZN (2007-2008)
- Director Programme in Computational Physics, UKZN (1999-2008)
- Faculty representative on Senate, UKZN (2005-2008)

- Senate representative on Council, UKZN (2006-2008)
- Acting Head of Physics Department, University of Pretoria (2010)
- NRF Group Executive: Astronomy (2011-2014)
- NRF Deputy Chief Executive Officer: Astronomy (2014-present)
- Chair of Executive Committee African School of Electronic Structure Methods and Applications, ASESMA (2010-2016)

#### Institutional service

- Elected to Senate, UKZN (2000 , 2003 and 2005)
- Served on University Information Technology Task Team, UKZN (2000-2002)
- Served on University Merger Task Team, UKZN (2001-2002)
- Director Programme in Computational Physics, UKZN (1999- 2008)
- Webmaster for School of Chemical and Physical Sciences, UKZN (1999-2004)
- Member of School Publicity Committee, UKZN (1999- 2004)
- Member of the School Computer Committee, UKZN (1998-2001)
- Regularly served on selection committees for posts within the Faculty of Science and Agriculture, UKZN (1997-2008)
- Member of the Faculty of Science and Agriculture Board, UKZN (2000-2008)
- Member of the Independent Higher Education Monitoring Group, UKZN (2005-2008)
- Elected as Senate representative on UKZN Council (2006-2008)
- Served on Senate *ad hoc* committee investigating reasons behind the UKZN industrial action (2006)
- Chair Physics Research Committee, UP (2009-2012)

#### National service

- Member of the South African Institute of Physics (Current)
- Elected Council member of the South African Institute of Physics (2003-2009)
- Elected President of South African Institute of Physics (2007-2009)
- Elected to the South African Institute of Physics Management and Policy Committee which oversaw the international review of physics in South Africa (2003-2004)
- Elected to the South African Institute of Physics Transformation Committee (2001-2003)
- Member of the Executive Committee of the Solid State Physics and Materials Science Specialist Group (Past).
- Member of the organising committee of the 10<sup>th</sup>, 12<sup>th</sup> and 15<sup>th</sup> Chris Engelbrecht Theoretical Physics Summer Schools (Past). Chairman of the 16<sup>th</sup> Chris Engelbrecht Theoretical Physics Summer School (2005)
- Member of the organising committee of the International Union of Pure and Applied Physics Conference on Physics and Industrial Development, Durban (1998)
- Served on the selection panel for the NRF Prestigious Scholarship Programme, on the grant review panel for the NRF Materials Thrust and the NRF Rating Evaluation Committee for Physics (Past)
- Served on the NRF SARCHI selection panel (2006-2007)
- Served on the editorial board of the South African Journal of Science (Past)
- Progress monitor for Department of Arts, Culture, Science and Technology Innovation Fund (Past)
- Served on the South African Academy of Science's Think Tank on Science and Technology (Past)
- Member of the Royal Society of South Africa. (Current)
- Member of the Academy of Sciences of South Africa (Current)
- Member of the South African liaison committee for the International Union for Pure and Applied Physics (IUPAP) (Current). Member of the South African delegation to the IUPAP General Assembly held in Atlanta, Georgia USA (1999). Headed the South African delegation to the IUPAP General Assembly held in Berlin (2002).
- Elected member of the IUPAP C20 Commission on Computational Physics (2005-current)
- Advisory Board of the African Institute of Mathematical Sciences AIMS (Past)
- Board member of National Laser Centre (Past)
- Board member of National Institute of Theoretical Physics (Past)
- Board member of SA ICSU (2010-2013)
- Member of ICSU Regional Committee of Africa (2011-2013)
- Chair Local Organising Committee, Workshop on Easy Java Simulations, University of Pretoria (July 2011)
- Associate editor South African Journal of Science (2010-2012)
- NRF Group Executive for Astronomy (2011-2014)
- NRF DCEO for Astronomy (2014-current)

#### International collaborations

- Prof Reiner Driezler, Goete University of Frankfurt (Past)
- Prof Hugues Dreyse, CNRS, Strasbourg, France (Past)
- Dr Mathias Herrmann, IKTS, Dresden, Germany (Past)
- Prof Gaute Einevoll, Agriculture University of Norway (Past)
- Prof Robert Ziff, University of Michigan, USA (Past)
- Prof Richard Martin, University of Illinois, USA (Current)
- Prof Wolfgang Christian, Davidson College, USA (Past)

### Research Interests

- Quantum mechanical studies of solid state systems, density functional theory, the plane-wave pseudopotential method, Brookhaven Electronic Structure package (BEST), Vienna Atomistic Simulation Package (VASP), Quantum Espresso (QE), (Current)
- Deriving approximate total energy methods from first principles (Past)
- Bulk properties, defects, surfaces, energetics of solids, metals, alloys, semiconductors, elastic properties (Current)
- Graphene, boronitrene, silicon-carbide, carbon nanotubes, alloys involving 5d transition metal systems, titanium, alloys of actinides and lanthanides (Current)
- Computational modelling of the processes of coarsening and sintering (Past)
- Percolation and random systems (past)
- Computational physics education research, numerical and computational algorithm development, computational solid state physics, computational statistical physics, computational quantum mechanics; developing paradigms of the electronic structure problem (Current)

