

RESEARCH OUTPUTS FROM 1997

PE NGOEPE

SCIENTIFIC PAPERS READ AT LOCAL CONFERENCES

1. P.E. Ngoepe, "Computational modelling facilities at the University of the North", Workshop on Computational Modelling in Metallurgy, organised under the auspices of FRD/Royal Society Initiative", Mattek Division, CSIR, January 1997, Pretoria.
2. K.R. Kganyago and P.E. Ngoepe, "Electronic and structural effects on lithium intercalated graphite: A density functional approach", Density Functional Theory Summer School of Theoretical Physics, January 1997, Hermanus.
3. P.E. Ngoepe, "Transport and elastic properties studies of ionic conductors", FRD/Royal Society - Materials Modelling Meeting, April 1997, University of the North, Sovenga.
4. K.R. Kganyago and P.E. Ngoepe, "First-Principle study of electronic and structural properties of pure and lithium intercalated graphite", FRD/Royal Society - Materials Modelling Meeting, April 1997, University of the North, Sovenga.
5. P.S. Ntoahae and P.E. Ngoepe, "Application of computer simulation methods to the study of electronic, structural and optical properties of platinum group minerals", South African Institute of Physics Conference, July 1997, Durban.
6. N.E. Hlungwani and P.E. Ngoepe, "Computer modelling studies of the electronic and optical properties of yttrium stabilized zirconia solid solution", South African

Institute of Physics Conference, July 1997, Durban.

7. K.R. Kganyago and P.E. Ngoepe, "Ab initio molecular dynamics study of LiC₆: Harris functional approach", South African Institute of Physics Conference, July 1997, Durban.
8. K.R. Kganyago and P.E. Ngoepe, "Electronic and structural effects on LiC₆: A density functional approach", South African Institute of Physics Conference, July 1997, Durban.
9. H.M. Sithole P.E. Ngoepe, D. Nyugen-Mahn and D.G. Pettifor, "Pressure dependence of electronic and optical properties of FeS₂", South African Institute of Physics Conference, July 1997, Durban.
10. K.R. Kganyago and P.E. Ngoepe, "Electronic and structural properties of lithium intercalated graphite: A density functional approach", Structural Chemistry Indaba II, August 1997, Kruger National Park.
11. P.S. Ntoahae and P.E. Ngoepe, "Computer simulation studies of platinum group minerals", Structural Chemistry Indaba II, August 1997, Kruger National Park.
12. P.E. Ngoepe, "Computational modelling in materials", Iscor Seminar Series, Iscor, Pretoria, August 1997.
13. P.E. Ngoepe. "Ab-initio predictions of phase stabilities in alloys", Columbus Stainless Seminar Series, Columbus Stainless, Middelburg, October 1997.
14. P.E. Ngoepe, "Computational modelling in materials", Armscor, Pretoria, November 1997.

15. K.R. Kganyago and P.E. Ngoepe, "Electronic and structural studies of LiC_6 ", Second FRD/Royal Society (UK) Materials Modelling Meeting, 4-5 May 1998, University of the North, Sovenga.
16. K.R. Kganyago and P.E. Ngoepe, "Ab initio molecular dynamics studies of lithium in LiC_6 : A Harris Functional Approach" Second FRD/Royal Society (UK) Materials Modelling Meeting, 4-5 May 1998, University of the North, Sovenga.
17. M.F. Phala, P.E. Ngoepe, "Computer modelling studies of bulk and nano TiO_2 ", Second FRD/Royal Society (UK) Materials Modelling Meeting, 4-5 May 1998, University of the North, Sovenga.
18. T.T. Netshisaulu, P.E. Ngoepe and A.V. Chadwick, "Computer modelling and EXAFS studies of mixed-metal fluorides", Second FRD/Royal Society (UK) Materials Modelling Meeting, 4-5 May 1998, University of the North, Sovenga.
19. H.M. Sithole and P.E. Ngoepe, "Calculation of equilibrium geometry of ion sulphides: A density functional approach", Second FRD/Royal Society (UK) Materials Modelling Meeting, 4-5- May 1998, University of the North, Sovenga.
20. P.S. Ntoahae and P.E. Ngoepe, "The effect of pressure on electronic and structural properties of platinum sulphides", Second FRD/Royal Society (UK) Materials Modelling Meeting, 4-5 May 1998, University of the North, Sovenga.
21. H.R. Chauke, P.E. Ngoepe and H.M. Sithole, "Ab initio calculations of structural electronic and optical properties of NiS_2 and CoS_2 ", Second FRD/Royal Society (UK) Materials Modelling Meeting, 4-5 May 1998, University of the North, Sovenga.
22. D. Mkhonto, P.E. Ngoepe and K.R. Kganyago, "Computer Modelling of Ilmenite

