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Hydrophobic gating in a model nanopore : from Molecular Dynamics simulations to Coarse Grained models

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Depending on their geometry and surface chemistry, hydrophobic nanopores may exist in a wet state in which water molecules fill the pore, or in a dry state in which a vapor bubble nucleates inside the pore [1]. Although the nanopore may remain for a long time in one of the states, the transition is very fast (<1ns), it is reversible and thermally activated. The transport processes across the pore are highly affected by its wetting. This is particularly relevant for electric conduction, as translocation of charged species is energetically unfavorable in the dry state, giving rise to an on/off signal modulated by the presence of a bubble. This phenomena is known as hydrophobic gating and plays a crucial role in several biological channels [2], as well as in solid state nanopore devices [3].

We studied a model hydrophobic nanopore in a 0.5M NaCl solution using Molecular Dynamics (MD) to compute the free energy and the diffusivity of the system [4] as a function of two variables: the axial position of a tagged ion, and the number of water molecules filling the pore. This approach revealed the existence of two stable states (wet and dry), and of a large free energy barrier for the ion translocation in the dry state, which is dramatically reduced in the wet state. Based on the results of the MD simulations, Coarse Grained (CG) Langevin simulations were used to compute the filling dependent pore conductivity and the rates of the drying/wetting transitions which involved timescales difficult to reach with MD simulations (~0.1s).

These results suggest that our system can be used as a proxy for the study hydrophobic gating in extreme confinement. The CG simulations can be used to study the kinetics of hydrophobic gating in more complex solid state or biological nanopores, possibly bridging the gap between the timescales of all-atom simulations and experiments.

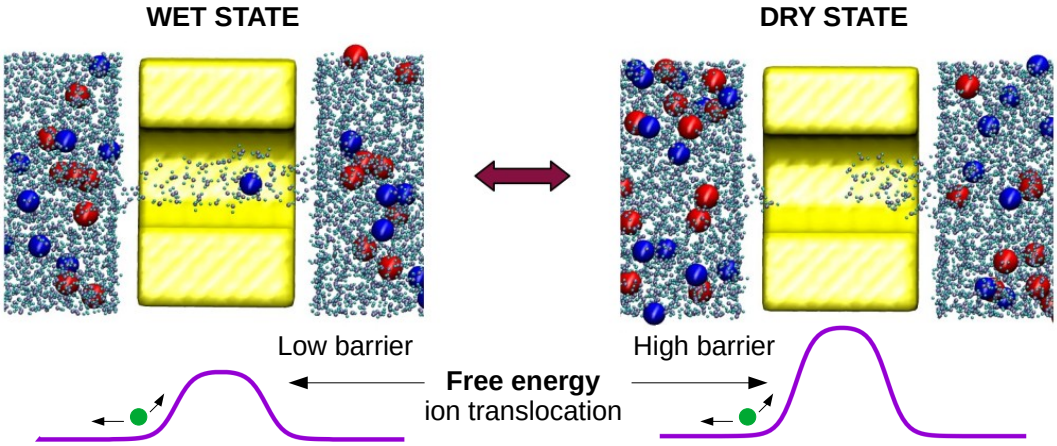

Figure: Coarse grained model of hydrophobic gating in terms of diffusion on a free energy landscape

[1] A.Tinti et al., PNAS (2017)
[2] P. Aryal et al., J. Mol. Biol. (2015)
[3] M.R. Powell et al., Nat. Nanotechnol. (2011)
[4] F. Zhu and G. Hummer, J. Chem. Theory Comput. (2012)

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