

## PHD POSITION IN THEORETICAL CHEMISTRY

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Company: VU Amsterdam

Location: Amsterdam

Category: computer-and-mathematical

Do you want to understand the physics that drives and controls chemical bonding and reactivity on the interface of surfaces? Are you interested in developing powerful and robust models to analyze these chemical phenomena? Then apply for this PhD position at Vrije Universiteit Amsterdam (VU).

**Location:** AMSTERDAM

**FTE:**1

### **Job description**

This project will focus on understanding the physical mechanisms governing chemical phenomena that take place on the interface of surfaces by using quantum chemical techniques. Theoretical studies devoted to surface chemistry are rapidly growing in the past decades due to the enormous advancement of computer technology. Nevertheless, the models used to study these chemical processes are, up to now, underdeveloped, hampering the ability to obtain the causality behind the observed chemical phenomena. This project aims to develop state-of-the-art models, rooted in Kohn-Sham density functional theory, to study chemical processes that take place at the interface of surfaces. These models will, in turn, be used to study a wide variety of chemistries occurring on surfaces, ranging from self-assembly of supramolecular polymers to heterogeneous catalysis.

### **Your duties**

Performing (periodic) density functional theory calculations

Developing and coding new models

Analyzing chemical processes on surfaces

Assisting in computational chemistry courses

Supervising B.Sc. and M.Sc. research projects

Attending national and international conferences

Writing scientific publications

### **Requirements**

We are looking for an outstanding, highly motivated, and creative candidate with the following qualifications:

Successfully completed an M.Sc. program in theoretical chemistry or a related field.

Experience in performing periodic density functional theory calculations.

Having a strong understanding of surface chemistry and band theory is a valuable advantage.

The ability to code proficiently in Python.

You have good writing skills and excellent communication skills.

### **What are we offering?**

A challenging position in a socially involved organization. The salary will be in accordance with university regulations for academic personnel and amounts €2,770 (PhD) per month during the first year and increases to €3,539 (PhD) per month during the fourth year, based on full-time employment. The job profile is based on the university job ranking system and is vacant for at least 1 FTE.

The appointment will initially be for 1 year. After a satisfactory evaluation of the initial appointment, the contract will be extended for a duration of 4 years. Additionally, Vrije Universiteit Amsterdam offers excellent fringe benefits and various schemes and regulations to promote a good work/life balance, such as:

a maximum of 41 days of annual leave based on full-time employment

8% holiday allowance and 8.3% end-of-year bonus

solid pension scheme (ABP)

possibility to save holiday hours, for sabbatical leave

child daycare facilities available on campus

## **About Vrije Universiteit Amsterdam**

The ambition of Vrije Universiteit Amsterdam is clear: to contribute to a better world through outstanding education and ground-breaking research. We strive to be a university where personal development and commitment to society play a leading role. A university where people from different disciplines and backgrounds collaborate to achieve innovations and to generate new knowledge. Our teaching and research encompass the entire spectrum of academic endeavor – from the humanities, the social sciences and the natural sciences through to the life sciences and the medical sciences.

Vrije Universiteit Amsterdam is home to more than 31,000 students. We employ over 5,000 individuals. The VU campus is easily accessible and located in the heart of Amsterdam's Zuidas district, a truly inspiring environment for teaching and research.

## **Diversity**

We are an inclusive university community. Diversity is one of our most important values. We believe that engaging in international activities and welcoming students and staff from a wide variety of backgrounds enhances the quality of our education and research. We are always looking for people who can enrich our world with their own unique perspectives and experiences.

## **The Faculty of Science**

Working at the Faculty of Science means working together with students, PhD candidates and scientists who are focused on their discipline, yet also have a broad view of the world. We are proud of the collegial working environment within the faculty, which is characterised by an ambitious and pragmatic attitude with commitment to the bigger picture. At the Faculty of Science, scientists and students work on fundamental and complex social issues for a sustainable and healthy future. From forest fires to big data, from obesity to malnutrition,

from genetics to pharmaceuticals and from molecules to the moon: our teaching and research cover the full breadth of the natural sciences. Scientific teaching and research is highly experimental, technical, computational and interdisciplinary in nature. This is why we collaborate extensively with leading research institutes and industry. The faculty has over 11,000 students studying across 40 educational programmes and employs over 1,600 staff spread over 10 scientific departments, making us the largest science faculty in the Netherlands.

### **About the department, institute, project**

You are part of the group within the Theoretical Chemistry (TC) division of the Chemistry and Pharmaceutical Sciences (CPS) department. The TheoCheM group offers a dynamic and interactional environment. Learn more about the dynamics of the TheoChem group . Our research spans from the development of new methods for computation chemistry, via the development of physical models for understanding and predicting structures and reactivity, to application to intriguing chemical and biological problems. The subgroup Predictive Surface Chemistry of Complex Systems is a new part of the TC division, where we study chemical processes at the interface of surfaces.

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