

UNIVERSITY OF THE
FREE STATE
UNIVERSITEIT VAN DIE
VRYSTAAT
YUNIVESITHI YA
FREISTATA



NAGOCAT
FOR 2213

DFG Deutsche
Forschungsgemeinschaft

PhD and Postdoc Positions in Computational Chemistry, South Africa

The Department of Chemistry at the **University of the Free State, Bloemfontein, South Africa**, is seeking **a postdoc and a PhD student** to work in the area of computational materials science and catalysis. The positions are offered in the newly established group of Prof. Lyudmila Moskaleva. The PhD position is offered for 3 years. The postdoc position is offered for 1 year with the possibility of extension up to 3 years subject to successful performance during the first year. The positions are available immediately and will remain open until filled.

Job description

You will work on a collaborative project within a research unit NAGOCAT (Nanoporous Gold – A prototype for a rational catalyst design) funded by the German Research Foundation (DFG). Apart from our research group, which is based at the University of the Free State in South Africa, the research unit comprises eight research groups from four universities in Northern Germany. The joint research program combines experimental and theoretical approaches.

You will carry out research on catalytic properties of nanoporous gold using DFT, ab initio MD simulations, and microkinetic modelling. You will be part of an international team to explore the molecular-level basis for processes that control chemical reactivity in complex systems associated with catalysis. The project will involve travel to Germany (1 – 2 times a year).

Related publications

- Tomaschun, G., Dononelli, W., Li, Y., Bäumer, M., Klüner, T., Moskaleva, L. V., Methanol oxidation on the Au(310) surface: A theoretical study, [J. Catal. \(2018\) 364, 216-227](#)
- Li, Y., Dononelli, W., Moreira, R., Risse, T., Bäumer, M., Klüner, T., Moskaleva, L., Oxygen-Driven Surface Evolution of Nanoporous Gold: Insights from Ab Initio Molecular Dynamics and Auger Electron Spectroscopy, [J. Phys. Chem. C \(2017\) 122, 5349-5357](#)
- Hoppe, S., Li, Y., Moskaleva, L. V., Müller S., How silver segregation stabilizes 1D surface gold oxide: a cluster expansion study combined with ab initio MD simulations, [Phys. Chem. Chem. Phys. \(2017\) 19, 14845-14853](#)
- Moskaleva, L.V., Röhe, S., Wittstock, A., Zielasek, V., Klüner, T., Neyman, K. M., Silver residues as a possible key to a remarkable oxidative catalytic activity of nanoporous gold, [Phys. Chem. Chem. Phys. \(2011\), 13, 4529-4539](#)

- Wittstock, A., Zielasek, V., Biener, J., Friend, C. M., Bäumer, M., Nanoporous gold catalysts for selective gas-phase oxidative coupling of methanol at low temperature, [Science \(2010\) 327, 319-322](#)

Your profile

Applicants **at the postdoctoral level** should have a Ph.D. degree in Physics, Chemistry, Chemical Engineering, or a related field. Experience with QM codes such as VASP, CP2K, CRYSTAL is required. Working experience in compiling and running programs in Linux environment is desirable. Proficiency in at least one programming language and shell scripting would be a plus.

Demonstrated oral and written communication skills (in English). Ability to make clear presentations. Relevant research accomplishments documented by publications in scientific literature. You are able to work independently, yet be a good team player. You are highly motivated, ambitious and driven to succeed. You are flexible and ready to work under the pressure of deadlines.

Applicants **at the PhD level** are required to have a university Master's degree in Chemistry, Physics or related discipline and a strong background in physical and theoretical chemistry paired with high motivation and curiosity. Experience with the above QM codes and/or Monte-Carlo or microkinetic modelling, or programming experience are not required but candidates with such experience will be given preference.

In the cover letter of your application, please explain in detail your specific interests and the experience that qualifies you for the position.

We offer

- Attractive remuneration (your salary is negotiable and will depend on your qualifications)
- A welcoming, dynamic international environment
- Work in a small team of enthusiastic researchers on intellectually challenging tasks
- Work with experts in the field
- Flexible working hours and various models to ensure the compatibility of family and career
- University of the Free State offers vibrant campus life and diverse recreational facilities

Bloemfontein is located in central South Africa and lies on the main road, rail and air links between north and south, east and west. It is a vibrant area but a peaceful place, perfect for those who love to feel that they are living a country lifestyle, but are still in a big city. The cost of living is among the most competitive in the country.

Useful websites

<https://www.ufs.ac.za/>

<https://www.ufs.ac.za/natagri/departments-and-divisions/chemistry-home>

<https://www.places.co.za/html/bloemfontein.html>

<https://www.expatistan.com/cost-of-living/bloemfontein?currency=EUR>

http://www.nagocat.uni-bremen.de/typo3_src-6.2.14/index.php?id=3

https://www.iapc.uni-bremen.de/baeumer/index.php?id=CV_LM&lang=de

<https://scholar.google.ca/citations?user=2b3wubQAAAAJ&hl=en>

How to apply

Please, send your cover letter, CV and a copy of transcript of records by email to Prof. Lyudmila Moskaleva, lyudmila.moskaleva@gmail.com

Only short-listed candidates will be contacted.