and Hematite", Second FRD/Royal Society (UK) Materials Modelling Meeting, 4-5 May 1998, University of the North, Sovenga.

23. L.R.M. Segooa and P.E. Ngoepe, "Small penetrants diffusion in polysiloxanes", Second FRD/Royal Society (UK) Materials Modelling Meeting, 4-5 May 1998, University of the North, Sovenga.
24. H.M. Sithole and P.E. Ngoepe, "Pressure dependence studies of structural and optical properties of iron sulphides", Second FRD/Royal Society (UK) Materials Modelling Meeting, 4-5 May 1998, University of the North, Sovenga.
25. K.R. Kganyago and P.E. Ngoepe, "Structural, electronic and lithium diffusion studies of LiC_6 ", South African Institute of Physics Annual Conference, 8-10 July 1998, Cape Town.
26. M.F. Phala and P.E. Ngoepe, "Computer modelling studies of lithium insertion in TiO_2 and LiTi_2O_4 ", South African Institute of Physics Annual Conference, 8-10 July 1998, Cape Town.
27. H.R. Chauke, P.E. Ngoepe and H.M. Sithole, "Calculation of equilibrium geometry of iron sulphides: A density functional approach", South African Institute of Physics Annual Conference, 8-10 July 1998, Cape Town.
28. H.R. Chauke, P.E. Ngoepe and H.M. Sithole, "First-Principle study of transition metal sulphides", South African Institute of Physics Annual Conference, 8-10 July 1998, Cape Town.
29. D. Mkhonto, P.E. Ngoepe and K.R. Kganyago, "First-principle study of transition metal sulphides", South African Institute of Physics Annual Conference, 8-10 July 1998, Cape Town.

30. L.R.M Segooa, P.E. Ngoepe and G. Goldbeck-Wood, "Atomistic simulation of sorption and diffusion of small molecules in polysiloxanes", South African Institute of Physics Annual Conference, 8-10 July 1998, Cape Town.
31. P.S. Ntoahae, P.E. Ngoepe, D. Nyugen-Mahn and D.G. Pettifor, "Computer simulation studies of platinum sulphides", South African Institute of Physics Annual Conference, 8-10 July 1998, Cape Town.
32. LRM Segooa and PE Ngoepe, "Computational modelling of small penetrants in polysiloxanes", 3rd FRD/Royal Society (UK) Materials Modelling Meeting, 8-9 March 1999, University of the North, Sovenga.
33. SP Ntoahae and PE Ngoepe, "Computer modelling studies of platinum sulphides:", 3rd FRD/Royal Society (UK) Materials Modelling Meeting, 8-9 March 1999, University of the North, Sovenga.
34. TT Netshisaulu and PE Ngoepe, "Computer modelling studies of CdF₂ (xPbF₂), 3rd FRD/Royal Society (UK) Materials Modelling Meeting, 8-9 March 1999, University of the North, Sovenga.
35. KR Kganyago and PE Ngoepe, "Optical properties of pure and intercalated graphite", 3rd FRD/Royal Society (UK) Materials Modelling Meeting, 8-9 March 1999, University of the North, Sovenga.
36. MF Phala and PE Ngoepe, "Ab-initio study of lithium intercalation in Li-Ti-O", 3rd FRD/Royal Society (UK) Materials Modelling Meeting, 8-9 March 1999, University of the North, Sovenga.
37. PE Ngoepe, "Computer simulation of stabilized cubic zirconia", 3rd FRD/Royal

Society (UK) Materials Modelling Meeting, 8-9 March 1999, University of the North, Sovenga.

