

The **Faculty of Science** and the **Leiden Institute of Chemistry** are looking for a **PhD student (1.0 fte)** for the research project entitled:

### **Multi-Scale Computational Insight in Precise Targeting of the Blood-Brain Barrier**

**Vacancy number:** (wordt door HRM ingevuld)

#### **Description of the project** (Max. 120 woorden in bullets of korte tekst)

A PhD position is available immediately in the Biophysical Organic Chemistry (BPOC) group at the Leiden Institute of Chemistry (LIC), for a cross-disciplinary project that is supervised by dr. Agur Sevink. The project is a collaboration between this group and the Supramolecular and Biomaterials Chemistry (SBC) group of prof. Alexander Kros, and aims at employing theory and modern multi-scale computational techniques for obtaining a deeper molecular understanding of the role of lipid structure and selective protein binding in the experimentally observed targeting of the blood-brain barrier (BBB) by binary liposomes with a very specific lipid composition.

Selective targeting of the BBB is an important topic in drug delivery research, owing to the poor affinity of many therapeutic drugs towards this barrier (giving rise to dosing issues and potentially leading to tissue damage) and the observation that a series of acceptors on the membrane render it an ideal target for selective drug delivery. The research in this project will focus on applying and extending coarse-grained/hybrid computational techniques for obtaining a deeper understanding of membrane binding and liposome structuring in terms of the lipid chemistry and composition, both by theory and by employing an efficient MD-SCF/MPCD computational method that was recently developed in the BPOC group and uniquely enables simulation of relevant liposomes with molecular resolution. The second aim is to obtain insight in the function of lipoprotein lipases (LPL) in binding to these liposomes and in their transport along the BBB.

The computational work will be performed in a synergetic feedback loop with experimental characterization activities that are already taking place in the SBC group, meaning that the candidate is expected to have good communication skills and basic knowledge of (physical organic) chemistry, apart from expertise in coding (C or C++, Python), modern computational modelling approaches and thermodynamics/statistical physics.

The BPOC group hosts experts in diverse topics in a vibrant intellectual environment, ranging from state-of-the-art computational techniques at the electronic (QM), atomistic (MM, MD) and coarse-grained (CGMD, DPD, SCFT) scales to experimental imaging and characterization techniques at a variety of length and time scales (with a focus on NMR). The shared goal is to uncover the fundamentals of key biophysical phenomena, with a clear focus on natural and artificial photosynthesis. The candidate will have to participate in teaching activities within the group and within the Chemistry curriculum at the LIC.

Starting date is open and the position will be filled once suitable candidates are found.

#### **Selection Criteria** (Max 120 woorden in bullets)

- We are looking for highly qualified and motivated graduates holding a master's degree (or equivalent) in chemistry, physics, engineering or related areas with excellent grades.
- Good communication skills and good to excellent proficiency in English.
- The candidate must have a keen interest in carrying research at the frontier of chemistry, physics and biology in a multidisciplinary environment, and should be able to work independently.
- The candidate should be strongly interested to expand their horizon beyond the specific field of their major and should have demonstrated an excellent educational track record.
- The candidate should have a strong computational background and preferably ample experience with coding in C/C++ and Python. Experience in molecular dynamics and/or modern coarse-grained methodologies is a plus.
- The PhD research needs to start before December 2018

## **Host institution**

Leiden University (LU) is ranked in the top 70 of leading Universities worldwide and belongs to the highest ranked European Universities. LU is the oldest university in the Netherlands, offering education to about 15,000 students in a wide range of studies. The faculty of science has currently 1044 employees and 4022 students and covers a broad range of disciplines such as Astronomy, Biology, Bio-pharmaceutical Science, Chemistry, Computer Science, Environmental Sciences, Mathematics and Physics.

## **Research at our faculty**

The Faculty of Science is a world-class faculty where staff and students work together in a dynamic international environment. It is a faculty where personal and academic development are top priorities. Our people are committed to expand fundamental knowledge by curiosity and to look beyond the borders of their own discipline; their aim is to benefit science, and to make a contribution to addressing the major societal challenges of the future.

The research carried out at the Faculty of Science is very diverse, ranging from mathematics, information science, astronomy, physics, chemistry and bio-pharmaceutical sciences to biology and environmental sciences. The research activities are organized in eight institutes. These institutes offer eight bachelor's and twelve master's programs. The faculty has grown strongly in recent years and now has more than 1,300 staff and almost 4,000 students. We are located at the heart of Leiden's Bio Science Park, one of Europe's biggest science parks, where university and business life come together.

The chemistry and life science research in the Leiden Institute of Chemistry (LIC) is organized around two major research areas: 'Chemical Biology' and 'Energy & Sustainability'. The institute's research themes illustrate the central position of chemistry between biology, medicine and physics. The various research topics carried out within these themes are ideal for executing interdisciplinary research.

For more information, see [www.universiteitleiden.nl/en/science](http://www.universiteitleiden.nl/en/science) and <http://workingat.leiden.edu/>

## **Terms and conditions**

We offer a full-time position for initially one year. After a positive evaluation of the progress of the thesis, personal capabilities and compatibility the appointment will be extended by a further three years. Salary range from [ Lian check nieuwe CAO ] gross per month (pay scale P in accordance with the Collective Labour Agreement for Dutch Universities).

Leiden University offers an attractive benefits package with additional holiday (8%) and end-of-year bonuses (8.3%), training and career development and sabbatical leave. Our individual choices model gives you some freedom to assemble your own set of terms and conditions. Candidates from outside The Netherlands may be eligible for a substantial tax break.

All our PhD students are embedded in the Leiden University Graduate School of Science [www.graduateschools.leidenuniv.nl](http://www.graduateschools.leidenuniv.nl). Our graduate school offers several PhD training courses at three levels: professional courses, skills training and personal effectiveness. In addition, advanced courses to deepen scientific knowledge are offered by the research school.

Leiden University is strongly committed to diversity within its community and especially welcomes applications from members of underrepresented groups. We particularly encourage women to apply.

## **Information**

If you have any questions about the procedure, please contact the HR adviser **Mrs. Eveline Castermans** ([e.castermans@science.leidenuniv.nl](mailto:e.castermans@science.leidenuniv.nl)), telephone: 071 5274189.

## **Applications**

For further information regarding the project and to apply for these positions, please send an email to

Dr. Agur Sevink (a.sevink[AT]chem.leidenuniv.nl)

Please ensure that you include in your application the vacancy number and the following additional documents:

- A cover letter explaining why you are interested in the position/research topic
- A recent Curriculum Vitae
- The letters of recommendation by 1 or 2 former supervisors
- The transcripts of your MSc studies

Only applications received **before June 30<sup>th</sup>, 2018** will be considered. The candidate can be appointed immediately if the conditions above are met.