

## PhD Project

### Wax<sup>+</sup>: Nanofiller-enhanced wax for heat storage

#### Project description:

A PhD position in the Center for Computational Energy Research (CCER), <https://www.ccer.nl/>, of the Eindhoven University of Technology is available with funding from the Open Technology Program (OTP) of Netherlands Organisation for Scientific Research (NWO). In the Netherlands, like in many countries, natural gas is extremely important for heating. However, with society shifting away from fossil fuels, sustainable materials for heating systems are essential. For example, organic Phase Change Materials (PCMs) such as paraffin wax can absorb and release heat during phase changes. Although these materials are promising, widespread application is limited by their low thermal conductivity. The project aims to increase it, using theoretical modelling and physical and chemical experimentation. The Wax<sup>+</sup> research team is made up of a number of CCER researchers and is supported by contributions from industrial partners such as Bosch, TNO-ECN, Nanocyl, and MDP Srl.

#### Aim of the PhD project:

The PhD project aims to computationally develop new nanofilled-waxes that can be used in future heat storage systems. Using classical and quantum-mechanical molecular dynamics modelling and DFT calculations, the PhD candidate will perform detailed simulations of the nanofiller network formation in paraffin melts and investigate its role in enhancing the overall heat transfer. Model parameters for the coarsened descriptions of the heat transfer will be extracted from these simulations, thereby creating a coherent multiscale approach.

#### Qualifications of applicant:

Talented, enthusiastic candidates with strong simulational skills holding a university degree (M.Sc.) in (Theoretical) Physics, Mechanical Engineering, Materials Science, Scientific Computing, or a closely related discipline are encouraged to apply. Preferably, the candidate has been exposed to any of these topics: statistical physics, computer simulation methods, and polymer physics. Proficiency in the C++ programming language is an advantage. Good knowledge of spoken and written English is an essential asset.

#### Appointment details:

We offer a full-time, four-year PhD position at a dynamic and ambitious university, with an immediate starting date. The project will be carried out in close collaboration with the Theory of Polymers and Soft Matter, Materials and Interface Chemistry, Transport in Permeable Matter, Molecular Materials and Nanosystems groups at Eindhoven University of Technology, and Multiscale Modelling and Simulation group at the University of Twente, the Netherlands. The candidate will collaborate closely with the industrial partners of the project. More information about this PhD position can be obtained from dr. Alexey Lyulin [a.v.lyulin@tue.nl](mailto:a.v.lyulin@tue.nl), tel. +31 (0) 40-247-4253. Application documents (pdf only) should be sent by email, including a letter of application, a short description of scientific/work experience, a full curriculum vitae, transcripts of B.Sc. and M.Sc. degrees, and contact information of two potential referees.