PhD

EINDHOVEN UNIVERSITY OF TECHNOLOGY

VACANCY COVERSHEET

Vacancy holder:	prof.dr. A. Lyulin, SMB group, APSE, TUe
Position category:	PhD
Irène Curie:	No
Beethoven:	No
Recruitment Group:	A. V. (Alexey) Lyulin, SMB, APSE, TU/e H. (Heiner) Friedrich, SPC, C&CE, TU/e H.P. (Henk) Huinink, TPM, APSE, TU/e B.J. (Bernard) Geurts, 3MS, EEMCS-AM, U Twente W.A.M. (Helmi) van Lieshout, SMB, APSE, TU/e
Working hours:	Fulltime
Type of employment:	Temporary position
Experience level:	Mid-senior level
Number of positions:	1

Pre-selection questions:

1. **I am currently an employee of Eindhoven University of Technology**
    - Yes
    - No

2. **Can you confirm that you do not hold any formal position, collaboration, or other affiliation with staff members of sanctioned universities, institutes, or research centers: EU sanctions regime? If you can confirm this, please click 'yes'.**
    - Yes (Desired/Qualified response)
    - No

PhD position
on Multiscale Modelling of Recycled Wax for Sustainable Thermal Storage (RecyWax+)

Short Description

To heat our houses and offices with a lower carbon footprint, efficient and low-cost heat storage solutions such as organic phase change materials (PCM) hold great promise. To design efficient and low-cost PCM composites the **RecyWax+** project combines multi-physics modelling approaches and physical experimentation of the thermal properties of the PCM composite. Throughout, theory is validated by synthesis and assembly of concrete PCMs. **RecyWax+** offers a PhD position for molecular-dynamics simulations of novel PCM systems for thermal storage.

Job Description

Recywax+ is supported within the Dutch Research Council NWO OTP programme, and is led by profs. **Alexey Lyulin**, **Heiner Friedrich** and **Henk Huinink** (all TU/e) and prof. **Bernard Geurts** (U Twente). The project explores how waste products can be turned into a sustainable battery for thermal storage. The idea is to combine waxes obtained through pyrolysis of plastic waste streams, with ultra-conductive graphene networks, i.e., nanometer sized carbon platelets that transport heat at tremendous conductivity. This creates a compact and efficient system for thermal energy storage, exploiting phase transition to store thermal energy in terms of an increased temperature, as well as a reversible change of phase from solid to liquid. Think of it as a heat battery that charges and discharges similarly to a regular battery, but with heat instead of electricity.
Recywax+ aims to develop the next generation of PCM composites extracted from upcycled polymer pyrolysis waste streams and thermally conductive fillers. In this PhD project we adopt a molecular modelling approach with which we address the following steps/questions:

- Characterize the molecular structure and molecular distribution of suitable polymer pyrolysis waste streams to aid modelling of filler-matrix interfaces;
- Modeling (using Gromacs and LAMMPS software packages and MARTINI-like upscaling) the filler-matrix interfaces to optimize thermal transport, e.g., by functionalization of the nanofiller surface;
- Simulate and advise on the ideal filler-filler contacts and filler-matrix interface structure; this interface should be such that the fillers are finely dispersed in the matrix, yet still enabling good filler-filler contacts;
- Connect sub-micron, atomistic properties of the interface to macroscopic network scales, predict thermal conductivity, and develop practical strategies to drastically increase thermal conductivity;

Job Requirements

Talented, enthusiastic candidates with strong simulation and/or experimentation interests and research-oriented attitude holding a university degree (M.Sc.) in (Theoretical) Physics, Applied Mathematics, Mechanical Engineering, Materials Science, Scientific Computing, Physical Chemistry, Polymer physics or a closely related discipline are encouraged to apply. Preferably, the candidate has been studying any of these topics: statistical physics, computer simulation methods, and polymer physics. Proficiency in the C++ and/or Python programming language is an advantage. Good knowledge of spoken and written English (C1 level) is an essential asset. The candidate should also be motivated to develop his/her own teaching skills and coach students in their MSc program.

Conditions of Employment

We offer a meaningful job at a dynamic and ambitious university, in an interdisciplinary setting and within an international network. You will work on a beautiful, green campus within walking distance of the central train station of Eindhoven. We offer you:

- Full-time employment for four years, with an intermediate evaluation (go/no-go) after nine months. You will spend 10% of your employment on teaching tasks.
- Salary and benefits (such as a pension scheme, paid pregnancy and maternity leave, partially paid parental leave) in accordance with the Collective Labour Agreement for Dutch Universities, scale P.
- A year-end bonus of 8.3% and annual vacation pay of 8%.
- High-quality training programs and other support to grow into a self-aware, independent scientific researcher. At TU/e we challenge you to take charge of your own learning process.
- An excellent technical infrastructure, on-campus children's day care and sports facilities.
- An allowance for commuting, working from home, and covering internet costs.
- A Staff Immigration Team and a tax compensation scheme (the 30% facility) for international candidates.

Information and application

About us

Eindhoven University of Technology is an internationally top-ranking university in the Netherlands that combines scientific curiosity with a hands-on attitude. Our spirit of collaboration translates into an open culture and a top position in collaborating with advanced industries. Fundamental knowledge enables us to design solutions for the highly complex problems of today and tomorrow.

Information

Additional information can be obtained by contacting prof. A. Lyulin, a.v.lyulin@tue.nl and Prof. H. Friedrich, H.Friedrich@tue.nl.
Do you recognize yourself in this profile and would you like to know more? Visit our website for more information about the application process or the conditions of employment. Are you inspired and would you like to know more about working at TU/e? Please visit our career page.

Application

We invite you to submit a complete application by using the apply button. The application should include a:
- Cover letter in which you describe your motivation and qualifications for the position.
- Curriculum vitae, including a list of courses you completed, a brief sketch of your graduation project, and the contact information of three references.

We look forward to receiving your application and will screen it as soon as possible. The vacancy will remain open until the position is filled.