38. HM Sithole, KV Wright, PE Ngoepe and DG Pettifor, "Computer simulation of iron sulphides: Interatomic potentials and elastic properties", 3rd FRD/Royal Society (UK) Materials Modelling Meeting, 8-9 March 1999, University of the North, Sovenga.
39. LR Segooa, PE Ngoepe and G Goldbeck-Wood, "Investigation of gas permeation through siloxanes polymer by molecular dynamics", 3rd FRD/Royal Society (UK) Materials Modelling Meeting, 8-9 March 1999, University of the North, Sovenga.
40. HM Sithole, D Nguyen-Manh, DG Pettifor and PE Ngoepe, "Internal relaxation, band gaps and elastic constant calculations of FeS₂", 3rd FRD/Royal Society (UK) Materials Modelling Meeting, 8-9 March 1999, University of the North, Sovenga.
41. NE Hlungwani, PE Ngoepe, MS Khan and MS Islam, "Computer simulations studies of stabilised cubic zirconia", 3rd FRD/Royal Society (UK) Materials Modelling Meeting, 8-9 March 1999, University of the North, Sovenga.
42. PS Ntoahae, PE Ngoepe, D Nguyen-Manh and DG Pettifor, "First principle studies of platinum group minerals", 3rd FRD/Royal Society (UK) Materials Modelling Meeting, 8-9 March 1999, University of the North, Sovenga.
43. D Mkhonto and PE Ngoepe, First principle studies of pressure on MgTiO₃", 3rd FRD/Royal Society (UK) Materials Modelling Meeting, 8-9 March 1999, University of the North, Sovenga.
44. PS Ntoahae, PE Ngoepe, D Nguyen-Manh and DG Pettifor, "Computer modelling studies of PtAs₂" 3rd FRD/Royal Society (UK) Materials Modelling Meeting, 8-9

March 1999, University of the North, Sovenga.

45. HR Chauke, PE Ngoepe, D Nguyen-Manh and DG Pettifor, "Electronic structure and stability of pentlandites: Co_9S_8 ", 3rd FRD/Royal Society (UK) Materials Modelling Meeting, 8-9 March 1999, University of the North, Sovenga.
46. SM Maphalla, PE Ngoepe, D Nguyen-Manh and DG Pettifor, "Phase stability studies of Al-Re systems", 3rd FRD/Royal Society (UK) Materials Modelling Meeting, 8-9 March 1999, University of the North, Sovenga.
47. J Muscat, D Mkhonto, NM Harrison and PE Ngoepe, "The structural, electronic and magnetic properties of ilmenite from ab-initio calculations" 3rd FRD/Royal Society (UK) Materials Modelling Meeting, 8-9 March 1999, University of the North, Sovenga.
48. KR Kganyago and PE Ngoepe, "Graphite and LiC_6 under pressure: equation of state and electronic structure" 3rd FRD/Royal Society (UK) Materials Modelling Meeting, 8-9 March 1999, University of the North, Sovenga.
49. HM Sithole, NH de Leeuw, SC Parker and PE Ngoepe "Modelling of surface stability and reactivity of pyrite (FeS_2)" 4th NRF/Royal Society (UK) Materials Modelling Meeting, 11-12 April 2000, University of the North, Sovenga.
50. SP Ntoahae and PE Ngoepe "Computer modelling studies of PtAsS " 4th NRF/Royal Society (UK) Materials Modelling Meeting, 11-12 April 2000, University of the North, Sovenga.
51. KR Kganyago and PE Ngoepe "Computational modelling studies of hexagonal metal sulphides" 4th NRF/Royal Society (UK) Materials Modelling Meeting, 11-12 April 2000, University of the North, Sovenga.

