Supplementary information

GROMACS Commands

The following Gromacs commands were used:
Simulations with Explicit Water:
(1) Preparing the Gromacs files:
pdb2gmx -f NaCl.pdb -water tip3p
(2) Creating the box (Box size of 3nm):
The geometrical center for the box is calculated from the nine numbers found in the .gro file, numbered here box1 - box9:
editconf -f in.gro -o out.gro -center 0.5*(box1 + box6 + box8) 0.5*(box2 + box4 + box9) 0.5*(box3 + box5 + box7)
In our system:
editconf -princ -center 5.021 5.161 2.433 -f conf.gro -bt dodecahedron -d 3.0 -o box.gro
genbox -cp box.gro -cs spc216.gro -p topol.top -o solvated.gro
(3) Energy Minimization:
grompp -f em.mdp -p topol.top -c solvated.gro -o em.tpr
mdrun -nice 0 -v -deffnm em
The em.mdp files we used:

```
------em.mdp------
integrator      = steep
nsteps          = 20000
nstlist         = 10
rlist           = 1.0
coulombtype     = pme
rcoulomb        = 1.0
vdwtype         = Cut-off
rvdw            = 1.0
nstenergy       = 10
define          = -DFLEXIBLE
------------------
```

(4) Equilibrating the water around the NaCl molecule:
grompp -f pr.mdp -n index.ndx -p topol.top -c em.gro -o pr.tpr
mdrun -nice 0 -v -deffnm pr

The pr.mdp file we used:

```
------pr.mdp------
integrator      = md
nsteps          = 2500
dt              = 0.002
nstlist         = 10
rlist           = 1.0
coulombtype     = pme
rcoulomb        = 1.0
vdwtype         = Cut-off
rvdw            = 1.0
tcoupl          = v-rescale
tc_grps         = Salt SOL
tau_t           = 0.1 0.1
ref_t           = 298 298
```

Pcoupl = Berendsen
tau_p = 1.0
compressibility = 5e-5 5e-5 5e-5 0 0 0
ref_p = 1.0
nstenergy = 100
define = -DPOSRES

(5) Running the simulation:
grompp -f run.mdp -p topol.top -c pr.gro -o run.tpr
mdrun -nice 0 -v -deffnm run
The run.mdp file we used: (example of 450^0K simulations)
------run.mdp------
integrator = md
nsteps = 500000
dt = 0.002
nstlist = 1
rlist = 1.0
coulombtype = pme
rcoulomb = 1.0
vdwtype = Cut-off
rvdw = 1.0
tcoupl = v-rescale
tc_grps = SOL non-Water
tau_t = 0.1 0.1
ref_t = 450 450
energygrps = Ion_chain_A Ion_chain_B
gen_vel = yes
gen_temp = 450
ld_seed = -1
gen_seed = -1
nstxout = 100
nstvout = 100
nstxtcout = 100
nstenergy = 100

Simulations with implicit water:
(1) Preparing the Gromacs files:
pdb2gmx -f 2NaCl.pdb (option 14 opls-aa force field followed by option 6: none – for no water in the system)
(2) Energy Minimization:
grompp -f em.mdp -p topol.top -c conf.gro -o em.tpr
mdrun -nt 8 -nice 0 -v -deffnm em
The em.mdp file we used:
------em.mdp------
integrator = steep
nsteps = 2000
implicit_solvent = GBSA
gb_algorithm = Still
sa_algorithm =
pbc = no
rgbradii = 0

ns_type = simple
nstlist = 0
rlist = 0
coulombtype = cut-off
rcoulomb = 0
vdwtype = cut-off
rvdw = 0
nstenergy = 100
emtol = 0

(3) Running the simulation:
grompp -maxwarn 2 -f run.mdp -n index.ndx -p topol.top -c em1longer.gro -t em1longer.trr -o run.tpr
mdrun -pd -nt 8 -nice 0 -v -deffnm run
The run.mdp file we used:
------run.mdp------
integrator = md
nsteps = 500000
dt = 0.002
implicit_solvent = GBSA
pbc = no
nstlist = 0
ns_type = simple
rlist = 0
rgbradii = 0
coulombtype = Cut-off
rcoulomb = 0
vdwtype = Cut-off
rvdw = 0
tcoupl = v-rescale
tc_grps = system
tau_t = 0.1
ref_t = 450
energygrps = Ion_chain_A Ion_chain_B
gen_vel = yes
gen_temp = 450
ld_seed = -1
gen_seed = -1
nstxout = 100
nstvout = 100
nstxtcout = 100
nstenergy = 100
