Patrick Senet
Maria Daniela Barrios Perez, Patrice Delarue, Vincent Meunier*, Adrien Nicolaï
Laboratoire Interdisciplinaire Carnot de Bourgogne UMR 6303 CNRS-Université de Bourgogne Franche-Comté, 9 Avenue Alain Savary, BP 47870, F-21078 Dijon Cedex, France

*Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, 110 8th street, Troy, NY 12180, USA.

psenet@u-bourgogne.fr

Monitoring the translocation of single polypeptides through MoS_2 nanopores from ionic current fluctuations, lessons from all-atom molecular dynamics simulations

Solid-state nanopores (SSN) have emerged as versatile devices for single-molecule biomolecule detection and sequencing [1]. SSNs offer promises as high-rate and low cost sequencing devices of DNA and proteins with potential applications for early diagnosis of diseases. The idea behind nanopores sequencing is based on experimental ultrafast monitoring of the ionic current through nanometer-sized channels [2]. Because the channel conductance of the ionic flow through nanopores scales inversely with the membrane thickness, few-atoms thick materials are ideal candidates with an expected high signal-to-noise ratio [3]. Beyond graphene, transition metal dichalcogenides such as molybdenum disulfide (MoS_2) are potentially advantageous due to their rich optoelectronic and mechanical properties. This study reports the results of all-atom molecular dynamics simulations that investigate the feasibility of using MoS_2 nanopores for protein sequencing. First, we investigate the dynamics of KCl ions through MoS_2 nanopores using non-equilibrium molecular dynamics (NEMD) simulations. MoS_2 nanopores with different diameters, from 1.0 to 3.0 nm and nanoporous membranes with different thicknesses, from single-layer to trilayers MoS_2 are studied. We provide open pore benchmark signals and new models for ionic conductance of such devices for further translocation simulations/experiments [4]. Second, we investigate uding NEMD simulations the translocation of model peptides in the presence of an electric field. The aim is to estimate the performances of MoS_2 nanopores for protein sequencing applications.

References

[1] C. Dekker, Nat. Nanotechnol., 2 (2007) 209–215
[2] J. K. Rosenstein, M. Wanunu, C. A. Merchant, M. Drndic , K. L. Shepard, Nat. Methods, 9 (2012) 487–492
[3] H. Arjmandi-Tash, L. Belyaeva and G. Schneider, Chem. Soc. Rev., 45 (2016) 476–493
[4] M. D. Barrios Perez, P. Senet, V. Meunier, A. Nicolaï, 16 (2017) 35-44