### Major Awards

- Fulbright Fellowship for graduate studies to the USA (1985-1986)
- National Research Foundation President's Award (1997-2000)
- Fulbright Fellowship for sabbatical leave to the USA (2004)

### Invited Talks

- CECAM workshop on Semiconductor Heterojunctions, University of Orsay, France (November 1990)
- Computational Methods in Physics, Trieste, Italy (February 1991)
- Colloquium, Technical University of Norway, Trondheim (March 1991)
- Workshop on Electronic Structure, SUNY, Stony Brook, USA (November 1992)
- CECAM workshop on MD Simulations of High-Temperature/High-Pressure systems, University of Orsay, France (April 1993)
- Solid State seminar, University of Connecticut, Storrs, USA (November 1993)
- Solid State seminar, Kansas State University, Manhattan, USA (November 1993)
- Workshop on Electronic Structure, SUNY, Stony Brook, USA (November 1994)
- Hume Rothery Symposium, Las Vegas, USA (February, 1995)
- Solid State seminar, Sandia National Laboratory, USA (February 1995)
- Workshop on Electronic Structure, University of Western Cape, South Africa (May 1996)
- Solid State seminar, University of Stellenbosch, South Africa (May 1996)
- Solid State seminar, University of Witwatersrand, South Africa (July 1996)
- Lecturer, Summer School for Theoretical Physics, Meerensee, South Africa (January 1997)
- Workshop on Materials Modelling, University of the North, South Africa (May 1997)
- Solid State seminar, University of Cape Town, South Africa (October 2001)
- Workshop on Spinel Nitrides, Rudesheim, Germany (September 2002)
- 2<sup>nd</sup> African-MRS Conference, Johannesburg, South Africa (December 2003)
- Solid State seminar, University of Cape Town, South Africa (October 2006)
- Seminar on Computational Physics at Nelson Mandela Metropolitan University (March 2008)
- Suppressed Bond-site percolation, Conference in Computational Physics, Conference on Computational Physics, Ouro Preto, Brazil (2008).
- Lecture on Computational Physics, Tribute to Prof AO Animalu, Abuja Nigeria (August 2008)
- 50<sup>th</sup> annual TB Davie Academic Freedom Lecture, University of Cape Town (August 2009)
- New modalities for scientific engagement in Africa, Conference in Computational Physics, Trondheim, Norway (2010).
- Critical Slowing Down of Entropy, Conference in Computational Physics, Kobe, Japan (2012)
- Colloquium North West University, Potchefstroom (November 2013).
- Colloquium University of Cape Town (November 2013).
- Invited talk, International Centre for Materials Research, University of California, Santa Barbara (July 2014).
- Graduation Address, North West University, Mafikeng (May 2015).
- Opening address IRSF Conference (March 2016).
- Address NASSP Winter School Awards Function (June 2016).
- Opening address UKZN-NAOC Astronomy Workshop (November 2016).
- Invited guest speaker, UKZN Research Awards Function (November 2016).

### Research students

#### Graduated Masters

- Ms Trisha Salagaram, Supervised by **N. Chetty**, Masters degree awarded with distinction April 2003
- Mr Leonard Nduwayo, Supervised by **N. Chetty** and co-supervised by Dr. R. Lindebaum, MSc degree awarded with distinction April 2003
- Mr Byren Archary, Supervised by **N. Chetty** and co-supervised by Prof Diane Grayson, MSc degree awarded April 2003
- Mr Miguel Cavero, Supervised by **N. Chetty** and co-supervised by Dr R. Lindebaum, MSc degree awarded with distinction April 2006

- Mr Daniel Cunnama, Supervised by **N. Chetty** and co-supervised by Dr. R. Lindebaum, MSc degree awarded April 2009
- Mr Edwin Mapasha, Supervised by **N. Chetty**, MSc degree awarded April 2011

#### Graduated Doctoral

- Ms Sharon Grussendorff, Supervised by **N. Chetty**, PhD degree awarded December 2003
- Ms Trisha Salagaram, Supervised by **N. Chetty**, PhD degree awarded April 2008
- Mr Leonard Nduwayo, Supervised by **N. Chetty** and co-supervised by Dr R. Lindebaum, PhD degree awarded April 2008
- Mr Miguel Cavero, Supervised by **N. Chetty** and co-supervised by Dr R. Lindebaum, PhD degree awarded in April 2012
- Mr Richard Andrew, Supervised by **N. Chetty** and co-supervised by Prof Max Bruan, PhD degree awarded in April 2013
- Mr Edwin Mapasha, Supervised by **N. Chetty**, PhD degree awarded in April 2014
- Mr Kingsley Obodo, Supervised by **N. Chetty**, PhD degree awarded in April 2014
- Mr Cecil Ouma, supervised by Prof Walter Meyer and co-supervised by **N. Chetty**, PhD degree awarded in April 2015