52. MF Phala, PE Ngoepe and N Quirke "Computer modelling studies of TiO₂ clusters in the rutile structure" 4th NRF/Royal Society (UK) Materials Modelling Meeting, 11-12 April 2000, University of the North, Sovenga.
53. KE Rammutla, JD Comins, TT Netshisaulu, PE Ngoepe and AV Chadwick "Optical spectroscopy and computer modelling studies of Ba_{1-x}La_xF_{2+x}" 4th NRF/Royal Society (UK) Materials Modelling Meeting, 11-12 April 2000, University of the North, Sovenga.
54. D Mkhonto and PE Ngoepe "Computer modelling studies of ilminite-like structures MeTiO₃ (Me: Mg, Zn, Mn)", 4th NRF/Royal Society (UK) Materials Modelling Meeting, 11-12 April, University of the North, Sovenga.
55. SM Maphalla, PE Ngoepe, D Nguyen-Mahn, DG Pettifor, L Cornish "Theoretical studies of phase stability studies in Al-Re binaries" 4th NRF/Royal Society (UK) Materials Modelling Meeting, 11-12 April, University of the North, Sovenga.

SCIENTIFIC PAPERS READ AT INTERNATIONAL CONFERENCES

1. H.M. Sithole, P.E. Ngoepe, D. Nyugen-Mahn and D.G. Pettifor, "Electronic structure pressure dependence and optical properties of FeS₂", 1997 Materials Research Society Fall Meeting, 1-5 December 1997, Boston, Massachusetts, Boston, U.S.A.
2. K.R. Kganyago and P.E. Ngoepe, "Study of transport, electronic and structural properties of the first stage lithium intercalated graphite: A density functional approach", Polar Solids Meeting, 14-15 December 1997, Liverpool, U.K.
3. K.R. Kganyago and P.E. Ngoepe, "Study of transport, electronic and structural properties of the first stage lithium intercalated graphite: A density functional

approach", Institute of Physics Annual Solid State Physics Conference, 16-18 December 1997, Exeter, U.K.

4. P.E. Ngoepe, "Elastic and transport properties of oxygen and fluorine ion conductors", Polar Solids Meeting, 30 March - 1 April 1998, Mansfield College, Oxford, U.K.
5. T.T. Netshisaulu, P.E. Ngoepe and A.V. Chadwick, "Molecular dynamics studies of $\text{CdF}_2(\text{xPbF}_2)$ ", Materials Research Society Spring Symposium, 13-17 April 1998, San Francisco, U.S.A.
6. K.R. Kganyago and P.E. Ngoepe, "Transport studies in lithium intercalated graphite: A Harris Functional Approach", Materials Research Society Spring Symposium, 13-17 April 1998, San Francisco, U.S.A.
7. T.T. Netshisaulu, M. Melle-Franco, P.E. Ngoepe and A.V. Chadwick, "EXAFS studies of disorder in $\text{CdF}_2(\text{xPbF}_2)$ ", European Conference on Defects in Insulating Materials (EURODIM '98), 6-10 July 1998, Keele, U.K.
8. K.R. Kganyago and P.E. Ngoepe, "Study of transport, electronic and structural properties of first stage lithium intercalated graphite: Density functional approach", 9th International Meeting on Lithium Batteries, 13-17 July 1998, Edinburgh, U.K.
9. M.F. Phala and P.E. Ngoepe, "Computer modelling studies of Li-Ti-O systems", 9th International Meeting on Lithium Batteries, 13-17 July 1998, Edinburgh, U.K.
10. LRM Segooa, PE Ngoepe and G Goldbeck-Wood, "Atomistic Simulation of Small Molecules in Polysiloxane" MSI Polymer Consortium Meeting, 28 March 99 to 01 April 99, San Diego, Carlifornia.

11. PE Ngoepe "Computational Modelling of Metal Sulphides", French-South African Workshop on Advanced Materials, 15-19 November 1999, Strausbourg, France.
12. LRM Segooa, PE Ngoepe and G Goldbeck-Wood "Atomic simulation of gas phase atoms with small radii through polysiloxanes" 14th International Conference on Defects in Insulating Materials, 3-7 April 2000, Johannesburg, Midrand.
13. EK Rammutla, JD Comins, TT Netshisaulu, PE Ngoepe and AV Chadwick "Correlation of light scattering and molecular dynamics in superionic Ba_{1-x}La_xF_{2+x}" 14th International Conference on Defects in Insulating Materials, 3-7 April 2000, Johannesburg, Midrand.

