Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

How physical properties of bacterial porins match environmental conditions

Ion density We calculated the free energy from the density of ions averaged over the MD trajectories, using:

$$F(z) = -k_{BT} ln(\rho(z)/\rho_0),$$

with respect to the density ρ_0 outside the pore; we calculated the density in a cylinder containing a single monomer,

$$\rho(r,z)_{(0<r<17;-40<z<40)},$$

before to integrate it along r, and considering the three monomers as independent. The free energies for potassium and chloride ions were calculated for the replica at 300K, see Fig. S**??**. We remind that from electrophysiology both OmpF and OmpC are cation selective, and the selectivity is more pronounced in OmpC that also has lower conductivity. The free energies show for cations small barriers for both pores, comparable to k_BT, and larger for anions. OmpC has always larger barrier than OmpC. It is interesting to note how both OmpF and OmpC have a large region in the periplasmic eyelet region that favours the accumulation of potassium. Thus, major differences are present in the extracellular eyelet region, controlled by the long extracellular loops.

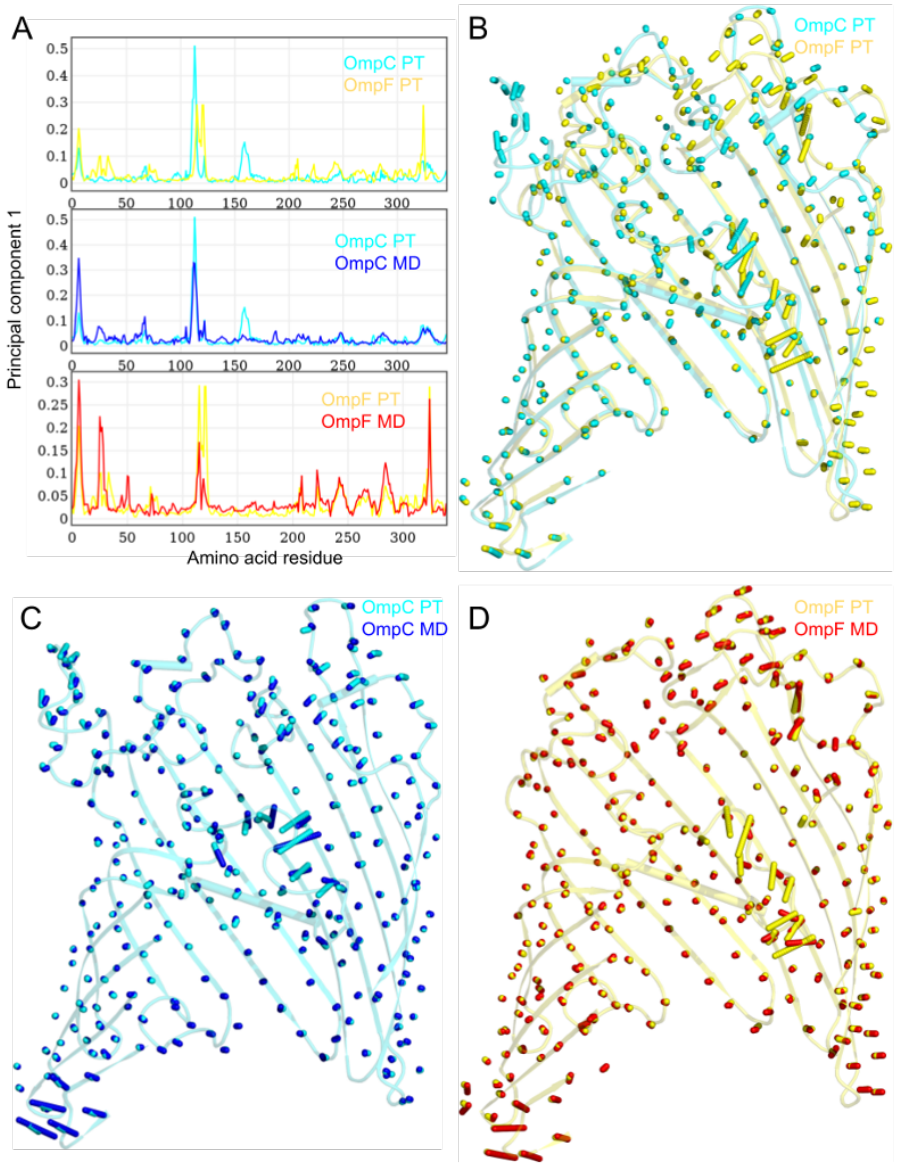

Figure S1 (A) The first principal component comparison among various setups. (B-D) The molecular graphics depiction of the first principal component differences.

