

Postdoctoral Fellowship Opportunity NITheCS North Node

Joint project between North-West University and Sol Plaatje University, South Africa

The National Institute for Theoretical and Computational Sciences (NITheCS) North Node invites applications for a Postdoctoral Fellowship in **Data-Driven Multiscale Modelling of Polymer Nanocomposites for Energy and Space Applications**.

The project is a collaboration between **Prof Lynndle Square at North-West University (NWU)** and **Prof Regina Maphanga at Sol Plaatje University (SPU)**. It will integrate atomistic modelling and machine learning to investigate structure–property relationships in advanced polymer nanocomposites, with applications in renewable-energy and space environments.

The fellowship forms part of the NITheCS Focus Area **Computational Modelling of Functional Materials for Driving Sustainable Innovation**. The fellow will participate in research activities at both NWU and SPU and will have access to suitable computational infrastructure, including high-performance computing resources.

Key responsibilities

- Conduct independent and collaborative research in computational materials science and data-driven materials design.
- Curate and integrate data from density functional theory (DFT), molecular dynamics (MD), relevant experiments and published literature.
- Develop suitable descriptors for polymer chemistry, nanofiller characteristics, interfaces, morphology and environmental conditions.
- Develop and evaluate machine-learning models for predicting thermomechanical properties, including elastic response, thermal conductivity, glass-transition behaviour and thermal stability.
- Use data-driven analysis to identify influential structure–property relationships and guide further atomistic calculations.
- Conduct targeted MD and/or DFT simulations to generate training data and assess model predictions.
- Develop reproducible computational workflows incorporating appropriate code, data-management and documentation practices.
- Participate in collaborative research, postgraduate mentoring and knowledge-sharing activities across NWU, SPU and the NITheCS community.
- Publish research findings in peer-reviewed journals and present results at conferences, seminars and NITheCS events.

Minimum Requirements

- A PhD in Physics, Materials Science, Computational Chemistry, Engineering, Data Science or a closely related discipline, obtained within the past five years.
- Demonstrated research experience in computational materials modelling, machine learning, scientific computing or a related field.
- A publication record in peer-reviewed journals appropriate to the applicant's career stage.
- Proficiency in Python and scientific computing environments.
- The ability to work independently and contribute effectively to a multidisciplinary collaborative project.

Fellowship Value:

- R350,000 per annum (tax-free)

- R50,000 per annum research expenses
- Once-off relocation allowance of R20,000

Application Deadline: 23 October 2026

Application Requirements:

- Detailed CV including publication list
- Cover letter outlining research interests and alignment
- Contact details of at least two referees

Applications and enquiries should be directed to:

Prof Lynndle Square
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