#### Current Masters

- Ms Eva Khoza, Supervised by **N. Chetty**, MSc degree (retired)
- Ms Mupumelo Basi, Supervised by Dr Donald Mkonto and co-supervised by **N. Chetty**, MSc degree **Deceased 23 June 2013**

#### Current Doctoral

- Mr Gilbert Mashapa, Supervised by **N. Chetty** and co-supervised by Dr Ray Superakas, PhD degree (retired)
- Ms Felana Andriambelaza, Supervised by **N. Chetty** and co-supervised by Dr Edwin Mapasha (2015-current)

#### Current Postdoctoral Fellows

- Dr Edwin Mapasha, Supervised by **N. Chetty**, NRF Fellowship, First principles studies of bi-layer graphene (2014-current)

#### Past Postdoctoral Fellows

- Dr Trisha Salagaram, Supervised by **N. Chetty**, NRF Fellowship, Computational Physics Research (2010-2012)
- Dr Aniekam Ukpong, Supervised by **N. Chetty**, UP Fellowship, Quantum Mechanical studies of novel materials (2011-2013)
- Dr Mahlangu Molepo, Supervised by **N. Chetty**, Special NRF Fellowship, Theoretical studies of real material systems (2012-2015)
- Dr Kingsley Obodo, Supervised by **N. Chetty**, NRF Fellowship, Quantum mechanical modelling of alloys involving actinides and lanthanides (2014)
- Dr Richard Andrew, Supervised by **N. Chetty**, University of Pretoria Fellowship, Quantum mechanical simulations of graphene and boronitrene, and Computational Physics Education Research (2013-2016)

## Publications

Citations from Web of Science determined on 20 Dec 2016

h=15

1. Use of composite sample configurations in order to determine the thermal conductivity of materials under pressure, by **N. Chetty**, R.J. Gummow and I. Sigalas, J. Phys. E: Sci. Instrum. **20** 512-515 (1987). (citations=1)
2. First principles elastic constants of AlAs, by **N. Chetty**, A. Munoz and R. M. Martin, Phys. Rev. **B40** (17), 11934-11936 (1989). (citations=39)
3. Modification of heterojunction band offsets by thin layers at interfaces: the role of the interface dipole, by A. Munoz, **N. Chetty** and R. M. Martin, Phys. Rev. **B41** (5), 2976-2981 (1990). (citations=105)
4. Determination of integrals at surfaces using the bulk crystal symmetry, by **N. Chetty** and R. M. Martin, Phys. Rev. **B44** (11), 5568-5571 (1991). (citations=19)
5. First principles energy density and its applications to selected polar surfaces, by **N. Chetty** and R. M. Martin, Phys. Rev. **B45**, 6074-6088 (1992). (citations=68)
6. A study of GaAs (111) and (-1-1-1) surfaces, and GaAs/AlAs (111) heterojunction using a local energy density, by **N. Chetty** and R. M. Martin, Phys. Rev. **B45**, 6089-6100 (1992). (citations=56)
7. Optimized and transferable densities from first principles local density calculations, by **N. Chetty**, K. W. Jacobsen and J. K. Norskov, Letter, J. Phys. Condens. Matter **3** 5437 (1991). (citations=19)
8. *Ab Initio* Potential for Solids, **N. Chetty**, K. Stokbro, K.W. Jacobsen and J.K. Norskov, Phys. Rev. **B46**, 3798-3809 (1992). (citations=34)
9. *Ab Initio* Effective Medium Theory for Al, Springer Series in Solid State Science, Interatomic Potential and Structural Stability, J.K. Norskov, K. Stokbro, N. Chetty, K.W. Jacobsen, Vol 114, 15-22 (1993). (citations=2)
10. Construction of transferable spherically-averaged electron potentials, K. Stokbro, **N. Chetty**, K.W. Jacobsen and J.K. Norskov, J. Phys. Condens. Matter **6** 5415 – 5421 (1994). (citations=4)
11. First Principles Pseudopotential Calculations on Aluminum and Aluminum Alloys, J.W. Davenport, **N. Chetty**, R.B. Marr, S. Narasimhan, J.E. Pasciak, R.F. Peierls and M. Weinert, Alloy Modeling and Design, eds. G.M.Stocks and P.E.A. Turchi, J. of the Minerals, Metals, and Materials Society, Warrendale, Pennsylvania, pages 3 – 12 (1994). (citations=0)
12. Effective-Medium Tight Binding Model for Silicon, K. Stokbro, **N. Chetty**, K.W. Jacobsen and J.K. Norskov, Phys. Rev. **B50**, 10727-10741 (1994). (citations=19)
13.  $\text{TiTe}_2$ : Inconsistency between Transport and Photoemission, P.B. Allen and **N. Chetty**, Phys. Rev. **B50**, 14855-14859 (1994). (citations=17)
14. Vacancies and Impurities in Aluminum and Magnesium Using Large Supercell Total Energy Calculations, **N. Chetty**, M. Weinert, T.S. Rahman and J.W. Davenport, Phys. Rev. **B52**, 6313-6326 (1995). (citations=97)
15. Stacking Faults in magnesium, **N. Chetty** and M. Weinert, Phys. Rev. **B56**, 10844-10851 (1997). (citations=57)
16. First Principles Methods versus (Semi) Empirical Methods: Modelling the hierarchy of length scales in Material Systems, **N. Chetty**, Mol. Simul. **21**, 173-181 (1998). (citations=0)
17. Role of core-valence interaction for pseudopotential calculations with exact exchange, E. Engel, A. Höck, R. N. Schmid, R. M. Dreizler, and **N. Chetty**, Phys. Rev. **B64**, 125111-125123 (2001). (citations=32)

