

Project 4.3. Multiscale Simulation of spontaneous liquid motion on nanopatterned substrates (theoretical)

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Background:

Novel developments in experimental nanopatterning have enabled the design of substrates that can steer the motion of liquids, which is crucial for many applications, such as microfluidics, coatings, self-cleaning, self-healing, etc. The effects characterizing this kind of fluid motion on nanopatterned substrates are tiny and therefore can be captured by computer simulation. Thanks to the acquired knowledge in these phenomena at the microscopic scale, the creation of novel technological solutions of improved functionality and efficiency nanodevices will become possible.

Aim:

Our project will provide insight into the microscopic nature of liquids spontaneous motion on nanopatterned substrates. The planned research tasks in the frame of an OPUS NCN project will involve molecular dynamics (MD) simulation to investigate such motion as a function of liquid and substrate properties. The PhD student will work closely with other researchers in the group and will also have the opportunity to interact with the European consortium ThermaSMART (<https://thermasmart.eng.ed.ac.uk>) exploiting further opportunities. In addition to performing MD simulations, the student will also have an opportunity to learn the basics of mean-field theoretical methods through an international collaboration already established with the University of Virginia, with a possibility of brief visits to the USA, where this training will be performed.

Requirements:

- Master's degree in Natural Sciences or Engineering
- good knowledge of a programming language (e.g. Python, C++)
- good analytical skills
- experience in simulation or numerical work. Experience with molecular dynamics simulation is a plus.
- ability to work as a team and effectively communicate.

Funding:

Scholarship from an NCN grant with funding of 5000 PLN per month, before subtracting obligatory employer and employee social security contributions. For 48 months.

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