University of Groningen
Faculty of Mathematics and Natural Sciences
Zernike Institute for Advanced Materials

Profile report: Theoretical Chemistry

Discipline: Chemistry
Level: Full/Associate professor
Fte: 1.0

1. Discipline/ In general

Theoretical chemistry is a broad discipline concerned with the development and application of theoretical methods for describing the properties of atoms, molecules and solids. The predictive and interpretative outcomes are complementary to experimental research results. The development of new methods and increasingly efficient computational schemes, combined with the enormous growth in computing power, has in recent years caused an enormous expansion of the field.

2. Vacancy

Theoretical Chemistry plays a central role in the Chemistry Department and in the Zernike Institute. This position concerns the new leader of the Theoretical Chemistry group.

3. Selection committee

- *Prof.dr. T.T.M. Palstra*, Solid State Chemistry and Director Zernike Institute (chair), t.t.m.palstra@rug.nl
- *Prof.dr. B. Noheda*, Nanostructures of Functional Oxides, b.noheda@rug.nl
- *Prof.dr. S.J. Marrink,* Molecular Dynamics and Member of the Zernike Institute Board, s.j.marrink@rug.nl
- *Prof.dr. P. Rudolf,* Surfaces and Thin Films and Director Graduate School of Science, p.rudolf@rug.nl
- *Prof.dr. R.C. Chiechi*, Chemistry of Molecular Materials and Devices, r.c.chiechi@rug.nl
- *Prof.dr. M. Scheffler*, Director Theory Department Fritz Haber Institute, scheffler@fhi-berlin.mpg.de
- *M. van Putten*, Student member
- *A. van der Woude*, Advisory member, Human Resources, a.m.van.der.woude@rug.nl
- *Dr. J.P. Birkner*, Advisory member, Scientific Coordinator Zernike Institute, j.p.birkner@rug.nl

4. Short description

Theoretical chemistry is a field with a rich tradition and becomes more and more important to predict, design and model the properties of molecules and materials. New efficient quantum theoretical methods and an enormous growth of computing power have caused theoretical chemistry to play an essential role in chemistry and nanoscience. Worldwide, we see increased interest in well-trained theoretical chemists. In Groningen, Theoretical Chemistry plays a central role in the chemistry department and in the Zernike Institute.

The Faculty and Zernike Institute recognize the importance of Theoretical Chemistry and have opened a position for a full professor who performs teaching and internationally leading research in *the development and application of theory to treat molecular systems - in gas, fluid and solid phases, in solutions and on supports*.

5. Developments in the discipline and external situation

The discipline

Theoretical chemistry is a broad discipline, concerned with the development and application of theoretical methods for describing the properties of atoms, molecules and solids, with the fundamental laws for motion of electrons and nuclei as a starting point. An important sub-discipline is quantum theoretical chemistry, which aims at first-principles predictions of the electronic structure of such systems. Initially, such studies have largely relied on wave function descriptions of the electronic structure, while later also density functional theory and Green function methods have been developed and used. Presently these methods are applied not only to investigate ground state properties but also for the study of excited states and dynamic properties. New methods, combined with the enormous growth in memory and speed of modern computers, have brought about a revolutionary expansion of the field. It has allowed for unprecedented accuracy in the computed energy level diagrams of small molecules, with relativistic and quantum electro-dynamical corrections included. Such calculations serve to benchmark the state-of-the-art-methods in this field.

The enormous progress mentioned has also enabled the field to tackle problems that involve larger (groups of) molecules, relevant to materials science and life sciences and to study the chemistry and physics of molecular systems in an environment, such as a solvent or a substrate. In addition, an increased activity exists in accounting for nuclear motion, quantum mechanically or classically. In the latter case, one combines quantum chemical approaches with molecular dynamics, an approach that is particularly valuable for reactivity in a solvent and for systems of biological origin, such as functional groups in proteins. New directions in the field include also the first-principles calculation of non-equilibrium properties, such as conductivity and charge separation. In Groningen this has recently become of particular interest due to the growing interest in functional materials, for example with respect to new developments in increasing the efficiency of solar energy systems.