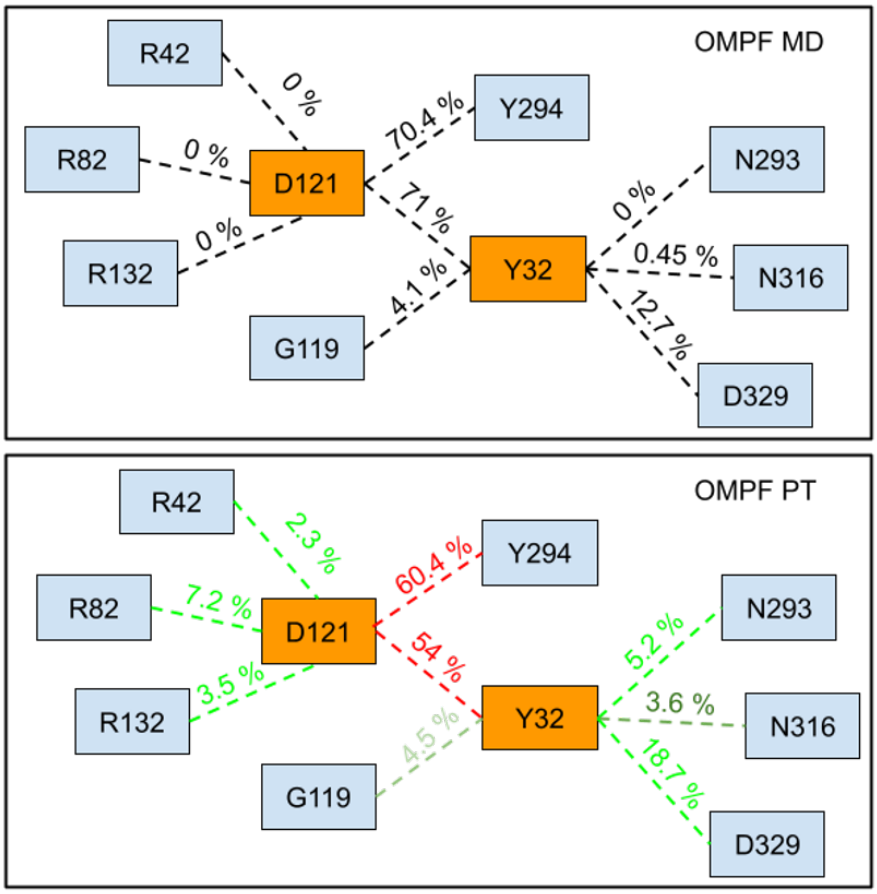

Figure S2 A schematic representation of the L3 loop hydrogen bonding interactions in (A) MD and (B) PT setups of the OMPF. Green and red colors of the lines representing hydrogen bonds stand for strengthening and weakening of the corresponding bond. The residue number refers to the OmpF sequence.

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sp|P02931|OMPF_ECOLI      AEIYNKDGNKVDLYGKAVGLHYFSKGNGENSYGGNGDMTYARLGFKGETQINSDLTGYGQ  60
sp|P06996|OMPC_ECOLI      AEVYNKDGNKLDLYGKVDGLHYFSDNKD-----VDGDQTYMRLGFKGETQVTDQLTGYGQ  55
                          **:*******:*****. ******..:.      :** ** *********:..:******