18. Perspectives on Physics and Industrial Development, **N. Chetty** and N. Comins, *Physica Scripta*, T97, 170-173 (2002). (citations=0)
19. Theoretical studies of Ir under pressure, Sharon Grussendorf, **N. Chetty** and H. Dreyse, *Journal of Physics (Condens. Matter)* 15 4127 — 4134 (2003). (citations=6)
20. Computational physics in South Africa, **N. Chetty**, F. Petruccione and R.J. Lindebaum, *South African Journal of Science*, 258-262, **101**, (2005). (citations=1)
21. Developing computational mathematics in Africa, **N. Chetty** and A.C. Bawa, *What mathematics from Africa? Polimetrica*, editor G. Sica, 35-52, ISBN 88-7699-023-2 (2005). (citations=1)
22. Physics for development, **N. Chetty**, S. Connell and A. C. Bawa, *Nature Physics* 747-749, vol 3, 11 November (2007). (citations=2)
23. Suppressed Bond-Site Percolation, L. Nduwayo, R. Lindebaum and **N. Chetty**, *Computer Physics Communications* vol 80 (4) 503-508 (2009). (citations=1)
24. Universities in a time of change, **N. Chetty**, *South African Journal of Science* Vol 105, No 9/10 325-327 (2009) (citations=0)
25. Ab initio studies of staggered Li adatoms on graphene, R.E. Mapasha and **N. Chetty**, *J. Comp. Mat. Sci.* Vol 49 (4), 787-791 (2010). (citations=16)
26. Material progress in Africa, **N. Chetty**, RM Martin, S Scandolo, *Nature Physics*, 830-832, vol 6, November (2010). (citations=0)
27. New modalities for scientific engagement in Africa – a case for computational physics, **N. Chetty**, *Computers Physics Communications* 182 (9) 2065-2070 (2011). (citations=0)
28. Enhancing the understanding of entropy through computation, T. Salagaram and **N. Chetty**, *Am. J. Phys.*, 79 (11), pp 1127-1132, (2011). (citations=2)
29. Modifying the bandoffset in boronitrene, K. Obodo, RC Andrew and **N. Chetty**, *Phys. Rev. B* **84** (15), 155308-155315, (2011). (citations=6)
30. Defect states of complexes involving a vacancy on the boron site in boronitrene, T. B. Ngwenya, A. M. Ukpong, and **N. Chetty**, *Phys. Rev. B* **84**, 245425-245437, (2011). (citations=9)
31. A theoretical investigation of the stability of crystalline silicon dicarbide, RC Andrew, M. Braun and **N. Chetty**, *J. Comp. Mat. Sci.* 55, pp186–191, (2012). (citations=1)
32. Ab initio studies of hydrogen on bilayer graphene, RE Mapasha, AM Ukpong and **N. Chetty**, *Phys. Rev. B* **85** 205402-205424 (2012). (citations=35)
33. The mechanical properties of graphene and boronitrene, RC Andrew, RE Mapasha, AM Ukpong and **N. Chetty**, *Phys Rev B*, Vol. 85, No. 12, pp. 125428(1)– 125437(9), (2012). (citations=59)
34. First principles molecular dynamics study of nitrogen vacancy complexes in boronitrene, A. M.Ukpong and **N. Chetty**, *Journal of Physics: Condensed Matter*, Vol. 24, No. 26, pp. 265002 (1) – 265002(10), (2012). (citations=2)
35. Density functional studies of the defect-induced electronic structure modifications in bilayer boronitrene, A. M.Ukpong and **N. Chetty**, *Journal of Physics: Conf Series*, Vol. 367, No. 1, pp. 012004(1) – 012010(6), (2012). (citations=0)
36. Half-metallic ferromagnetism in substitutionally doped boronitrene, A. M. Ukpong, and **N. Chetty**, *Phys Rev B*, Vol. 86, 19, 195409 9(1)-195422(13), (2012). (citations=2)
37. Ab initio studies of vacancies in (8,0) and (8,8) single-walled carbon and boron nitride nanotubes, G. Mashapa, **N. Chetty**, S. Sinha Ray, J. Nanoscience and Nanotechnology, 12:7030-7036 (2012). (citations=7)
