

**PhD and Post-Doctoral Fellow**  
**SCHOLARSHIPS FOR 2024**  
**MATERIAL SCIENCE AND CONDENSED MATTER PHYSICS**  
**UNIVERSITY OF THE FREE STATE**

**DEADLINE: 30 June 2023**

**Applications are invited for 1 PhD and 2 Post-Doctoral fellow positions for 2024.**

**RESEARCH TOPICS:**

**1) Safer nanomaterials through computational modelling and design**

The unique properties of nanomaterials (NMs), relative to their bulk form, have seen them used in a rapidly increasing number of commercial applications. However, with these novel properties of NMs come potential health and environmental hazards. Thus, as part of a responsible innovation approach, NMs potential risks must be assessed in parallel to the exploitation of their benefits. Due to their enormous variability, NM risk assessment needs advanced *in silico* methodologies capable of extraction of advanced descriptors of the materials reflecting their ability to interact with biomolecules and live tissues, and machine learning (ML) from experimental and computational datasets.

In nanotechnology applications involving biological tissues, the responses and impacts are believed to be induced and steered by interactions at the bio-nano interface. We expect that the interactions of NMs with water, amino acids, segments of lipids, sugars, and nucleic acids are especially important. The interactions with these representative fragments may constitute the material's fingerprint that is predictive of consecutive biological responses.

A significant effort has been made recently to evaluate the relevant NM properties and build predictive models. The materials models involved quantum chemical methods to evaluate the NM surface reactivity and parameterize atomistic force fields, evaluate the interactions between biomolecular fragments with inorganics surfaces, and quantify the surface hydrophilicity using atomistic simulations. Coarse-grained models were also proposed to predict the protein-NM interactions and the kinetics of the formation of NM protein corona.

## 2) Developing Infrared Sensors with nanorods and nanowires.

Short wave infrared (SWIR) and mid wave (MIR) infrared light are two spectral bands covering wavelengths from 1 to 5  $\mu\text{m}$ . The sun emits 30% of its power in this IR range, the night sky glows brightest in the SWIR. Different molecules can be identified by SWIR and MIR absorption bands, fog- or smoke-filled air better transmit SWIR light and data communication through optical fibers is most efficient with SWIR light. Hence the importance of technologies that enable interaction with SWIR and MIR light to make possible more efficient solar energy harvesting, automated visualization, identification and inspection of objects or imaging coupled with chemical analysis. In this project. In this international project, in collaboration with a European collaborator, nanowires and nanorods will be synthesised, exploiting the quantum confinement effects to engineer these nanostructure's optical properties, making use of intraband transitions to develop infrared sensors. *The PhD candidate will have the opportunity to a mini-sabbatical and visit our European collaborator's university lab* and gain valuable work experience. The post-doctoral fellow will also be afforded the opportunity to visit the European university workshop related to this project.

### APPLICATIONS

Applicants should email a **single PDF document** containing the following:

- Your CV.
- Transcripts of *all* university-level results.
- A brief statement of research interests (1 page). Please include all previous research experience, with details of the research project and supervisor. Please indicate which of the projects listed below you are interested in.

Applicants should also arrange for **1 reference letters** to be sent directly to us by the same closing date.

**Email:** [harrisra@ufs.ac.za](mailto:harrisra@ufs.ac.za)

**Deadline:** **30 June 2023**

### SCHOLARSHIP VALUES

Competitive scholarships are offered to successful applicants, for a PhD candidate and two post-doctoral fellows. More details about the scholarship values will be communicated directly to the applicant.

### SCHOLARSHIP CONDITIONS

Scholarships are granted on a year-by-year basis - i.e. continuing into the next year depends on satisfactory progress.