

## Faculty of Science and Engineering

**Profile report:** Multiscale modelling of multifunctional supramolecular materials  
(Multischaal modelleren van multifunctionele supramoleculaire materialen)

- Discipline: Computational Physics/Materials Science, Mechanical Engineering
- Level: tenure-track Assistant professor
- Fte: Full time (1,0)

### 1. Scientific discipline

Development of bio-inspired supramolecular and hybrid (nano-)materials is attracting much interest. Currently, there is a need for multiscale modelling techniques to (i) steer further development of hybrid and supramolecular materials towards target properties and to (ii) provide quantitative tools that will allow the full potential of these materials to be used in (bio-/medical-) engineering design. Such bottom-up hierarchical models will relate the macroscopic behaviour of supramolecular polymers to their structure at molecular and relevant mesoscopic levels.

### 2. Vacancy

This position is opened by the Board of the Faculty in the context of the sector plans and will be embedded in the Zernike Institute for Advanced Materials, research unit Micromechanics. 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.ir. C.H. van der Wal, scientific director of the Zernike Institute for Advanced Materials and professor Physics of Quantum Devices (Chair)  
Prof.dr. M. Kamperman, professor Polymer Science  
Prof.dr.ir. E. van der Giessen, professor Micromechanics  
Prof.dr.ir. P.R. Onck, Deputy director Physics/Applied Physics Masters education and professor Micromechanics of Cellular and Active Materials (Teaching)  
Prof.dr.ir. J.M.A. Scherpen, professor Discrete Technology and Production Automation  
Prof.dr. C. Storm, Theory of Polymers and Soft Matter (TU Eindhoven)  
Student member

Prof.dr. S.J. Marrink, (advisor, professor Molecular Dynamics)  
Dr. J.P. Birkner (advisor, Research Manager Zernike Institute)  
Ms. A. van der Woude (advisor, Human Resources)

### 4. Research area

Inspired by biomaterials, researchers of the Zernike Institute for Advanced Materials and associated institutes in Groningen have achieved breakthroughs in the development of supramolecular materials, while also hybrid nanomaterials are attracting much

interest in view of their potential applications in various branches of engineering. Both new classes of materials out-perform current materials in terms of multi-functionality and sustainability. Supramolecular polymers combine extreme deformability with high strength and self-healing abilities, and can readily be endowed with multiphysics actuation and sensing properties. Hybrid nanomaterials allow for extreme fine-tuning of the material nanostructure and therefore their properties, while offering unprecedented opportunities in interfacing with biomaterials and –systems. While modelling has so far essentially provided qualitative guidelines for material design, exploiting the full potential of these materials relies on quantitative, predictive models. Because of the vast difference between the internal material nanostructure and the macroscopic scale of engineering applications, these models have to be multiscale and to be able to connect emergent behavior at several scales. The models will also have to meet the ever-increasing requirements on quantitative lifetime predictability for engineering applications.

### **5. Embedding: institute (and base unit)**

The position will be embedded within the research unit Micromechanics at the Zernike Institute for Advanced Materials and strongly link to various education and research programmes, including Applied Physics, Biomedical Engineering and the new Mechanical Engineering programme.

The mission of the Zernike Institute for Advanced Materials lies in focused, curiosity-driven, symbiotic studies of functional materials involving researchers from physics, chemistry and bio-nanosciences. The Zernike Institute's main driving force is the desire to understand how things work at the microscopic level, i.e. the atomic and molecular scale. This is the realm of nanoscience and nanotechnology. In this field, the Zernike Institute for Advanced Materials covers the whole chain from synthesizing materials, building devices, characterizing materials and devices, and investigating the theoretical foundation of their properties. The institute performs interdisciplinary research with other Institutes of the Faculty of Science and Engineering and with the UMCG. The Berendsen Center for Multiscale modelling and Materials Design combines various theoretical and computational groups within the Zernike Institute, with the aim to establish high-throughput modelling platforms for design of advanced materials.

The research unit Micromechanics, participating in the Berendsen Center, is led by Profs. Van der Giessen and Onck. The group has ample experience with continuum modelling of polymers, mesoscopic biopolymer network models, as well as with atomistic and coarse-grained molecular dynamics of biopolymers. The research unit comprises around 10 PhD students and is supported by a system administrator and a secretary.

### **6. Local and (inter)national position**

The position is created to strengthen the Faculties profile in technology especially with respect to mechanical engineering. It connects research on multiscale modelling and on fundamental polymer science (Zernike Institute) with applications in biomedical engineering (Kolff Institute) and soft robotics (ENTEG). The focus of the position may open

further collaborative avenues with other institutes of the Faculty of Science and Engineering (e.g. GBB, Stratingh) and the medical faculty (UMCG, GRIP).

In the Netherlands complementary fundamental chemistry research on supramolecular materials is carried out at Eindhoven University of Technology, but the step of using multiscale modelling for the improved design of such materials for multifunctional engineering applications is not yet taken there.

Also internationally, there is much interest in the chemistry of supramolecular and hybrid nanomaterials, as evidenced by many papers on the topic in top-quality journals, but the next step to materials design for targeted applications is in its infancy. Examples of similar multiscale modelling research can currently be found in less than a dozen institutes, including MIT, National University of Singapore and Leibniz Institute Dresden.

### **7. Expected contributions to research**

The candidate is expected to initiate and develop his/her own research program in the field of Multiscale modelling of multifunctional supramolecular materials. She/he is expected to interact closely with experimental materials chemists and physicists for the synthesis of new materials, as well as with researchers in relevant application areas, such as biomaterials for biomedical applications and soft robotics.

The research should have a visibility both at the national and the international level and lead to scientific publications. The research is expected to cross-fertilize the existing research within the Zernike Institute, the Kolff Institute (UMCG) and ENTEG.

Obtaining substantial external funding is crucial. Supervision of PhD students is an important part of the research activities. The research is expected to strengthen the existing efforts within the Zernike Institute and ENTEG in the field of Multiscale modelling of multifunctional supramolecular materials and to take an international leadership role.

### **8. Expected contributions to teaching**

The candidate is expected to teach at the bachelor and master level and to contribute to the Topmaster program in Nanoscience organized by the Zernike Institute. She/he is expected to participate in the teaching program of specialized courses in relation to Multiscale modelling of multifunctional supramolecular materials and other related topics. Furthermore, the candidate will be involved in supervising bachelor, master and PhD students.

### **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.