Ice nucleation in neat and polluted water

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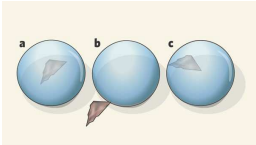
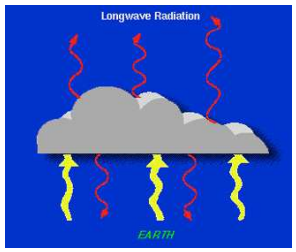
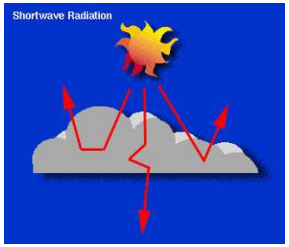
Motivation

- water in nature mostly freezes heterogeneously



- homogeneous nucleation controls the formation of cirrus and polar stratospheric clouds affecting directly radiative of the Earth

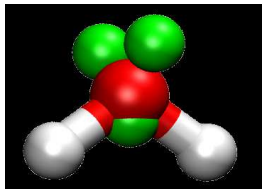




- Is homogeneous ice nucleation initiated preferentially at the surface or in the bulk?
- surface nucleation can not be confirmed using existing experimental data
- formation of ice nucleus can be affected by surface contamination

Methods

MD simulations

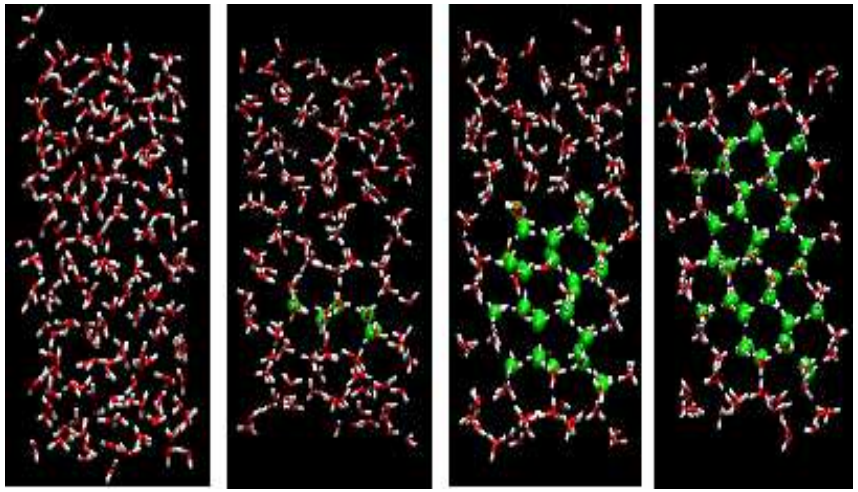


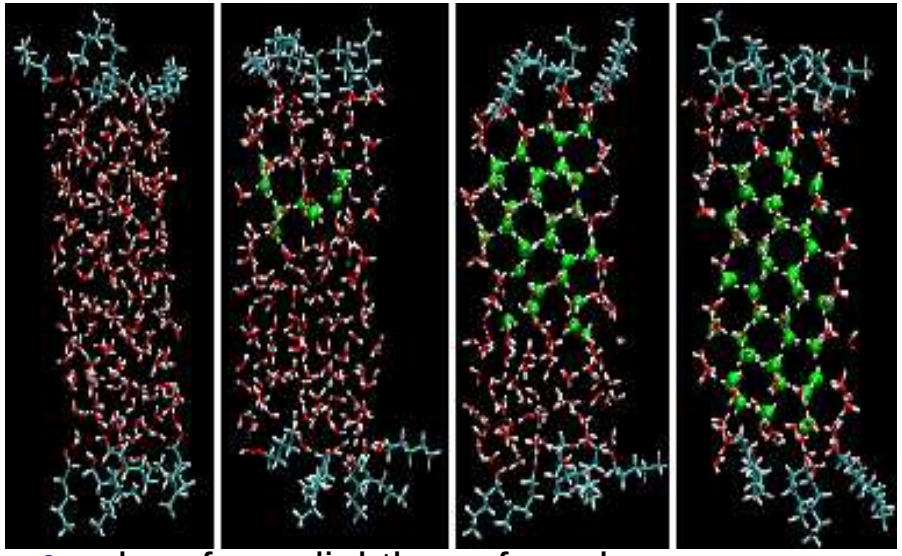
- NE6 water model
- meting temperature approx. 275 K

simulation cell

- Gromacs 3.3.1
- supercooled to 250 K
- periodic boundary conditions
- slab thickness 30 Å
- 192 water molecules
- 12 pentanol molecules (model of pollutant)
- long simulations (~100 ns)

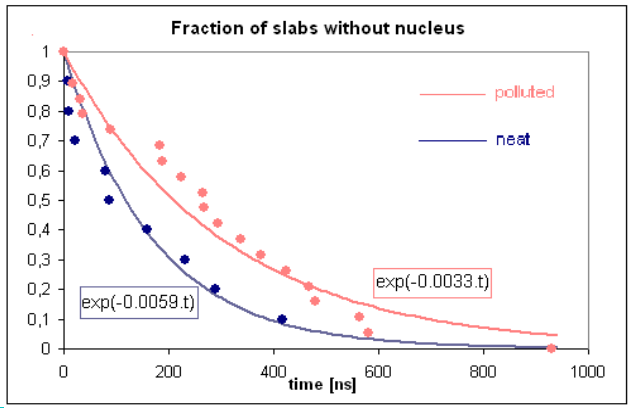
Results





- simulations indicate that freezing starts mostly in the subsurface
- freezing is faster, if nucleus is formed in the center of the slab
- average time of freezing: 36 ns

- subsurface slightly preferred
- average time of freezing: 49 ns



Conclusion

- freezing starts from the subsurface region, subsurface is preferred for neat water more than for polluted water
- freezing rate depends on the location of nucleus in both cases
- formation of nucleus takes longer time and freezing rate is slower for polluted water