External situation
Chemistry in The Netherlands has an excellent reputation as evidenced by several international rankings. A recent evaluation of chemistry research in the Netherlands placed a disproportionate number of overall excellent groups in Groningen. The National Science Foundation NWO considers research on the fundamental properties of materials of key-importance for enabling new technological developments. Therefore, Chemistry is selected as one of the NWO top-sectors. Furthermore, strong ties exist between academia and chemical industry. This has resulted in a new program supported by the Ministries of Education, Culture and Science and of Economy, Agriculture and Innovation, in which chemistry is recognized as one of the ten key technology areas (topsectoren).
Strong contacts exist between the groups that are active in the field of theoretical chemistry in the Netherlands. One of the most internationally visible sister groups in the field is hosted at the Free University Amsterdam (*L. Visscher/ F.M. Bickelhaupt)*, with research aimed at developing multi-level theories and methods for studying and designing molecules, nanostructures and materials. Theoretical chemistry research groups with a somewhat different focus are at Leiden University (*G-J. Kroes*; quantum dynamics of interactions of hydrogen and other small molecules with surfaces) and at the Radboud University Nijmegen (*G. Groenenboom*; dynamics of clusters and crystals of small molecules). After the retirement of the present associate professor at Utrecht University (*Van Lenthe*; Valence Bond theory and electronic structure studies of molecules and molecular complexes) the position will probably not be maintained. The Technical universities have no independent theoretical chemistry research groups, but strong researchers are embedded in larger programs. The U Twente hosts a Computational Materials Science group (*P.J. Kelly, G. Brocks*), with research focused on understanding the relationship between the chemical composition of condensed matter and the magnetic, optical, electrical, and mechanical properties.
The Groningen Theoretical Chemistry group has maintained an excellent reputation for more than forty years. Presently there are international research collaborations, with, for example, the Universities of Barcelona (*Sousa*), Brussels (*De Proft*), Düsseldorf (*Marian*), Kyoto (*Morokuma*), Leuven (*Nguyen* and *Pierloot*), Madrid (*Barandiaran and Seijo*), North Texas (*Bagus*), Oporto (*Ramos*), Perugia (*Lagana*), Sheffield (*Fowler*), Toulouse (*Guihery*) and Trieste (*Parmigiani* and *Stener*).

6. Research group, Chemistry Department and Zernike Institute
The current research interests within the Research Group are oriented towards the development and application of modern computational methods to describe molecules and solids with a focus on structure-property relations, electronic excitations, magnetic interactions and response properties. In this research the development of accurate but efficient *first principles* quantum chemical methods and computational schemes is combined with their application to timely, relevant problems. The group is also well-known for its pioneering work in combining the accurate treatments of electron correlation and relativistic effects.
Prof. R. Broer focuses her research on the treatment of systems with strong electron correlation effects, such as transition metal compounds. Prof. Broer is expected to retire in 2016. *Prof. C. de Graaf* is appointed as honorary professor (0.1 FTE), to study materials in which spins have a fundamental influence on the physical and chemical properties. The TC group in Groningen distinguishes itself from most other TC groups through the intensive collaborations with a variety of other experimental and theoretical groups within the Zernike Institute and the Chemistry Department