38. Defect complexes in carbon and boron nitride nanotubes, G. Mashapa, **N. Chetty**, S. Sinha Ray, J. Nanoscience and Nanotechnology, 12:7021-7029 (2012). (citations=0)
39. First-principles studies of extrinsic and intrinsic defects in boron nitride nanotubes, G. Mashapa, **N. Chetty**, S. Sinha Ray, J. Nanoscience and Nanotechnology, 12:7807-7814, October (2012). (citations=0)
40. Vacancy complexes in carbon and boron nitride nanotubes, G. Mashapa, **N. Chetty**, S. Sinha Ray, J. Nanoscience and Nanotechnology, 12:7796-7806, October (2012). (citations=1)
41. First principles LDA + U and GGA + U study of protactinium and protactinium oxides: dependence on the effective U parameter, K. Obodo and **N. Chetty**, *J. Phys.: Condens. Matter* 25, 145603-145614 (2013). (citations=8)
42. Probing the extensive nature of entropy, T. Salagaram and **N. Chetty**, *Journal of Physics: Conf Series*, vol 454, 012074 (2013) (citations=0)
43. The challenges of developing computational physics: The case of South Africa, T. Salagaram and **N. Chetty**, *Journal of Physics: Conf Series*, vol 454, 012075 (2013). (citations=0)
44. Mechanical properties of hydrogenated bilayer graphene R. C. Andrew, R. E. Mapasha and **N. Chetty**, *J. Chem. Phys.* 138 (24), (2013). (citations=0)
45. Van der Waals density-functional study of 100% hydrogen coverage on bilayer graphene: R.E. Mapasha, R.C. Andrew, **N. Chetty**, *J. Comp. Mat. Sci.* 1-8, 78 (2013). (citations=1)
46. A theoretical study of thorium titanium-based alloys, K.O. Obodo and **N. Chetty**, *J. Nuc. Mat.*, 440, 229–235 (2013). (citations=2)
47. Comparative investigations of lithium adatoms on AA and AB stackings of bilayer graphene: a van der Waals density functional study R. E. Mapasha, **N. Chetty**, *J. Comp. and Theo. Nanoscience*, Vol 11, Issue 4, 1211-1221 (2014). (citations=2)
48. GGA + U studies of the early actinide mononitrides and dinitrides, K.O. Obodo and **N. Chetty**, *J. Nuc. Mat.* 442(1-3), 235-244 (2013). (citations=6)
49. *Ab initio* studies of Th<sub>3</sub>N<sub>4</sub>, Th<sub>2</sub>N<sub>3</sub> and Th<sub>2</sub>N<sub>2</sub>(NH), K.O. Obodo and **N. Chetty**, *Solid State Comm.* Vol 193, 41-44 (2013).
50. First principles calculations of pentaheptite graphene and boronitrene derivatives, M.P. Molepo, R.E. Mapasha, K.O. Obodo and **N. Chetty**, *Computational Material Science* Vol 92, 395-400 (2014). (citations=0)
51. Simplified pseudopotential problems for the classroom, T. Salagaram, R. Andrew and **N. Chetty**, *J. Computing in Science and Engineering* Vol 17, Issue 1, 46-53 (2015). (citations=0)
52. Ab initio studies of isolated hydrogen vacancies in graphene, R.E. Mapasha, M.P. Molepo and **N. Chetty**, *Physica E: Low-dimensional Systems and Nanostructures*, Vol 79, 52-58 (2016). (citations=0)
53. Defect charge states in Si doped hexagonal boron-nitride monolayer, R.E. Mapasha, M.P. Molepo, R. C. Andrew and N. Chetty, *J. Phys: Condensed Matter*, **28** (5) (2016). (citations=0)
54. A hybrid density functional study of silicon and phosphorus doped hexagonal boron nitride monolayer, R. E. Mapasha, E. Igumbor, **N. Chetty**, *J. Phys. Conf. Series*, Vol 759 (1) (2016). (citations=0)
55. Visualizing higher order Brillouin zones with applications, R.C. Andrew, T. Salagaram and N. Chetty, <https://doi.org/10.1088/1361-6404/aa5e0d>, *Euro J. Phys* (2016). (citations=0)
56. First-principles studies of chromium line-ordered alloys in a molybdenum disulfide monolayer by F.N. Andriambelaza, R.E. Mapasha and N. Chetty, *submitted Modelling and Simulation in Materials Science and Engineering* (2017).

