

Centre Européen de Calcul Atomique et Moléculaire  
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In the context of the EU H2020 project FET NANOPHLOW we are seeking 4 highly qualified post-doctoral researchers for an exciting collaborative project on the fundamental challenges of thermodynamic gradient driven transport.

Increasingly, modern technology is addressing problems where fluid transport takes place in submicron sized channels, or in pores. The physical laws of transport in such channels are qualitatively different from those that determine bulk flow; they are poorly understood and, importantly, barely exploited. The aim of NANOPHLOW is to lay the basis for an entire novel technology where thermal gradients and concentration gradients along nano-sized channels are harnessed to drive devices that have no equivalent on the macroscopic scale. Such gradient-driven surface flows offer a huge scope for fundamental advances with very significant technological implications.

The postdoctoral positions will address complementary aspects related to the fundamental challenges of thermodynamic driving. The broad, theoretical approach will provide a systematic way to go beyond the state-of-the-art macroscopic descriptions of phoresis to capture the effects of the molecular nature of solvent and solute, solute size, solute and surface specificity, solute flexibility, surface wettability and heterogeneity, fluctuations and correlations.

The projects will be carried out under the supervision of Prof. I. Pagonabarraga (Univ. Barcelona), B. Rotenberg (Sorbonne Univ., Paris), E. Trizac (Univ. Paris-Sud, Orsay), and R. van Roij (Univ. of Utrecht). Specifically:

1. The work in Barcelona will focus on the development and use of mesoscopic computational models to study the transport and rectification of soft matter and of biomolecules under strong confinement. The project will address the role of entropic transport and of capillarity in nanoscale transport mechanisms. Please contact prof I. Pagonabarraga ([ipagonabarraga@ub.edu](mailto:ipagonabarraga@ub.edu)) for more information and applications.
2. The work in Sorbonne Université will focus on molecular aspects, to address surface- and fluid-specific effects on the flows induced by thermodynamic gradients at solid-liquid interfaces. This includes the development of molecular simulation strategies to evaluate osmotic flows, as well as the study of systems investigated experimentally within the NANOPHLOW consortium, such as flow through nanotubes. Please contact B. Rotenberg ([benjamin.rotenberg@sorbonne-universite.fr](mailto:benjamin.rotenberg@sorbonne-universite.fr)) for more information and applications.

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3. The work at Paris-Sud University will be analytically oriented, with possible computational aspects depending on taste, targeting the study of thermodynamic-gradient-driven phenomena. Charged as well as neutral systems will be investigated. Please contact prof. E. Trizac ([emmanuel.trizac@lptms.u-psud.fr](mailto:emmanuel.trizac@lptms.u-psud.fr)) for more information and applications.
4. The work in Utrecht will be largely based on the development of (dynamic) density functional theory for phoretic and osmotic transport through nanostructures as well as on the numerical calculation of solutions to the resulting Poisson-Nernst-Planck-Stokes-type equations of motion, where connection is to be made with ongoing experiments in the "Nanophlow" consortium. Please contact prof. R. van Roij ([r.vanroij@uu.nl](mailto:r.vanroij@uu.nl)) for more information and applications.

The project is strongly collaborative. The research activities will be carried out by the researchers at the institution their contract will be associated with: Univ. Sorbonne, Univ. Paris-Sud, Univ. Utrecht, Univ. Barcelona, but will also involve strong and frequent contact with the rest of the NANOPHLOW partners, which include two small and medium enterprises.

We seek motivated researchers, with theoretical and computational expertise.

Candidates should have a background in computer simulation (atomistic MD, coarse-grained MD), statistical mechanics, biophysics or soft condensed matter.

Candidates with an appropriate background, who are interested in a cutting-edge research at the interface between physics and the biological sciences, are invited to apply.

Postdoctoral positions are for a period of two years, with starting date as soon as possible, and in any case before Jan 2019

Positions will be filled as we identify suitable candidates.

Interested candidates can apply by sending their CV (including publication list) and a short research statement (with plans and motivations) by email to the PI of their interest in Barcelona, Paris, and/or Utrecht with subject: "Application Nanophlow".

Multiple applications are allowed.

Please help us distribute this announcement.

Best regards,

Ignacio Pagonabarraga, Benjamin Rotenberg, Emmanuel Trizac and René van Roij