SCIENTIFIC PUBLICATIONS

1. P.J. Chaba and P.E. Ngoepe, "Defects and ion transport properties of yttria doped zirconia", Materials Research Society Symposium Proceedings Vol 453 (Solid State Chemistry of Inorganic Materials), eds. P.K. Davies, A.J. Jacobson, C.C. Troradi, T.A. Vanderah, (Materials Research Society, June 1997) 549-553.
2. D. Nyugen-Mahn, D.G. Pettifor, H.M. Sithole and P.E Ngoepe, "Electronic structure, pressure dependence and optical properties of FeS₂", Materials Research Society Symposium Proceedings, volume 491. (Tight-Binding Approach to Computational Materials Science) eds. P.E.A. Turchi, Gonis, L. Colombo, (Materials Research Society, 1998) 401-406.
3. P.J. Chaba and P.E. Ngoepe, "Computer modelling studies of elastic and transport properties of yttria stabilised zirconia", Molecular Simulations (1998), Vol. 21, pp. 161-172.

4. T.T. Netshisaulu, P.E. Ngoepe and A.V. Chadwick, ‘Computer modelling and EXAFS study of disorder in CdF₂(xPbF₂) mixed systems’. *Molecular Simulation* (1999) Vol 22, pp. 1-21.
5. D.Nguyen-Manh, P.S. Ntoahae, D.G. Pettifor and P.E. Ngoepe. ‘Electronic structure of platinum-group minerals: prediction of semiconductor band gaps’. *Molecular Simulation* (1999), Vol 22, pp 23-30.
6. H.M. Sithole, D. Nguyen-Manh, D.G. Pettifor and P.E. Ngoepe, ‘Internal relaxation, band gaps and elastic constant calculations of FeS₂’. *Molecular Simulation* (1999) Vol.22, pp 31-37.
7. K.R. Kganyago and P.E. Ngoepe, Effects of local and gradient-corrected density approximations on the prediction of the interlayer lattice distance *c*, in graphite and LiC₆. *Molecular Simulation* (1999), Vol. 22, pp. 39-49.
8. T.T. Netshisaulu, M. Melle-Franco, P.E. Ngoepe and A.V. Chadwick, ‘Studies of disorder in Cd_{1-x}Pb_xF₂ mixed crystals’, *Radiation Effects and Defects in Solids*, (1999) Vol 149, pp. 243-248.
9. J.S. Braithwaite, C.R.A. Catlow, J.D. Gale, J.H. Harding and P.E. Ngoepe, ‘Calculated cell discharge curve for lithium batteries with a V₂O₅ cathode’, *J. Mater. Chem.* (2000) Vol 10, pp. 239-240.

SCIENTIFIC PAPERS SUBMITTED FOR PUBLICATION

1. H.M. Sithole, N.H. Leeuw, S.C. Parker and P.E. Ngoepe, “Modelling surface stability and reactivity of pyrite: Introduction of the new potential model”, Submitted for publication, Journal of Physical Chemistry.
1. LRM Segooa, PE Ngoepe and G Goldbeck-Wood “Atomistic simulation of gas phase atoms with small radii through polysiloxanes”. Accepted for publication, Radiation Effects and Defects in Solids.
2. EK Rammutla, JD Comins, TT Netshisaulu, PE Ngoepe and AV Chadwick “Correlation of light scattering and molecular dynamics in superionic $Ba_{1-x}La_xF_{2+x}$ ” Accepted for publication, Radiation Effects and Defects in Solids.

SCIENTIFIC PAPERS IN PREPARATION

1. K.R. Kganyago and PE Ngoepe. “Electronic and optical properties studies of graphite and intercalated graphite”.
2. SP Ntoahae, D Nguyen Mahn, PE Ngoepe and DG Pettifor. “Studies of electronic properties and equation of state of platinum sulphides”.
3. D Mkhonto and PE Ngoepe “First principles studies of electronic and structural properties of ilminite $MgTiO_3$ ”
4. NE Hlungwani, MS Khan, MS Islam and PE Ngope. “Molecular dynamics studies of co-doped yttria stabilised cubic zirconia”.
5. MF Phala, PE Ngoepe and N Quirke. “First principles studies of deformation charge density and charge transfer in Li-Ti-O systems”.
6. PE Ngoepe “Studies of electronic and structural properties of zirconia oxide

doped with sulphur”.