1. Energy density calculations applied to GaAs polar surfaces, Proceedings of Third International Conference on the Structure of Surfaces, University of Wisconsin-Milwaukee, USA, July 1990, Springer-Verlag (1991), **N. Chetty** and R.M. Martin.
2. Physics in South Africa – where do we stand? **N. Chetty**, Proceedings International Conference on the Development of Science and Technology, Durban 1998, editors AC Bawa, K. Lassila and L. Rule (2000)
3. Computational Materials Physics at the University of Natal, **N. Chetty**, *Proceedings of the 2<sup>nd</sup> African-MRS Conference*, University of Witwatersrand Press, Editors Ballim, Every, Luyckx and Levendis, ISBN 0-620-31513-X, December 2003.
4. Computational Physics at the University of KwaZulu-Natal, **N. Chetty**, Proceedings of the International Conference on Physics Education: What Physics should we teach?, Durban, South Africa ISBN 1-86888-359 (2005).

#### Books and chapters in books

1. Book: Research Activities in Physics and Related Fields in South Africa, I. Gertenbach, **N. Chetty** and L. Hasselgren, a catalogue published by The International Programme in the Physical Sciences, ISBN 91-506-1349-9 (1999).
2. Chapter in book: The importance of communicating freely, **N. Chetty**, *Undressing Durban*, ed. R. Pattman and S. Khan, Madiba Publishers 433-436 ISBN 0-947445-68-4 (2007)
3. Book: The Struggle for the soul of a South African University – The University of KwaZulu-Natal, Academic Freedom, Corporatisation and Transformation, **Nithaya Chetty** and Christopher Merrett, self-published ISBN 978-0-620-58600-9 (2014).

#### Other scholarly publications

1. PhD Thesis: First principles energy density and its applications to selected polar surfaces and interfaces, by **N. Chetty**, University of Illinois at Urbana-Champaign (1990).
2. Science as a basis for development in Africa, **N. Chetty** and A.C. Bawa, *APS News*, vol 14, **10** November 2005.
3. Shaping the future of Physics in South Africa, S. Connell, **N. Chetty**, H. Moraal, *APS News*, vol 17, **1**, January 2008.
4. Growing opportunities for international collaborations in South Africa, **N. Chetty**, S. Connell, H. Moraal, *APS News*, vol 17, **2** March 2008.

#### Reviews and Technical reports

1. Report: Review of the National Laser Centre Rental Pool Programme of the CSIR, **N. Chetty** (chair), A.W. Parker, I. Gledhill and T. Majozi, December 2005.
2. Report of the Senate ad hoc Committee looking into the causes of the industrial action of February 2006, I. Konyin (Chair), J. Aitchison, **N. Chetty**, R. de Kadt, N. Gqaleni, M. Green, J. May, J. Mubangizi, S. Ngubane, S. Ngwane, V. Sewpaul, A. Sitas, R. Vithal, A. von Kotze, September 2006.
3. Report: Review of the UKZN School of Religion and Theology, **N. Chetty** (chair), N. Hlongwa, J. Cochrane, M. Masenya, C. Steyn, D. Dziva, S. Chingondole, S. Mathieson and A. Walker, January 2008.

#### References

1. Prof Patricia Whitelock, SAAO, [paw@saao.ac.za](mailto:paw@saao.ac.za)
2. Prof Richard Martin, Physics, University of Illinois, [martin@uiuc.edu](mailto:martin@uiuc.edu)
3. Prof Johan Malherbe, Physics, University of Pretoria, [Johan.Malherbe@up.ac.za](mailto:Johan.Malherbe@up.ac.za)
4. Dr Albert van Jaarsveld, NRF CEO, [Albert@nrf.ac.za](mailto:Albert@nrf.ac.za)
5. Dr Michael Shara, Chair of the SALT Board, American Museum of Natural History, [mshara@amnh.org](mailto:mshara@amnh.org)
6. Dr Thomas Auf der Heyde, Deputy Director General, DST, [Thomas.AufderHeyde@dst.gov.za](mailto:Thomas.AufderHeyde@dst.gov.za)
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## CORPORATE



*Nithaya Chetty  
Physics Department, University of Pretoria  
and  
National Research Foundation of South Africa  
January 2017*

In July 2011, Nithaya Chetty was seconded to the National Research Foundation (NRF) as Group Executive: Astronomy, and in Oct 2014 he was appointed Deputy Chief Executive Officer: Astronomy. Chetty is responsible for playing a key role in:

- implementing and co-ordinating the national strategy for astronomy and related future national investments;
- overseeing the astronomy national facilities and the SKA-SA project within the NRF, and ensuring their synergistic interactions as well as the transfer of best practices amongst them, the rest of the NRF and other elements of the National System of Innovation (NSI);
- developing synergies between the astronomy facilities, universities and science councils, and the astronomy community at large, to address the country's transformation imperatives in terms of skilled resources and research capacity;
- playing a key role in creating a national long range planning culture for multi-wavelength astronomy infrastructure and equipment;
- promoting public awareness through appropriate outreach initiatives; and
- liaising with international partners, boards, and other major international facilities.