sp|P02931|OMPF_ECOLI      WEYNFQGNNSEGADAQTGNKTRLAFAGLKYADVGSFDYGRNYGVVYDALGYTDMLPEFGG  120
sp|P06996|OMPC_ECOLI      WEYQIQGNSAENE---NNSWTRVAFAGLKFQDVGSFDYGRNYGVVYDVTSWTDVLPEFGG  112
                          ***::***.:*.    ... **:******: ****************. .:**:******

sp|P02931|OMPF_ECOLI      DTAYSDDFFVGRVGGVATYRNSNFFGLVDGLNFAVQYLGKNERD--------------TA  166
sp|P06996|OMPC_ECOLI      DTYGSDNFMQQRGNGFATYRNTDFFGLVDGLNFAVQYQGKNGNPSGEGFTSGVTNNGRDA  172
                          **  **:*:  * .*.*****::*************** *** .               *

sp|P02931|OMPF_ECOLI      RRSNGDGVGGSISYEYEGFGIVGAYGAADRTNLQE-AQPLGNGKKAEQWATGLKYDANNI  225
sp|P06996|OMPC_ECOLI      LRQNGDGVGGSITYDYEGFGIGGAISSSKRTDAQNTAAYIGNGDRAETYTGGLKYDANNI  232
                           *.*********:*:****** ** .::.**: *: *  :***.:** :: *********

sp|P02931|OMPF_ECOLI      YLAANYGETRNATPITNKFTNTSGFANKTQDVLLVAQYQFDFGLRPSIAYTKSKAKDV-E  284
sp|P06996|OMPC_ECOLI      YLAAQYTQTYNATRV-----GSLGWANKAQNFEAVAQYQFDFGLRPSLAYLQSKGKNLGR  287
                          ****:* :* *** :     .: *:***:*:.  **************:** :**.*:: .

sp|P02931|OMPF_ECOLI      GIGDVDLVNYFEVGATYYFNKNMSTYVDYIINQIDSD---NKLGVGSDDTVAVGIVYQF   340
sp|P06996|OMPC_ECOLI      GYDDEDILKYVDVGATYYFNKNMSTYVDYKINLLDDNQFTRDAGINTDNIVALGLVYQF   346
                          * .* *:::*.:*****************  ** :*.:   .. *:.:*: **:*:****
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Figure S3 Alignment of the simulated sequences of OmpF and OmpC.

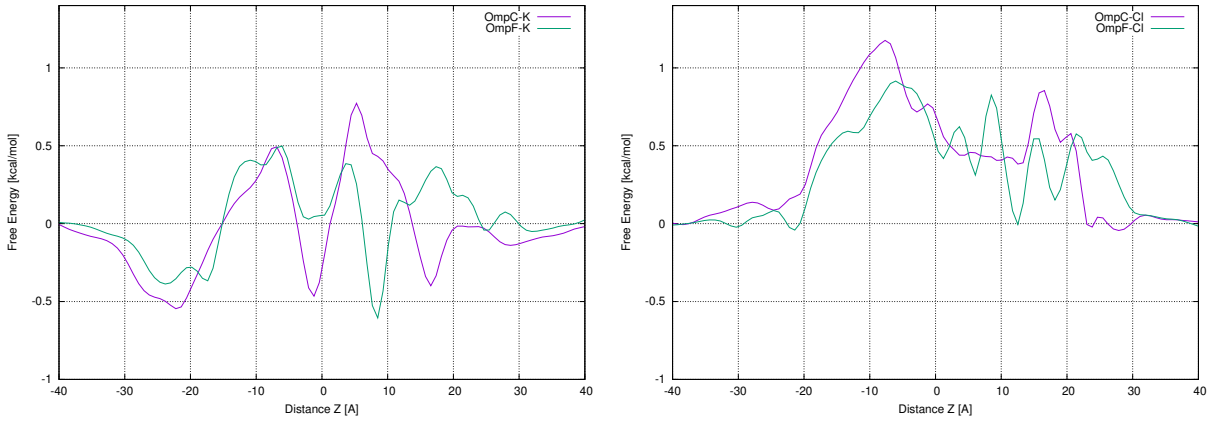

Figure S4 Free energy of potassium and chloride ions in OmpF and OmpC as function of distance z along the diffusion axis for the PT replica at 300 K.