on the design and characterization of (multi)functional materials.
At present, the TC group is, together with the groups "Chemistry of (Bio)Molecular Materials" and "Devices and Photophysics and Opto-Electronics" responsible for the FOM Focus Programme "Next Generation Organic Photovoltaics", to deliver the science for highly efficient, long-lived, and low-cost organic photovoltaic devices. The FOM Focus programme was started within the Zernike Institute under the directorship of *Prof. J.C. Hummelen* in 2011 and will run until at least 2021.
Closely related theoretical and computational research within the Zernike Institute is performed by (i) *Prof. R.A. de Groot*, who specializes in band-structure calculations and holds a honorary professorship in the group Solid State Materials for Electronics, (ii) the group Theory of Condensed Matter headed by *Prof. J. Knoester* and (iii) the Molecular Dynamics group headed by *Prof. S.-J. Marrink*.
The Chemistry Department of the Groningen University is world-leading, as shown by a recent evaluation of chemistry groups in the Netherlands, where overall excellence was recognized in the fields of organic chemistry, biochemistry, polymer chemistry and solid state chemistry.
The interdisciplinary Zernike Institute for Advanced Materials is one of the six top research schools in The Netherlands (selected by the Netherlands Organization for Scientific Research, NWO) and is supported financially by the Netherlands Ministry of Education, Culture and Science under the Bonus Incentive Scheme ("Center-of-Excellence Programme"). It is a combination of physics and chemistry research groups of the Zernike Institute proper, the Stratingh Institute for Chemistry and the Groningen Biomolecular and Biotechnology Institute. Recently, the Ministry of Education, Culture and Science has extended this status for the institute for the coming years.
Within the institute 21 groups from physics, chemistry and biology collaborate on two focus areas of research:
- Biomolecular and bioinspired functionality
- Advanced materials for electromagnetic functionality
The Zernike Institute focuses on curiosity-driven science and covers all aspects from synthesis to building of materials and devices, and characterization, both in experiment and theory. The institute has extensive infrastructure for preparation and characterization of organic, bioorganic and hybrid nanoparticle systems including the nanolab.
In-house collaborations:
In recent years collaborative work was done with the following partners:
a. *Prof. J.C. Hummelen, Dr. R.C. Chiechi*, design and evaluation of new molecular systems and materials for molecular photovoltaics;
b. *Dr. W.R. Brown, Prof. B.L. Feringa, Prof. P. Rudolf,* design and study of new catalysts and molecular switches and motors;
c. *Prof. M.A. Loi* organic semiconductors, organic/inorganic hybrid systems and their application in optoelectronic devices;
d. *Prof.P. Rudolf, Prof. T.T.M. Palstra, Prof. B. Noheda and Prof. R.A. de Groot*, organic/inorganic hybrid systems;
e. *Prof. S.-J. Marrink, Dr. A.H. de Vries,* molecular dynamics of biological and organic systems;
f. *Dr. T.L.C. Jansen and Prof. M. Mostovoy,* theoretical models of many-particle excitations and magnetic properties of oxides.

7. Expected contributions to teaching
The candidate is expected to contribute to the chemistry-related BSc and MSc

programmes. This includes the Top Master Programme Nanoscience of the Zernike Institute. Outreach activities form an important component of the activities of the scientific staff of the faculty.
The Theoretical Chemistry group participates in the Erasmus Mundus Master Programme in Theoretical Chemistry and Computational Modeling (TCCM). The other participants are Universidad Autónoma de Madrid (coordinator); Universidad de Valencia; Catholic University Leuven; Università degli Studi de Perugia; Université Toulouse III Paul Sabatier; Universidade do Porto.
He/she will also be actively involved in teaching and in the development of new courses for these programmes. Furthermore, the candidate will be involved in supervising master and PhD students.
An important aim for the coming years is to develop an Erasmus Mundus Doctorate Programme in Theoretical Chemistry and Computational Modeling, through a collaborative effort with thirteen European sister groups.

8. Expected contributions to research
The candidate is expected to develop a world leading research programme in theoretical chemistry with special focus on the development and application of theory to treat molecular systems - in gas, fluid and solid phases, in solution and on supports. The research is also expected to cross-fertilize the existing research within and between the research groups and should lead to a strengthening of the international reputation of the group and the institute.
Obtaining substantial external funding is thereby crucial. The main national sources for funding of research in theoretical chemistry are administered by the Netherlands Organization for Scientific Research (NWO), through their Chemical (CW) and Physical (FOM) Divisions. Cooperation with industry is encouraged, especially in the framework of NWO TOP-sector research programmes. International funding sources, such as the ERC abd Framework Programmes (FP7, Horizon 2020) administered by the European Union, play an increasingly important role.

9. Expected contributions to the organization
It is expected that the chair holder plays an active role in the general organization of research on the national and international level and within the faculty and the institute. Contributions to the organization of existing and new teaching programmes are also expected.

10. Career perspective
The position will be offered as full or associate professorship. The appointment level will be based on the previous performance and experience of the candidate. He/she will be the anticipated leader of the Theoretical Chemistry research group.