

Postdoctoral research positions in Computational Materials Science

Institution: University of South Africa (UNISA)

Applications are invited for two Postdoctoral Fellowship research positions in Computational Materials Science in the High Performance Computing research group led by Prof. Enrico Lombardi at UNISA.

Research Focus:

The postdoctoral researchers will pursue novel research in computational materials science to understand microscopic mechanisms underlying the properties of materials. Materials of interest range from two-dimensional solids to crystalline semiconducting materials. We are particularly interested in wide bandgap semiconductors such as diamond and, Ga₂O₃, etc., as well as heterostructures formed by van der Waals layered solids including their applications in spintronics, optoelectronics, energy, and gas sensing, amongst others. Density Functional Theory and its various extensions are the main computational approach. Since there are plethora of potential materials for these applications, high-throughput calculations (i.e., involving large amount of data) to screen materials may be necessary. Analysis of data may require knowledge of, and application of machine learning, data science or statistical techniques. Ultimately, the research will focus on the understanding of the behaviour of defects in these materials, and optimize the properties (composition, application of external perturbations, such as mechanical, electrical, magnetic, etc.) of selected materials for targeted applications.

Responsibilities:

- Conduct research on nanoscale structural, electronic, optical (excitons, plasmons, ...), magnetic properties of selected solids.
- Collaborate with other researchers and contribute to ongoing projects.
- Publish a minimum of 3 articles per annum in international accredited journals.
- Present research at local and international conferences, as well as internal seminars.

Requirements:

- PhD in Physics, in Computational Condensed Matter/Materials Physics, obtained within the last 5 years.
- Proven research track record with at least one article published in an accredited journal, and at least one conference presentation.
- Significant computational and data analysis skills are a strong recommendation, including experience in the use of Linux, scripting, and use of High Performance computing (HPC) resources for data-intensive calculations, and programming skills.
- Demonstrated experience in applying electronic structure calculations to materials systems, with proficiency in Density Functional Theory calculations (e.g. using codes such as Quantum ESPRESSO, CASTEP/Materials Studio, WIEN2k, or similar).
- Evidence of knowledge and application of machine learning and/or AI techniques, especially to materials science research, is highly recommended.

Position details:

 The first position is funded by the NRF for a period of 2 years. Depending on performance, the appointment may be extended for a 3rd year from UNISA funds, subject to funding availability. Remuneration (including UNISA top-up) is R 360 000 p.a. (non-taxable). Appointment to this position will be made in the research focus area of 2D solids and semiconducting materials.



2. The second position is funded by UNISA, for a period of up to 3 years, renewable annually depending on performance and funding availability. Remuneration is R 300 000 p.a. (non-taxable). This appointment will be made in the research focus area of diamond and other wide-bandgap semiconductors.

Both appointments are initially for a period of 1 year, and are renewable annually based on performance, subject to publication of at least three articles in accredited international journals (based on research that has been conducted at UNISA), a conference presentation and at least two internal seminars per annum.

Positions will be on the Unisa Main campus (Pretoria). Candidates may be expected to travel to the Science Campus (Florida, Johannesburg).

Applications:

Interested candidates are invited to apply for these positions by emailing applications to Mr M Myaka: <u>myakamp@unisa.ac.za</u>, with subject line "**Postdoc CSET - Prof. Lombardi**"

- 1. Covering letter, specifying the post(s) applied for, and detailing research interests, expertise, qualifications, and how the applicant meets the requirements.
- 2. Completed application from (forms obtainable from: https://tinyurl.com/2b9an5jk)
- 3. Detailed research plan with clear indication of research outputs for the period of the postdoctoral fellowship.
- 4. Curriculum Vitae, including a list of publications.
- Copies of degree certificates. (Degrees issues by foreign Universities must be accompanied by a SAQA evaluation of foreign qualification certificate <u>https://www.saqa.org.za/services/evaluation-of-foreign-qualifications/</u>)
- 6. Provide contact details of three potential referees. Candidates must arrange for three letters of reference to be forwarded to Mr Myaka <u>myakamp@unisa.ac.za</u>.
- 7. Additional documentation as specified in the application form.

The above should be merged as a single PDF document, or grouped as a single ZIP file.

Deadline for application: 11 December 2023, but the position will remain open until a suitably qualified candidate is found.

Enquiries: For enquiries or questions relating to this position, please contact us at: <u>lombaeb@unisa.ac.za</u> (Prof EB Lombardi) <u>rajiat1@unisa.ac.za</u> (Dr AT Raji) <u>benecem@unisa.ac.za</u> (Dr EM Benecha)

We look forward to receiving your application.