Chetty serves as the line management authority for the South African Astronomical Observatory (SAAO), Hartebeesthoek Radio Astronomy Observatory (HartRAO), Square Kilometre Array South Africa (SKA SA), South African Gamma Ray Astronomy Programme (SA-GAMMA), NASSP Programme, South African LSST Programme. He represents NRF on the Board of the Southern African Large Telescope (SALT) and serves on the South African Square Kilometre Array (SKA) Steering Committee. He leads South African interests in the High Energy Stereoscopic System (HESS), and led the support for Namibia's bid to host the Cherenkov Telescope Array (CTA) which was ultimately unsuccessful. Chetty provides the interface between South African academic community and NRF on matters related to astronomy and receives advice from the Astronomy Advisory Council which serves as the voice of the Astronomy research community in South Africa. Chetty speaks on behalf of astronomy in South Africa, and represents South Africa's interests in astronomy locally and internationally. He leads the management of South African astronomy cooperation with UK, USA, Holland, India, China and BRICS, and was instrumental in developing the modalities for research engagements between these countries. Chetty led the re-drafting of the terms of reference of the SKA SA Steering Committee, and has played a leading role in the merger process involving SKA SA and HartRAO to form the South African Radio Astronomy Observatory (SARAO).

# RESUMÉ



Nithaya Chetty  
Physics Department, University of Pretoria  
and  
National Research Foundation of South Africa  
January 2017

Nithaya (Full name Nithayanathan) Chetty was born on 25 September 1963 in Pietermaritzburg in KwaZulu-Natal Province, South Africa, and spent his early years in Umhlanga Road and in Thornville Junction where he attended primary school (1969-1975). The Chetty family then moved to Pietermaritzburg where he completed his high schooling (Raisethorpe 1976-1980). He was placed first in the national matriculation examinations in 1980 and represented South Africa at the International Youth Science Fortnight in London that year.

Chetty pursued his undergraduate studies at the University of Natal in Pietermaritzburg (1981-1984) under racial permit (7% of the student population at the U. Natal was allowed to be of colour at that time) where he passed his BSc (physics and applied mathematics) and BSc Honours (physics) degrees *cum laude*, having attained first class passes with certificates of merit in each of his subjects for all four years. Chetty was supported with a CSIR undergraduate bursary and several University of Natal scholarships. He served on the Students Representative Council in (1982-1983) and played cricket for the Royals Cricket Club, which was the oldest non-racial SACOS affiliated cricket club in Pietermaritzburg at that time.

In 1984 he was selected as the principal candidate in South Africa for the American Fulbright Fellowship. He studied at the University of Illinois at Urbana-Champaign where he completed his Masters degree in physics (GPA 4.968) (1986) and his PhD degree (1990) in the field of theoretical and computational solid state physics. He held post-doctoral research appointments at the Technical University of Denmark (1990-1992) and at the Brookhaven National Laboratory in the USA (1992-1995). He had written his own plane-wave pseudopotential code based on a preconditioned steepest descent method in collaboration with Michael Weinert (BEST – Brookhaven Electronic Structure code).

Chetty was a lecturer at the University of South Africa (1995-1996) where he served as the secretary of the academic affirmative action programme, and was elected to represent the faculty of science on the steering committee for transformation. He was the recipient of an NRF President's award (1997–2001).

He joined the physics department at the University of Natal in Pietermaritzburg as a senior lecturer in January 1997, and was appointed associate professor of physics in 2005. He directed the only Computational Physics Programme in the country at the University of KwaZulu-Natal (1999-2008). He was deputy head of the School of Physics at the UKZN (2008). He served as the deputy director of the National Institute for Theoretical Physics (2007-2008). He served on the University of Natal Task Team on the merger (2002). He served as a faculty representative on Senate and as a Senate representative on the UKZN Council (2006-2008). He served on the Senate *ad hoc* committee that investigated the reasons behind the industrial action (2006). Chetty chaired a panel review of the UKZN School of Religion and Theology (2007). He was an invited participant at a workshop organized by the Council on Higher Education Task Team on "Higher Education, Institutional Autonomy and Academic Freedom" (2007)

He serves (or has recently served) on the selection panel for the NRF Prestigious Scholarship Programme, on the grant review panel for NRF Materials Science Focus area and the NRF Evaluation Committee for physics. Chetty served on the editorial board of the South African Journal of Science and was a progress monitor for the Department of Arts, Culture, Science and Technology Innovation Fund (2001-2002). He has served on the Academy of Science of South Africa's Think Tank on Science and Technology. Chetty chaired an international panel review of the Rental Pool Programme of the National Laser Centre commissioned by the NRF and CSIR in December 2005. He served on the DST-NRF selection panel for the South African Research Chairs Initiative (2006 and 2007). He accompanied the deputy minister of Science and Technology, Mr Derek Hanekom, on a scientific mission to Eastern Europe to sign bi-national agreements with Romania and Slovakia where he represented South African interests in physics (2006). Chetty served on the board of the National Laser Centre (2007-2010), on the board the National Institute for Theoretical Physics (2009-2012), and the International Council on Science (ICSU) Board of South Africa (2011-2013). He is an associate member of the National Institute of Theoretical Physics. He was the associate editor of the South African Journal of Science (2010-2012). He is an elected member of the Academy of Sciences of South Africa. He is an elected member of the Royal Society of South Africa.

