

Faculty of Science and Engineering

Profile report: Tenure track assistant professor position in Computer-Aided Organic Synthesis (Computer-ondersteunde Organische Synthese)

- Discipline: *Organic Chemistry*
- Level: tenure-track Assistant professor
- Fte: Full time (1,0)

1. Scientific discipline

Computer-Aided Organic Synthesis is an emerging subfield of synthetic chemistry, in which computer-based approaches are used to develop strategies to identify design principles behind molecular reactivity, predict reactivities of individual molecules in different chemical environments, explore the landscape of potential reactions and to find the most promising synthesis pathways to complex molecules. These *in silico* approaches are complemented by lab work to implement these strategies experimentally and harness the added value of the computer-aided approach.

2. Vacancy

This position is opened by the Board of the Faculty of Science and Engineering in the context of the sector plans and will be embedded in the Stratingh Institute for Chemistry. The position falls within the framework of 'Career Paths in Science 4' ('Bèta's in Banen 4'). Please see link for [criteria and conditions](#).

3. Selection committee (BAC)

Prof. Dr. A.J. Minnaard, Director of the Stratingh Institute, Chair
Prof. Dr. S.R. Harutyunyan, Chair of the Board of the Stratingh Institute
Prof. Dr. W.R. Browne, Education Director of the Stratingh Institute
Prof. Dr. S. Otto, Stratingh Institute
Prof. J.G. Roelfes, Stratingh Institute
Dr. Anat Milo, Ben-Gurion University of the Negev
Andy Sardjan, MSc student
Added: L. Boomsma (HR) and Dr. Gaël Schaeffer, as advisors

4. Research area

Synthesis, the science of making molecules, is an essential part of chemistry. Being able to design, make, and therefore study molecules at will, addresses directly the overarching fundamental chemical enigma of how molecules react. However, i) classical physical organic molecular descriptors are not always adequate for addressing molecular reactivity and ii) the number of known reactions has increased so drastically in the last decades that the human brain is not able to handle all this information. Therefore, support from computational methods is needed to understand and predict reactivity in order to discover and optimize new synthetic pathways. This can be approached from various angles, such

as via a computational, statistical, automated and/or artificial intelligence approach in order to identify new strategies behind chemical design principles. The validation of this computer-aided approach by showing its added value in the synthesis of more complex molecules is a key step of the process, and experimental data acquired during the process can be used to refine the findings.

5. Embedding

The position will be embedded in the Stratingh Institute for Chemistry, where the candidate will be expected to contribute to its internationally leading research and education in organic chemistry. Depending on the profile of the candidate and her/his research interest, the position will be embedded in the base unit of Prof. Harutyunyan, or Prof. Otto.

The Stratingh Institute for Chemistry focuses on research in molecular and supramolecular chemistry, with overarching impact on biology, chemical engineering, and physics based on fundamental organic and inorganic chemistry. It covers three research areas:

- Chemistry of Life: this area concentrates on a molecular approach to the study of biological phenomena and medicinally relevant problems, including the synthesis of complex natural products, the design and synthesis of small molecules to study and steer biochemical and cellular processes, and emerging properties like self-organization and catalysis, including life itself.
- Chemical Conversion: this area investigates new synthesis and catalysis methods, including asymmetric catalysis and oxidation catalysis, designing artificial enzymes for new-to-nature reactions, the use of bio-based feedstock and development of sustainable processes, and homogeneous catalysis methods using earth-abundant metals.
- Chemistry of Materials: this area covers various topics in nanoscience with a focus on advanced functional materials, such as molecular switches and motors, photovoltaics, functional polymers, molecular electronics, supramolecular materials, functional surfaces and artificial membrane components.

6. Local and (inter)national position

The new independent group will closely cooperate with other groups in the Stratingh Institute (Minnaard, Harutyunyan, Otto, Feringa and others), and potentially groups from the Engineering and Technology Institute Groningen (ENTEG) or other research institutes from the Faculty of Science and Engineering.

The Stratingh Institute for Chemistry has built over the years an extensive collaboration network nationally and worldwide. Research groups within the Stratingh Institute take part in national research consortia, e.g., the Gravitation Program Functional Molecular Systems, the National Institute for Catalysis (NIOK), ARC-CBBC, the Origins Center, and in local research networks such as the CoFund program ALERT and the FOM-FOCUS group Organo Photovoltaics. The Stratingh Institute for Chemistry has a long tradition of cooperative projects with industry (DSM, Unilever, AKZO/NOBEL, Shell,

Solvay) and participates in many international projects (e.g. Harvard Univ., Univ. of Leuven, ECUST Shanghai, Nagoya Univ., EMPA Zurich, Univ. Bologna, Univ. Colorado, UCLA, Univ. Tokyo).

The Stratingh Institute for Chemistry has an (inter-)national excellent position in synthetic chemistry and catalysis in the Dutch chemical landscape, and is recognized as a stronghold for synthesis. Members of the Stratingh Institute were among the founding fathers of the national ARC-CBBC and recognized among the three hubs (Utrecht, heterogeneous catalysis; Eindhoven, chemical engineering; Groningen, synthesis, homogeneous catalysis, materials).

7. Expected contributions to research

The candidate is expected to build her/his own independent research group in the emerging field of organic chemistry supported by computer methods. The candidate and his/her team are expected to develop new tools or approaches to understand and predict molecular reactivity and/or molecular pathways, surpassing the knowledge of any organic chemist. Knowledge and skills in organic chemistry will allow this research group to prove experimentally the added value of the computer-aided approach and validate the results by synthesizing the compounds in the laboratory. Supervising PhD students and post-doctoral researchers, as well as obtaining substantial extramural funding is key to attaining the above objectives.

8. Expected contributions to teaching

The candidate will teach in the BSc Chemistry & Chemical Engineering and in the Master Chemistry. The candidate will contribute to teaching in the field of organic chemistry as well as computational methods relevant to this field. Supervision of bachelor and master students in their research projects is also part of the teaching contribution.

9. Expected contributions to the organization

The candidate is expected to have an active interest and to provide a positive contribution to the management and organizational tasks of the institute. At the level of the FSE, the candidate will contribute to the organization of the faculty, for example by participating in working groups and committees, in the fields of teaching, research and management. The candidate will participate in relevant national and international organizations.