

Ionic conductance and selectivity of hydrophobic nanopores

Leonhard M. Henkes,¹ Martin Urban,¹ Florian Mrugalla,¹ Serena Smeazzetto,²
Gerhard Thiel,³ Stefan M. Kast¹

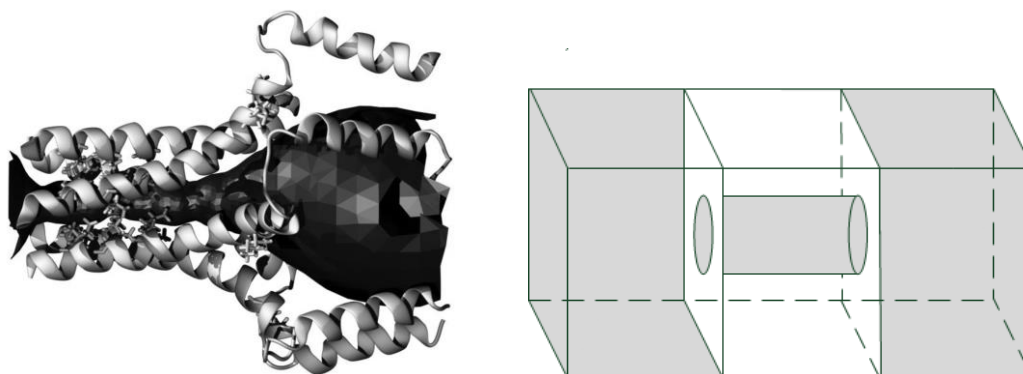
¹*Physikalische Chemie III, TU Dortmund, D-44227 Dortmund, Germany*

²*Dipartimento di Chimica, Università di Firenze, I-50019 Sesto Fiorentino, Italy*

³*Fachbereich Biologie, TU Darmstadt, D-64287 Darmstadt, Germany*

Over the last years various hydrophobic pores with selectivity features were identified, including ion channels. [1-3] Yet the origin of their intrinsic ion discrimination is still not understood, while properties such as overall pore geometry, chemical detail of the interior, or wall charges all play a role for modulating ion conductance. One controversially discussed example of a hydrophobic nanopore that exhibits ion channel properties is the pentameric membrane protein phospholamban (PLN) [4], for which available structures reveal a narrow constriction that is only slightly larger than the diameter of passing ions. [5]

Here we apply three-dimensional reference interaction site model (3D RISM) integral equation theory for deriving the relevant free energy surface governing ion translocation, the potential of mean force (PMF) at finite electrolyte concentration. Combined with an expression connecting the equilibrium PMF with ion conductance [3] we obtain selectivity orders in agreement with experimentally measured values. Together with ion-specific partition coefficients along the translocation pathway we construct a coherent picture of ionic selectivity for this particular channel, supplemented by results from a simplified nanopore model comprised of hard-wall interactions between pore lining and the solvent.



- [1] C. Song, B. Corry, *J. Phys. Chem. B*, **2009**, *113*, 7642-7649.
- [2] S. M. Kast, T. Kloss, S. Tayefeh, G. Thiel, *J. Gen. Physiol.*, **2011**, *138*, 371-373.
- [3] F. Zhu, G. Hummer, *J. Chem. Theory Comput.*, **2012**, *8*, 3759-3768.
- [4] K. Oxenoid, J. J. Chou, *Proc. Nat. Acad. Sci. USA*, **2005**, *102*, 10870-10875.
- [5] S. Smeazzetto, A. Saponaro, H. S. Young, M. R. Moncelli, G. Thiel, *PLoS ONE*, **2013**, *8*, e52744.