He served on the South African Institute of Physics (SAIP) Transformation Committee (2001-2003). He was elected to serve on the Management and Policy Committee in 2003 which oversaw the international review of physics in South Africa. He is a member of the Council of the SAIP and was president of the SAIP (2007-2009). He is an honorary member of the SAIP.

He was a co-organizer for the 1997, 1999 and 2004 Chris Engelbrecht theoretical physics Summer schools, and he chaired the 2005 Summer school on Advanced Scientific Computing. He is an elected member of C20 which is the Commission for Computational Physics of the International Union for Pure and Applied Physics (IUPAP) where he is serving a fourth term (2005-2008, 2008-2011, 2011-2014, 2015-2018). He was a member of the International Advisory

Committee for the Commission for Computational Physics 2007, 2008, 2010, 2011 and 2014 annual conferences held in Belgium, Brazil, Norway, USA and USA respectively.

He was a member of the South African delegation to the IUPAP General Assembly held in Atlanta, Georgia USA in 1999. He headed the South African delegation to the IUPAP General Assembly held in Berlin in 2002. He was co-organiser of the inaugural African School on Electronic Structure Methods and Applications (ASESMA) in 2010. He was chair of the executive committee of ASESMA (2010-2015).

He is or was a referee for the Physical Review B, Physical Review Letters and the Journal of Applied Physics. He has given invited talks including a presentation at the Computational Physics Workshop in Trieste, Italy (1991) and the Hume Rothery Symposium in Las Vegas, USA (1995). Chetty has more than 50 peer-reviewed publications and has had or currently has international collaborations with institutions in Germany, France, Norway, India, Japan and the USA. Chetty served as a member of the Centre of Excellence in Strong Materials which is headquartered at the University of Witwatersrand, Johannesburg, working on theoretical studies of 5d transition metal alloys.

Chetty was a visiting professor at the Goethe University of Frankfurt (December 1997-January 1998). He spent a sabbatical leave at the University of Illinois at Urbana-Champaign in 2004 on a Fulbright Researcher's grant where he worked with Prof Richard Martin on the use of the localized basis set quantum mechanical scheme SIESTA. He entered into research collaborations with the CSIR to study Ti-based alloys (2005-2008). He has received funding from de Beers and Element Six for his work on semi-empirical modeling of the process of sintering.

Chetty's current research interests include first principles quantum mechanical studies of silicon carbide, carbon nanotubes, graphene, boronitrene, transition metal alloys and alloys involving actinides and lanthanides using plane wave pseudopotential methods. He has also recently worked on computational studies of percolating systems. He is involved in promoting computational physics education in South Africa and in Africa. He pursues research in Computational Physics Education. His teaching interests include Solid State Physics, Quantum Mechanics, Statistical Physics, Classical Mechanics, Mathematical Methods in Physics and Computational Physics. Chetty has graduated six MSc students and seven PhD students. He has supervised four postdoctoral fellows. Chetty is full professor in physics at the University of Pretoria.

He served as the National Research Foundation (NRF) Group Executive for Astronomy (2011-2014), and is currently on secondment to the NRF as Deputy CEO: Astronomy. As DCEO: Astronomy, he provides strategic leadership and management oversight for SKA South African project, the South African Astronomical Observatory (SAAO), the Hartebeesthoek Radio Astronomy Observatory (HartRAO), the Southern African Large Telescope (SALT), the South African Gamma Ray Astronomy Programme, the National Astrophysics and Space Science Programme (NASSP), the South African LSST Programme, various South African international bi-lateral agreements in Astronomy (including the USA, UK, Holland, India and China) as well as BRICS Astronomy, etc.

He is a strong advocate for Academic Freedom. He delivered the 2009 TB Davie Academic Lecture at the University of Cape Town. His book on *The Struggle for the Soul of a University: The University of KwaZulu-Natal, Academic Freedom, Corporatisation and Transformation* by Nithaya Chetty and Christopher Merrett ISBN 978-0-620-58600-9 was self-published in 2014.

He is an occasional columnist for the Witness, Mail and Guardian and the Cape Times. He is married to Anashree Chetty (born Govender 11 March 1973). His son, Arjuna Alexander Kolkur Sorensen (born 04 March 1993) lives in Copenhagen, Denmark.