Nanopore based devices have been revolutionizing several key-applications such as energy harvesting [1], water treatment and biosensing [2]. Technological advancements are hindered by our lack of control and understanding of the coupling between hydrodynamics, electrokinetics and chemical effects that govern the mass and charge motion at nanoscale. An additional challenge is the nanometric scale of the pore that raises questions on the validity of standard continuum hydrodynamic models.

In this framework, atomistic simulation constitutes a powerful tool to get information on the nanoscale dynamics. Presently, we are working on atomistic models of a single nanopore under aimed at understanding the complex interplay between surface charge, pore shape and ionic concentration [3]. These simulations are expected to provide an unprecedented picture of the process that will allow to set the range of validity of existing theories and, in case, stimulate the development of nanoscale corrections.

References