7. HM Sithole, K Wright, DG Pettifor and PE Ngoepe “Computer simulations studies of FeS₂, their potentials and elastic properties”.
8. HR Chauke, D Nguyen Mahn, PE Ngoepe and DG Pettifor “Electronic structure and stability of pentlandites: Co₉S₈ and the related alloys”
9. SM Maphalla, PE Ngoepe, D Nguyen-Mahn and DG Pettifor, “Phase stability study in Al-Re binary systems”.

CONFERENCES ORGANISED

1. Co-Chairperson of an International Advisory Committee for the 14th International Conference on Defects in Insulating Materials (ICDIM 2000), 1996-2000. Also co-chairperson of this conference which was held at the Eskom Conference Centre, Midrand, from 3-7 April 2000, and was attended by approximately 200 delegates from all over the world. The conference ran successfully.
2. Co-editor of the Proceedings of ICDIM 2000.
3. Chairperson for four Materials Modelling Meetings, held annually at the University of the North, from 1997 to 2000. These annual symposiums are attended by approximately 50 delegates from universities, science councils and industry from South Africa, and mainly the United Kingdom, and other parts of the world. The symposiums are supported by the National Research Foundation and The Royal Society (UK).
4. Guest editor of two proceedings of the First and Second Materials Modelling Meetings.

5. Organised a workshop on “Thermodynamic Calculation of Phase Diagrams”, run by Prof. B Sundman, from the Royal Institute of Technology, Sweden, February 1998, and was attended mainly by metallurgists from universities, science councils and industry.

SCIENTIFIC COMMITTEES

3. Member of the Solid State Physics and Materials Science Specialist Group of the South African Institute of Physics, 1994-
4. Member of the Council of the South African Institute of Physics, 1995-1999.
3. Member of the Editorial Board of Molecular Simulations (Journal), Gordon and Breach, U.K., 1997 - .
4. Evaluator on Materials Proposals - Innovation Fund, run by Department of Arts, Culture, Science and Technology, 1998, 1999, 2000
5. Member of the Research Committee of South African Universities Vice-Chancellors' Association, 1998 –
6. Member of the Manufacturing and Materials Sector Working Group, National Research and Technology Foresight Project, 1997-1999
5. Member of the South African Power Utility Research Advisory Board Committee, 1998 –
6. Member of the Foundation for Research and Development Council, 1995–1999
7. Member of the Personnel Committee for the Foundation for Research and Development Council, 1995-1999
8. Member of the National Research Foundation Board, 1999 -
9. Member of the Personnel Committee for the National Research Foundation Board, 1999 -

A. MEMBERSHIP OF SOCIETIES

1. Member of the South African Institute of Physics
2. Member of the Academy of Science for Southern Africa
3. Member of the Solar Energy Society of Southern Africa
4. Member of the Materials Research Society

1. **POST GRADUATE STUDENTS**

MSc

P.J. Chaba	"Computer Simulations Studies of Yttria Stabilised Cubic Zirconia". Degree awarded with a distinction in April 2000
K.R. Kganyago	"First Principle studies of Lithium Intercalated Graphite" . To complete June 2000
P.S. Ntoahae	"Computer Modelling of Platinum Sulphides". To complete September 2000
L.R.M. Segooa	"Molecular Dynamics Simulation of Small Molecules in Polymers". To complete June 2000
D. Mkhonto	"Computer Modelling Studies in Mixtures of Ilmenite and Hametite". To complete September 2000
H.R. Chauke	"Computer Modelling Studies of Transition Metal Sulphides". To complete September 2000
S.M. Maphalla	"Theoretical Studies of Phase Stabilities in Al-Re

Binary Systems". To complete December 2000.

R.R. Maphanga "Computational Modelling and EXAFS Studies of Electrolytic Manganese Dioxides". To complete December 2001.

M.A. Mahladisa "Computational Modelling of Nanocrystalline TiO₂ Structures". To complete December 2001.

Ph.Ds

H.M. Sithole "Atomistic and Electronic Structure Studies of FeS₂". To complete June 2000.

T.T. Netshisaulu "Computer Modelling and EXAFS Studies of Mixed-Metal Fluorites". To complete December 2000